

CHEMISTRY

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Supporting Information

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Selective Formation of 2-Imidazolines and 2-Substituted Oxazoles via a Three-Component Reaction.

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Orru*

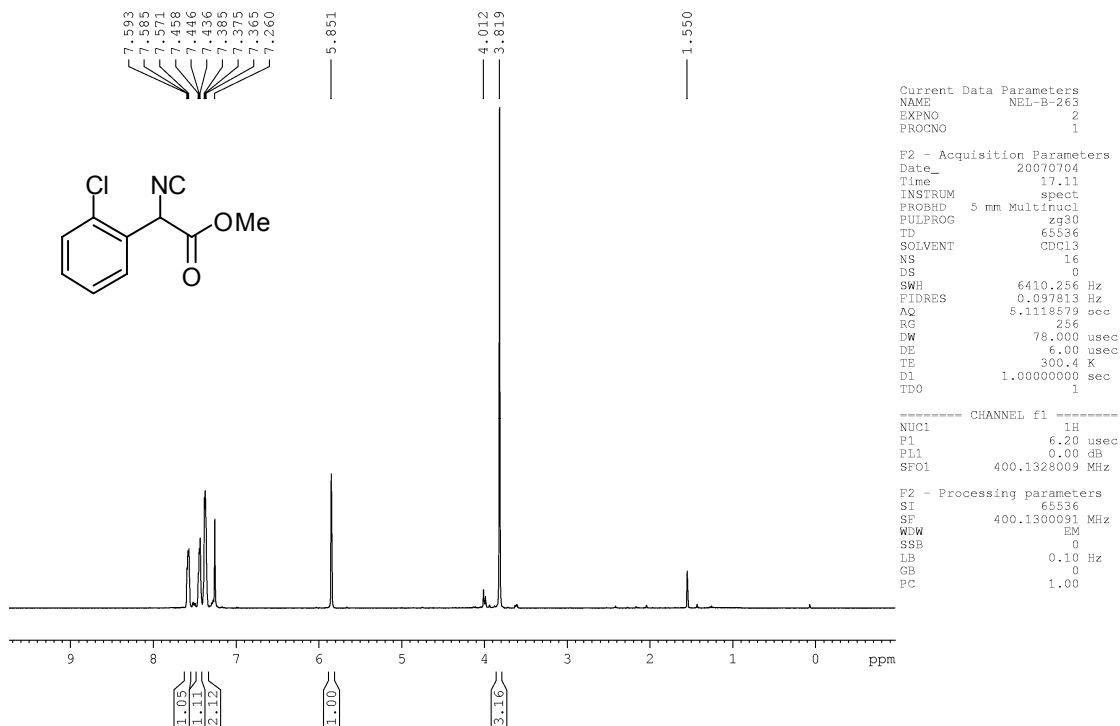
*Department of Chemistry & Pharmaceutical Sciences
Vrije Universiteit Amsterdam
De Boelelaan 1083, 1081 HV Amsterdam*

¹H NMR and ¹³C NMR spectra of all new compounds.

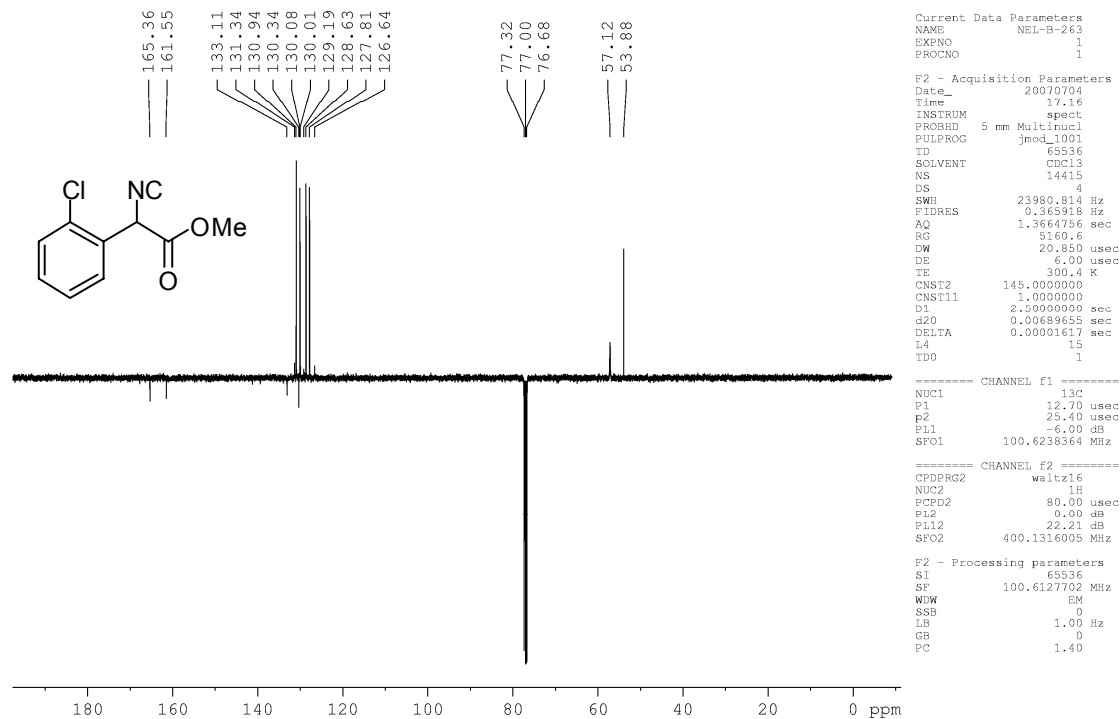
Compound	Page	Compound	Page
Isocyanide (1f)	3	Oxazole (5b)	20
Isocyanide (1g)	4	Oxazole (5c)	21
Isocyanide (1h)	5	Oxazole (5d)	22
Isocyanide (1i)	6	Oxazole (5e)	23
Isocyanide (1j)	7	Oxazole (5f)	24
Imidazoline (4a)	8	Oxazole (5g)	25
Imidazoline (4c)	9	Oxazole (5h)	26
Imidazoline (4e)	10	Oxazole (5i)	27
Imidazoline (4f)	11	Oxazole (5l)	28
Imidazoline (4g)	12	Oxazole (5m)	29
Imidazoline (4h)	13	Oxazole (5n)	30
Imidazoline (4i)	14	Oxazole (5o)	31
Imidazoline (4j)	15	Oxazole (5p)	32
Imidazoline (4k)	16	Oxazole (5q)	33
Imidazoline (4l)	17	Oxazole (6)	34
Imidazoline (4n)	18	Oxazole (7)	35
Oxazole (5a)	19	Oxazole (8)	36

Methyl 2-(*o*-chlorophenyl)-2-isocyanoacetate (1f):

¹H NMR (400.13 MHz, CDCl₃)

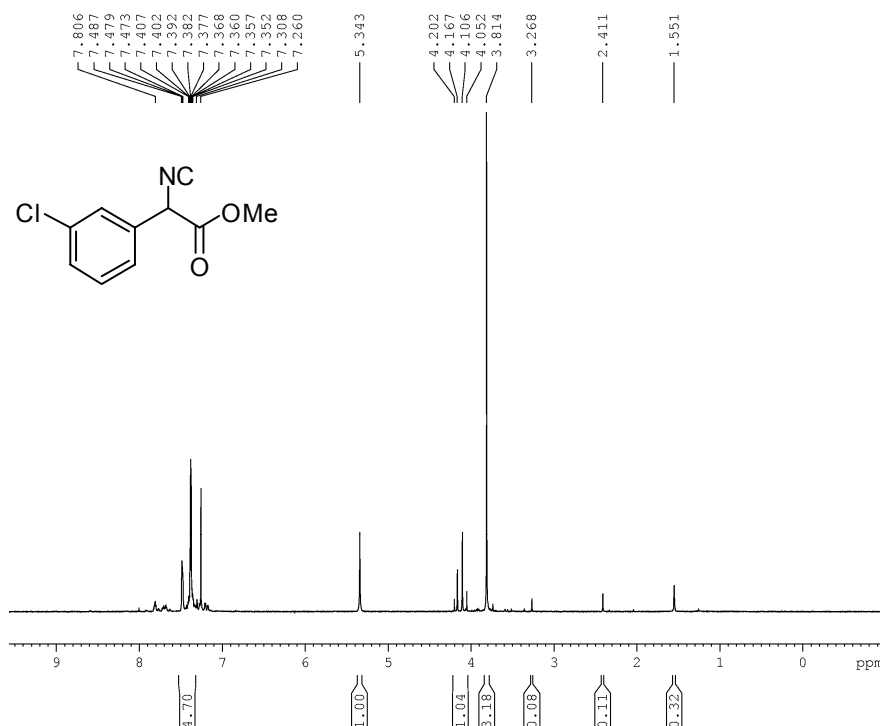


¹³C{¹H} NMR (100.62 MHz, CDCl₃)



Methyl 2-(*m*-chlorophenyl)-2-isocyanoacetate (1g):

¹H NMR (250.13 MHz, CDCl₃)



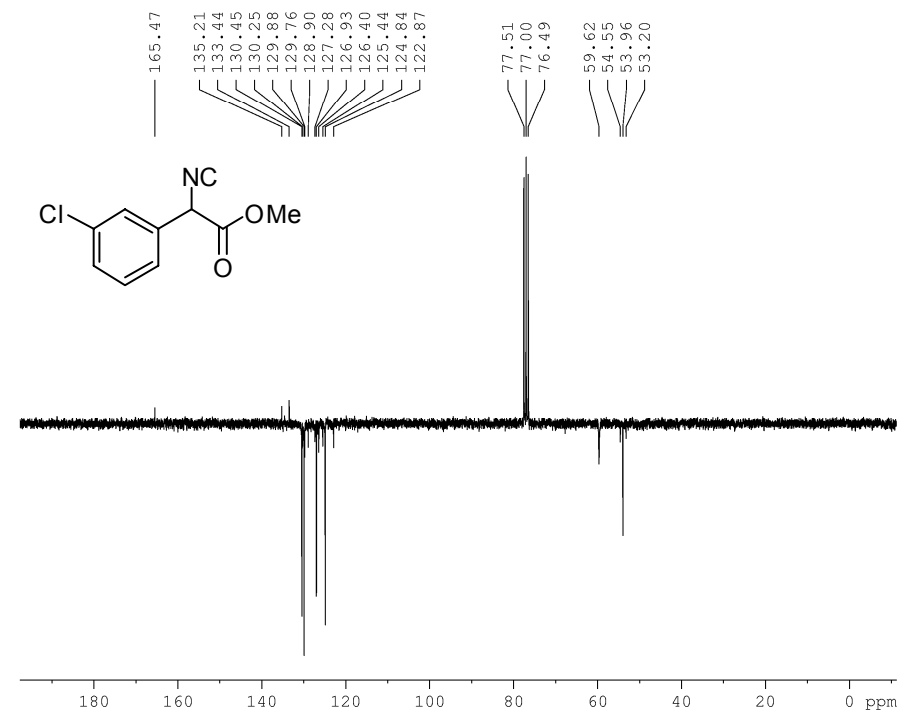
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¹³C{¹H} NMR (62.90 MHz, CDCl₃)



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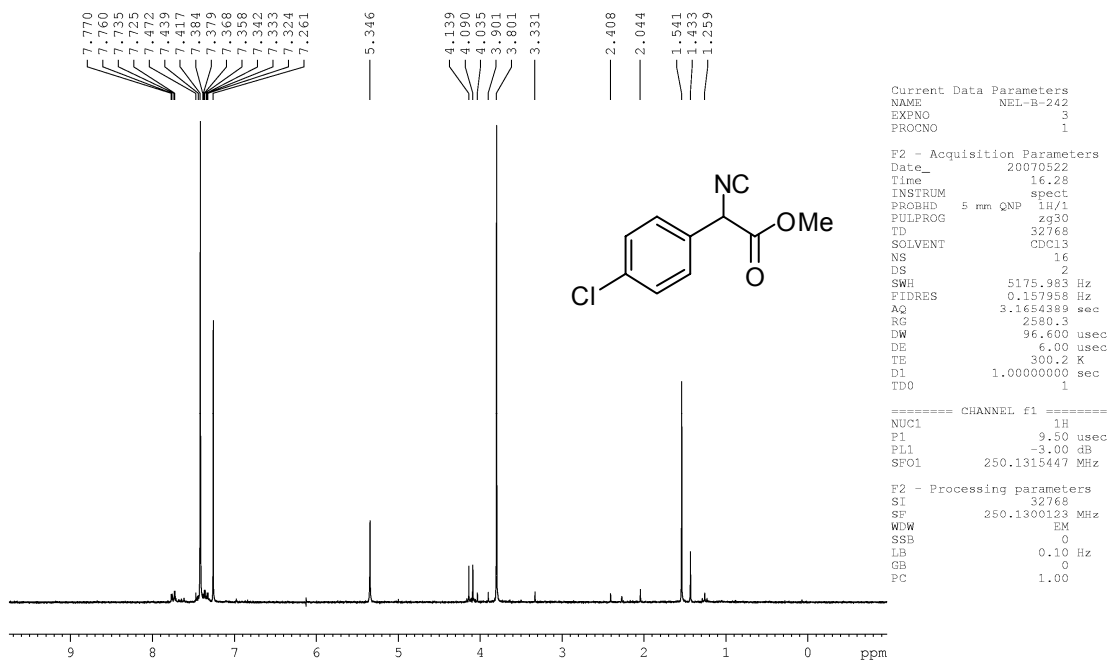
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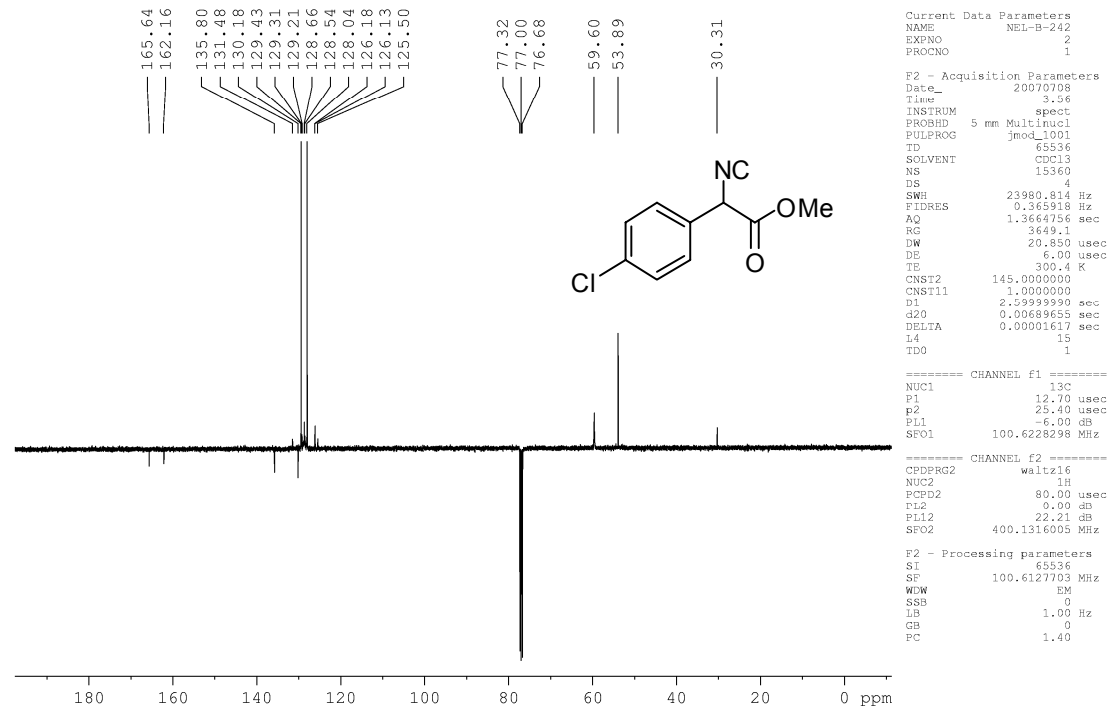
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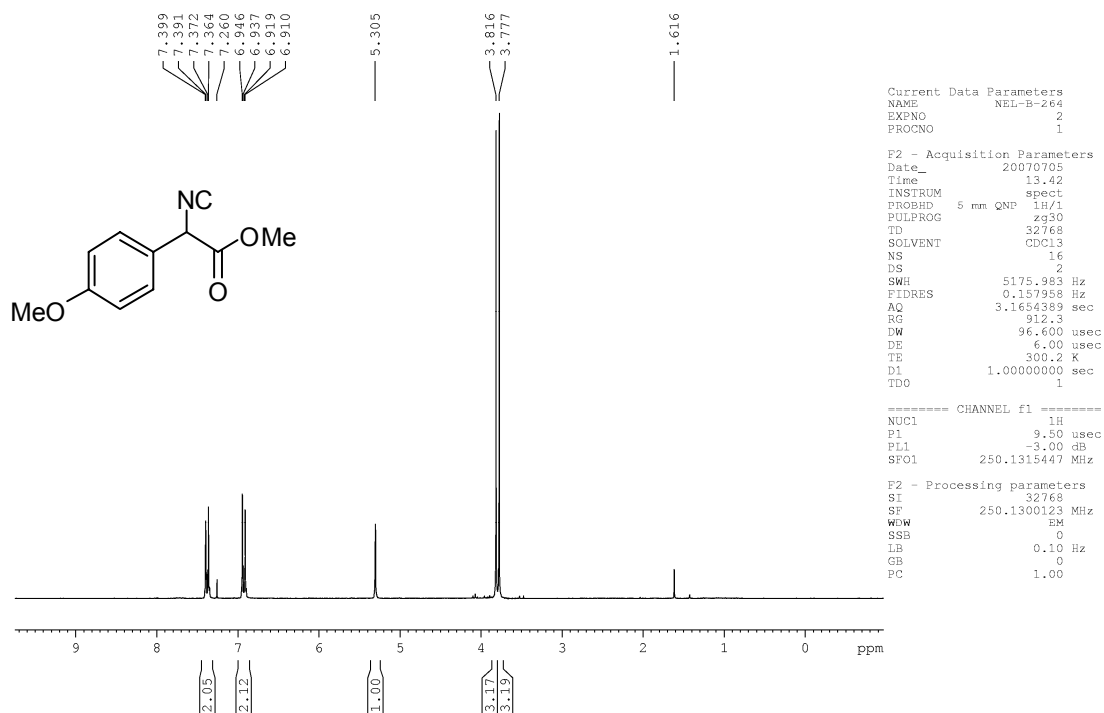
^1H NMR (250.13 MHz, CDCl_3)



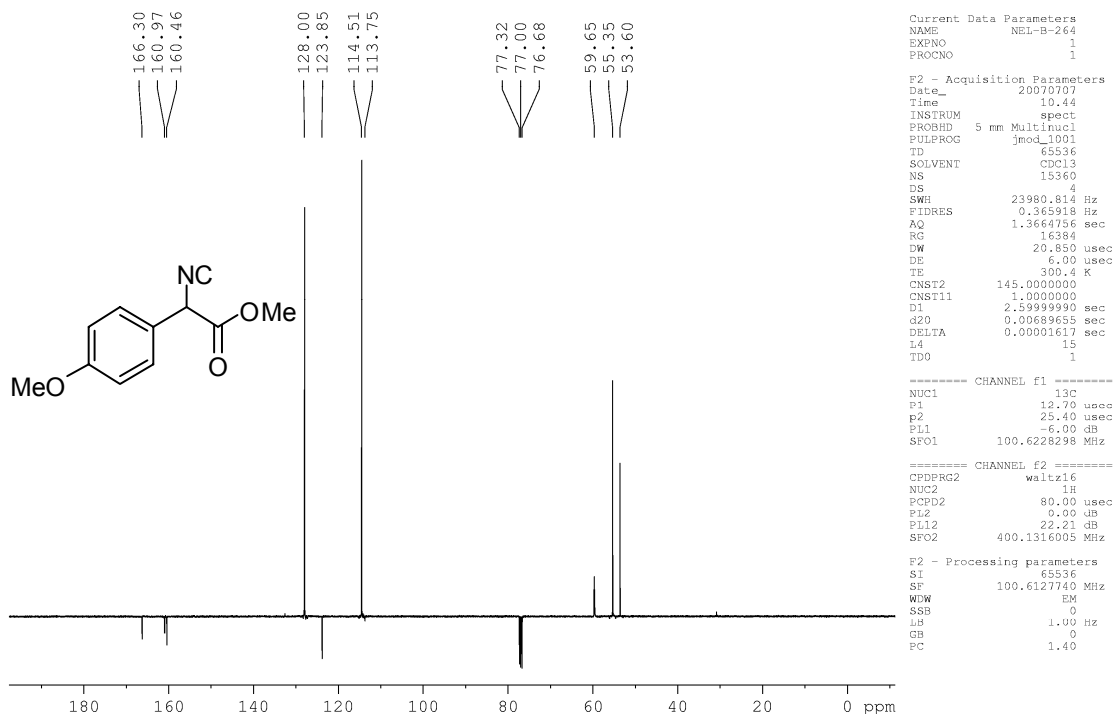
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl_3)



Methyl 2-(*p*-methoxyphenyl)-2-isocyanoacetate (1i):
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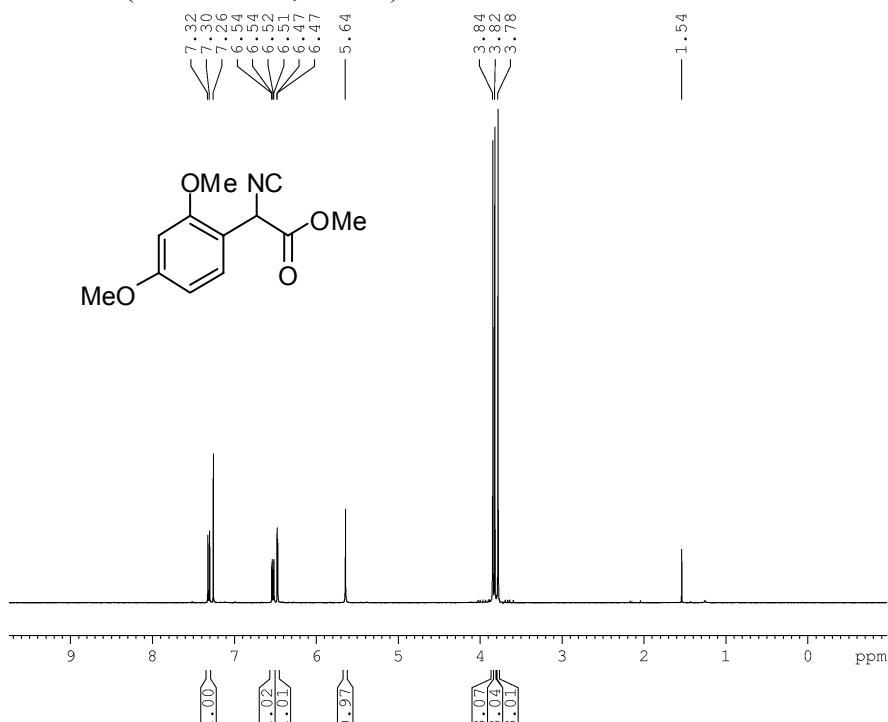


¹³C{¹H} NMR (100.62 MHz, CDCl₃)



Methyl 2-(*o,p*-dimethoxyphenyl)-2-isocyanoacetate (1j):

¹H NMR (400.13 MHz, CDCl₃)



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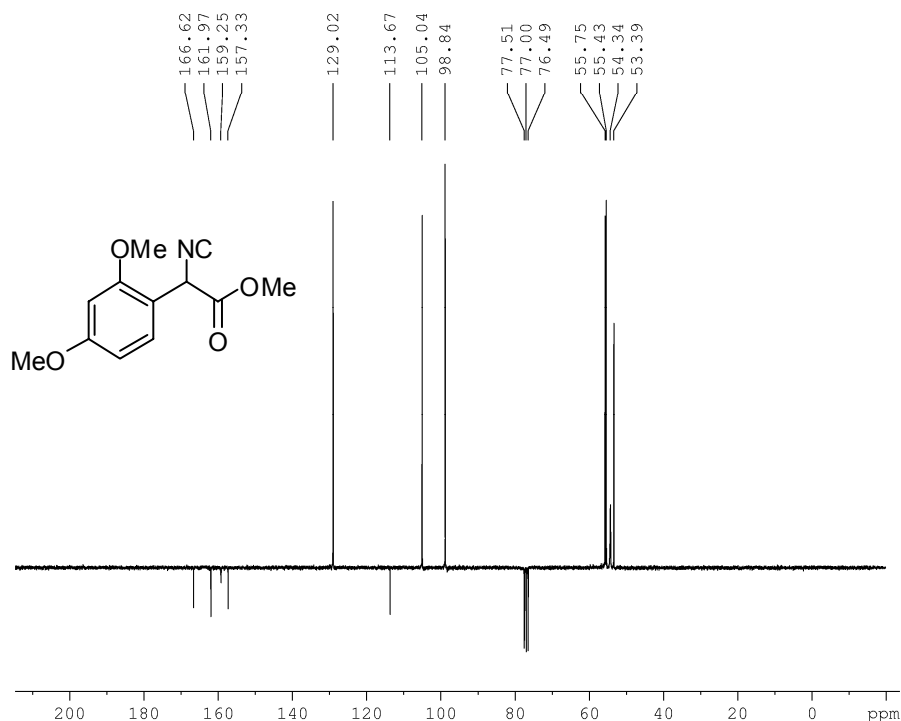
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¹³C{¹H} NMR (62.90 MHz, CDCl₃)



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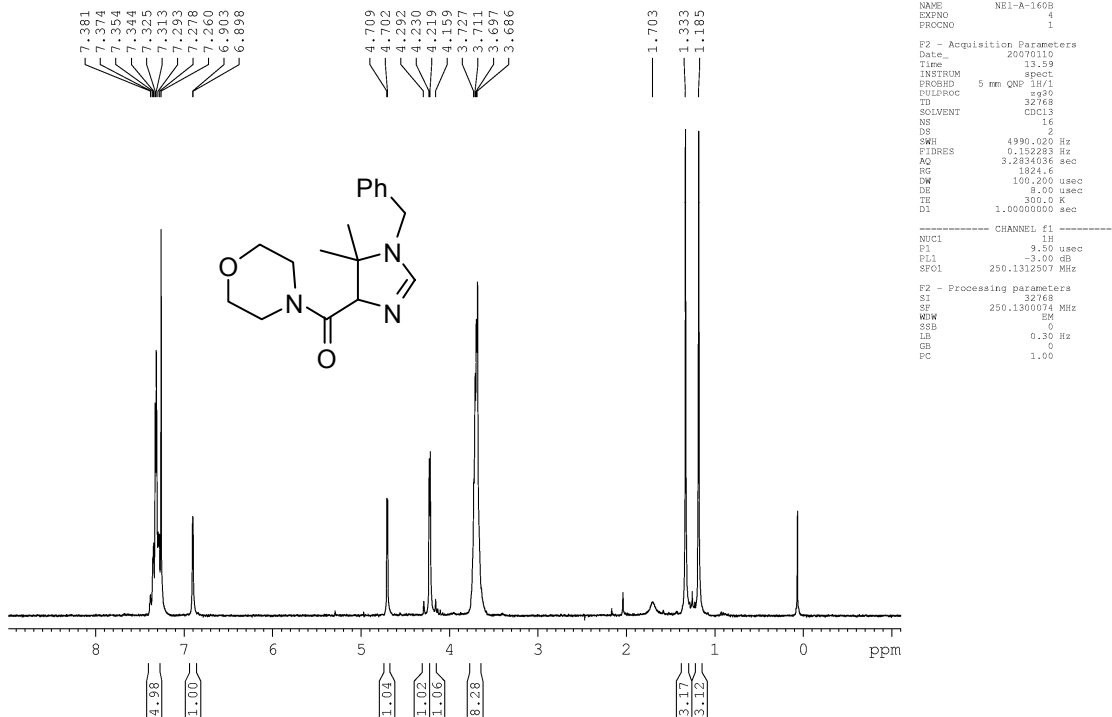
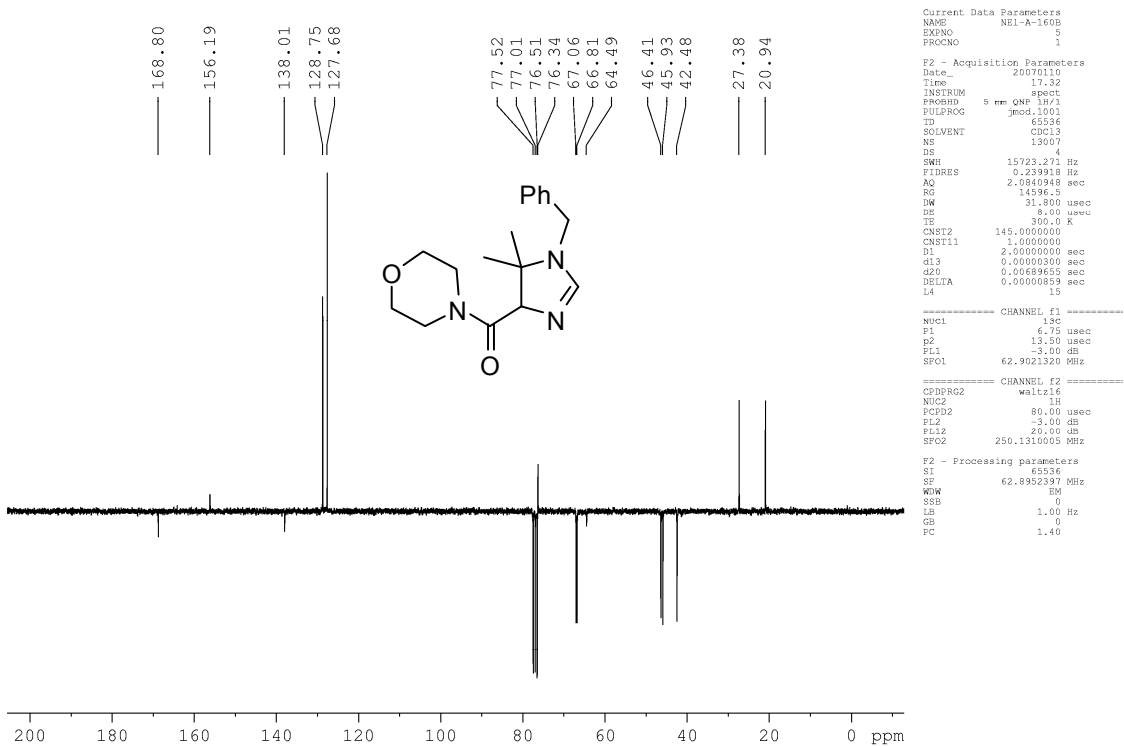
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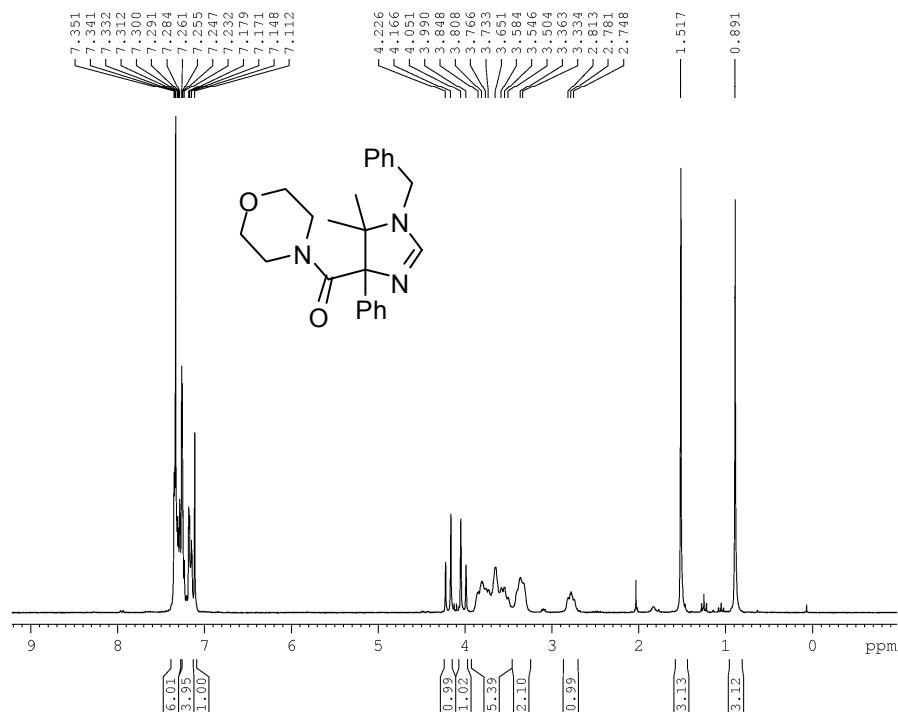
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P2         13.50 usec
PL1        -3.00 dB
SFO1       62.9015280 MHz

===== CHANNEL f2 =====
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NUC2       1H
PCPD2     80.00 usec
P12       -3.00 dB
PL12      20.00 dB
SFO2      250.1310005 MHz

F2 - Processing parameters
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SF         62.8952444 MHz
WDW        EM
SSB        0
LB         1.00 Hz
CB         0
PC         1.40
    
```

¹H NMR (250.13 MHz, CDCl₃) $^{13}\text{C}\{^1\text{H}\}$ NMR (62.90 MHz, CDCl_3)

(1-benzyl-5,5-dimethyl-4-phenyl-4,5-dihydro-1H-imidazol-4-yl)(morpholino)methanone (4c):
¹H NMR (250.13 MHz, CDCl₃)



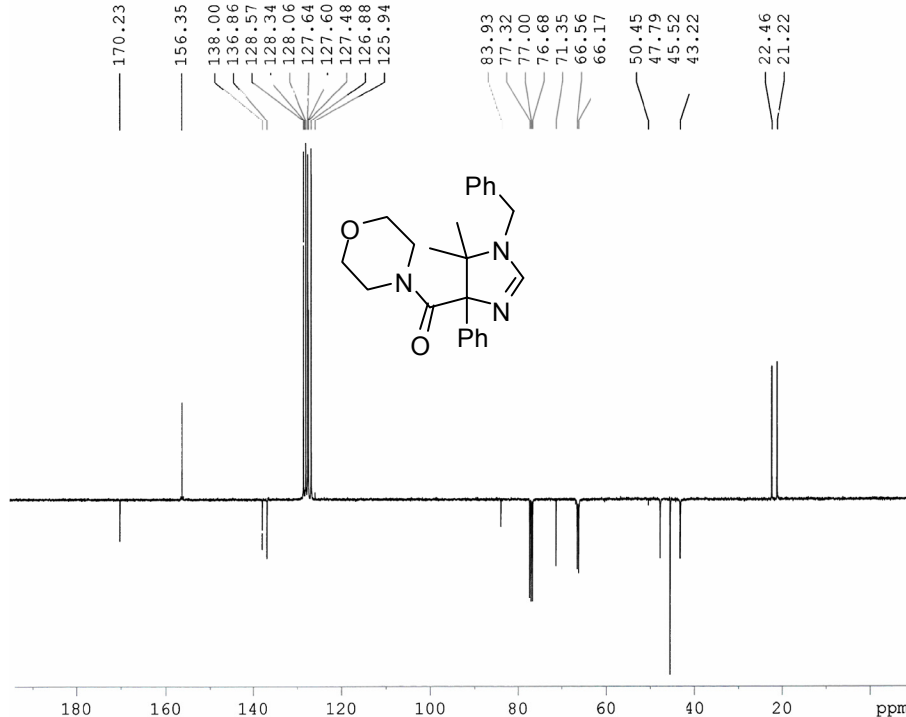
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 TE 300.2 K
 D1 1.00000000 sec
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===== CHANNEL f1 =====
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¹³C{¹H} NMR (100.62 MHz, CDCl₃)



Current Data Parameters
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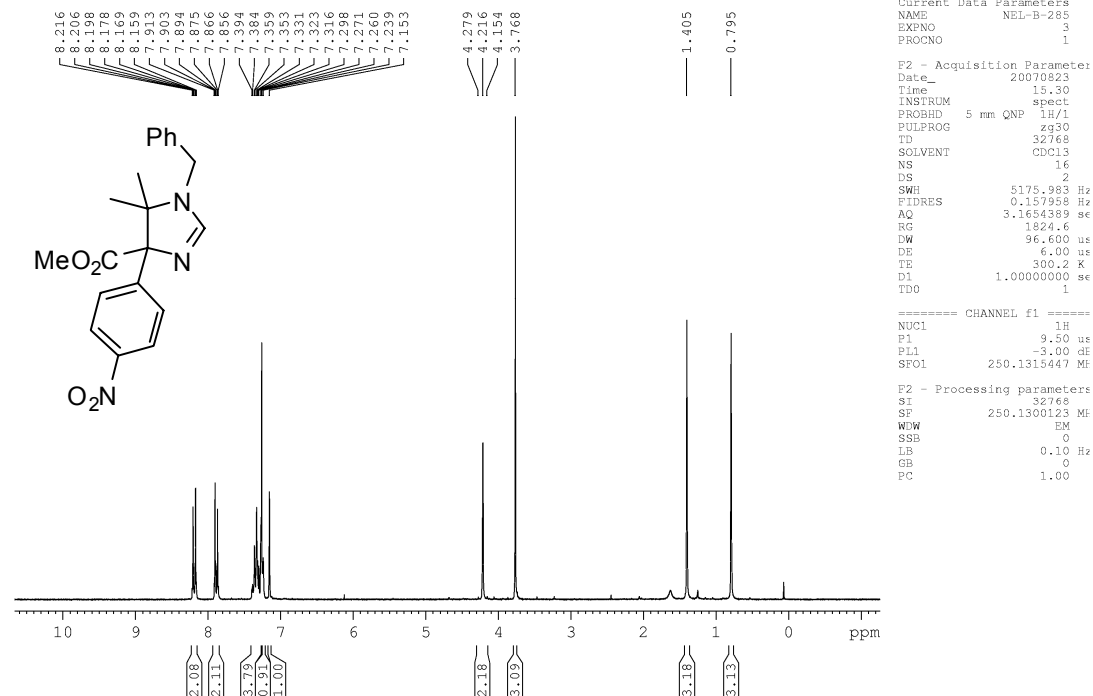
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 SFO2 400.1316005 MHz

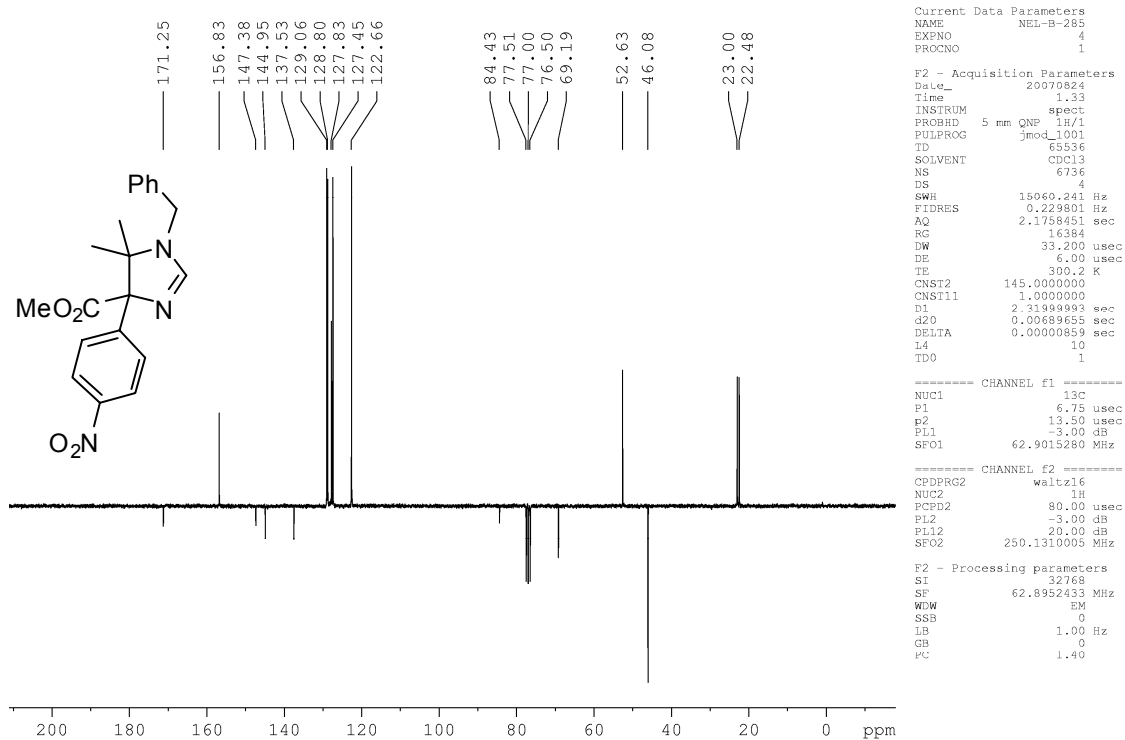
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Methyl 1-benzyl-5,5-dimethyl-4-(4-nitrophenyl)-4,5-dihydro-1H-imidazole-4-carboxylate (4e):

^1H NMR (250.13 MHz, CDCl_3)

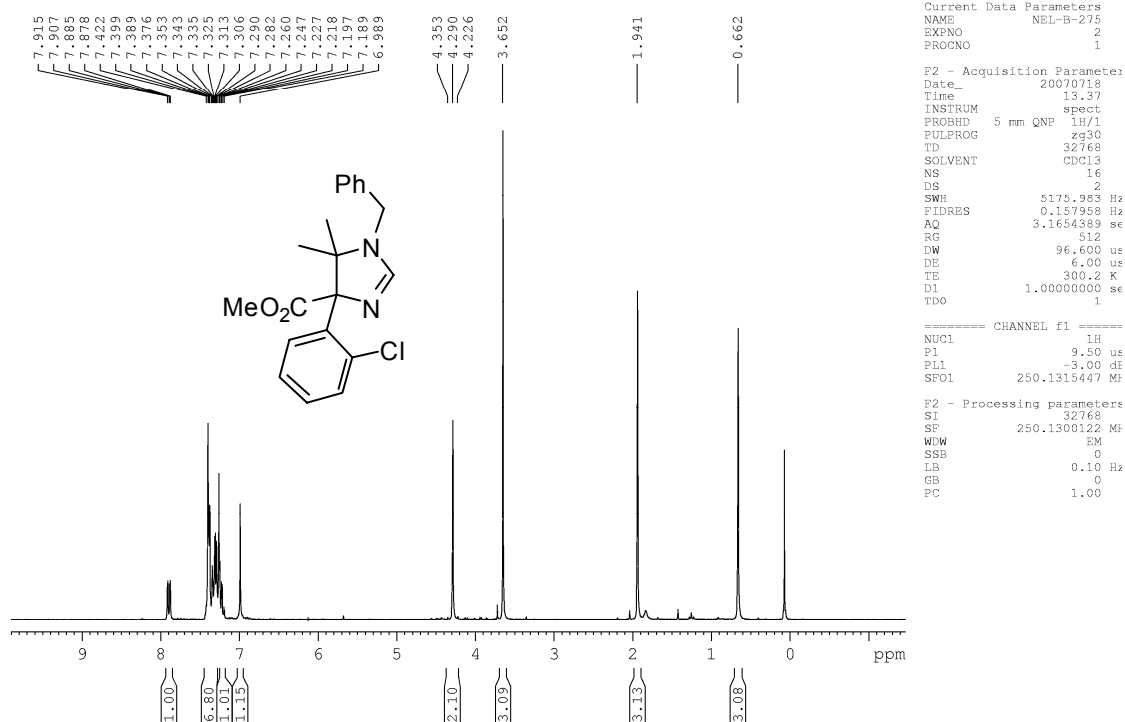


$^{13}\text{C}\{^1\text{H}\}$ NMR (62.90 MHz, CDCl_3)

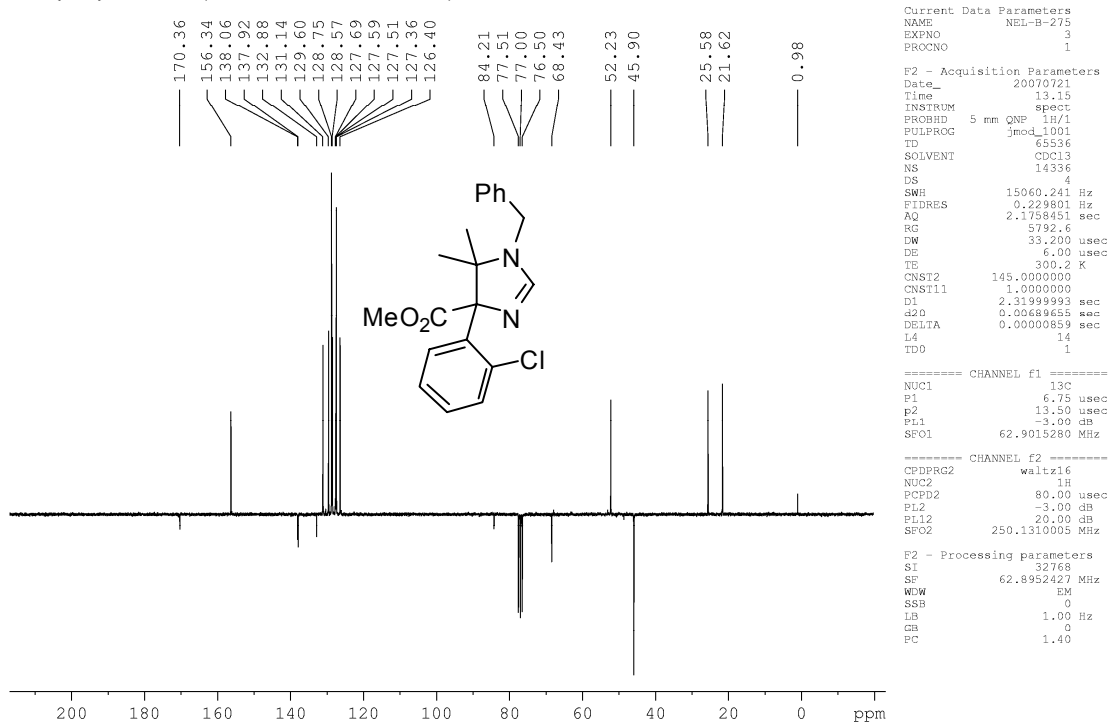


Methyl 1-benzyl-4-(2-chlorophenyl)-5,5-dimethyl-4,5-dihydro-1H-imidazole-4-carboxylate (4f):

^1H NMR (250.13 MHz, CDCl_3)

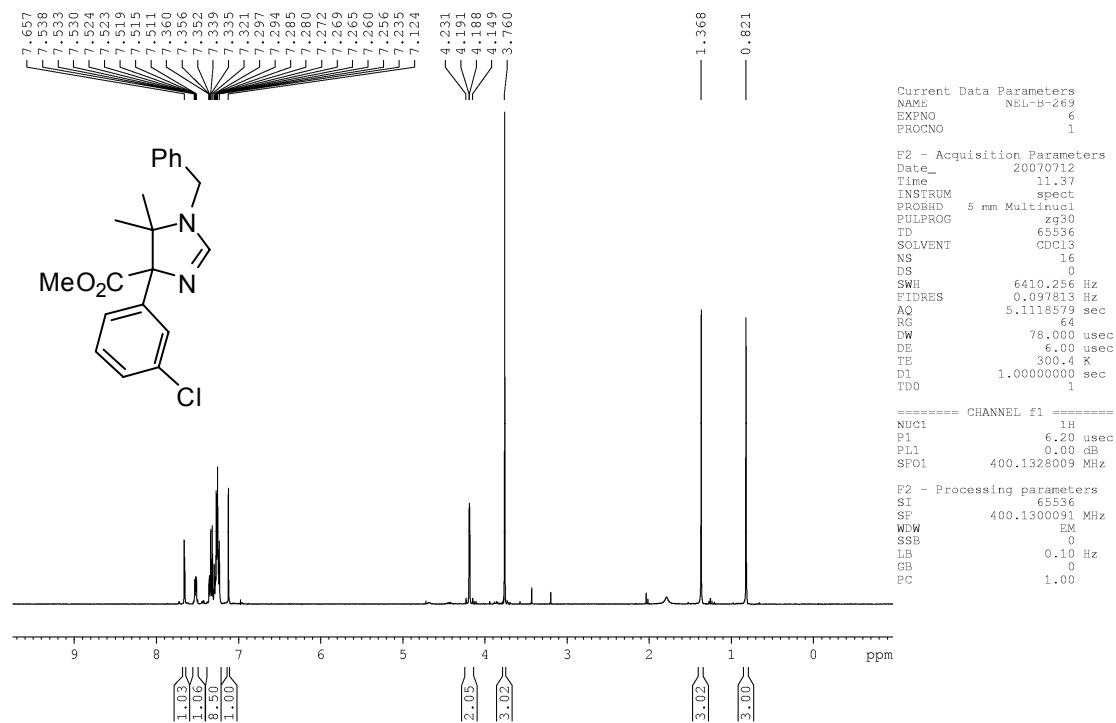


$^{13}\text{C}\{^1\text{H}\}$ NMR (62.90 MHz, CDCl_3)

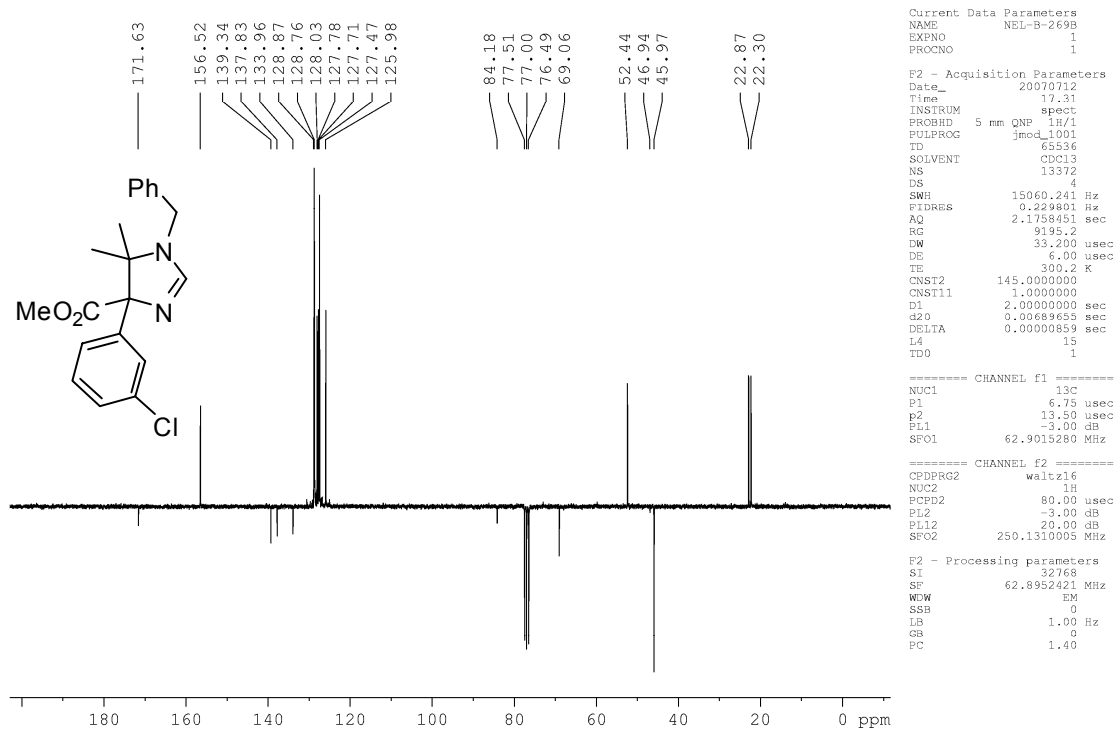


Methyl 1-benzyl-4-(3-chlorophenyl)-5,5-dimethyl-4,5-dihydro-1H-imidazole-4-carboxylate (4g):

^1H NMR (400.13 MHz, CDCl_3)

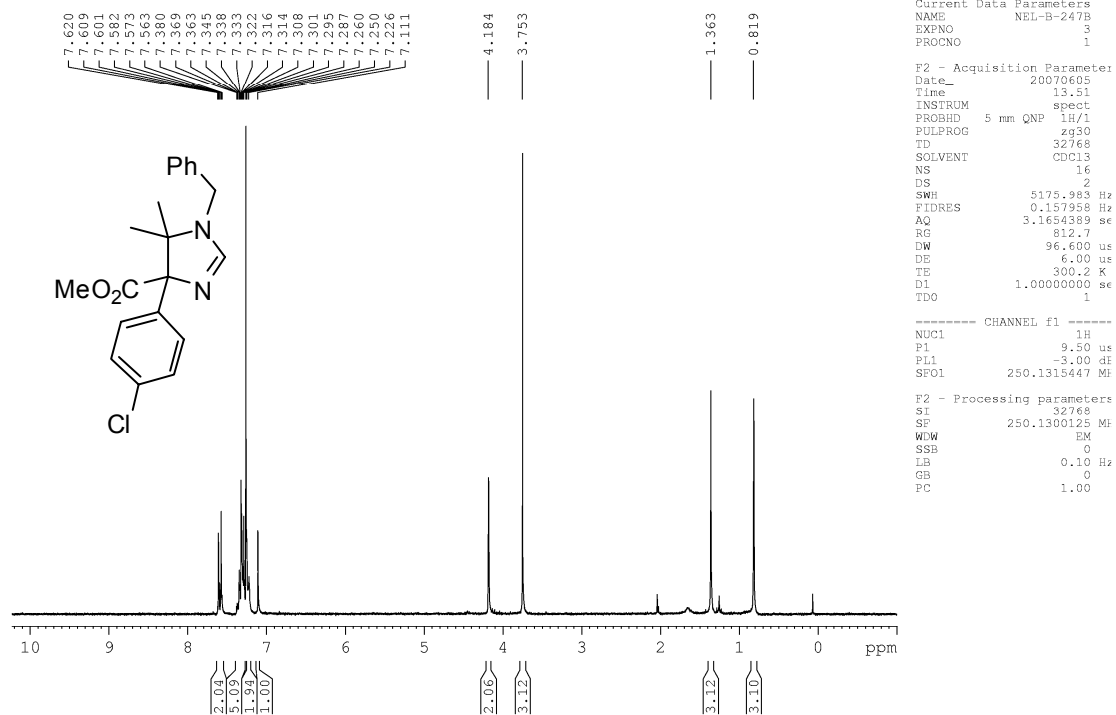


$^{13}\text{C}\{^1\text{H}\}$ NMR (62.90 MHz, CDCl_3)

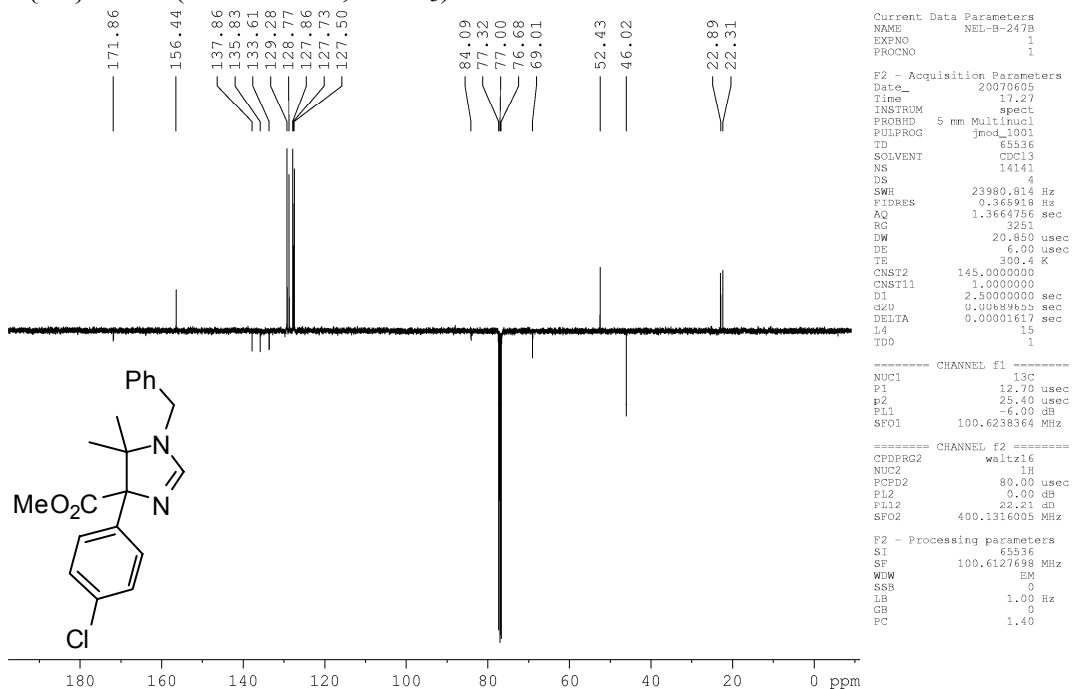


Methyl 1-benzyl-4-(4-chlorophenyl)-5,5-dimethyl-4,5-dihydro-1H-imidazole-4-carboxylate (4h):

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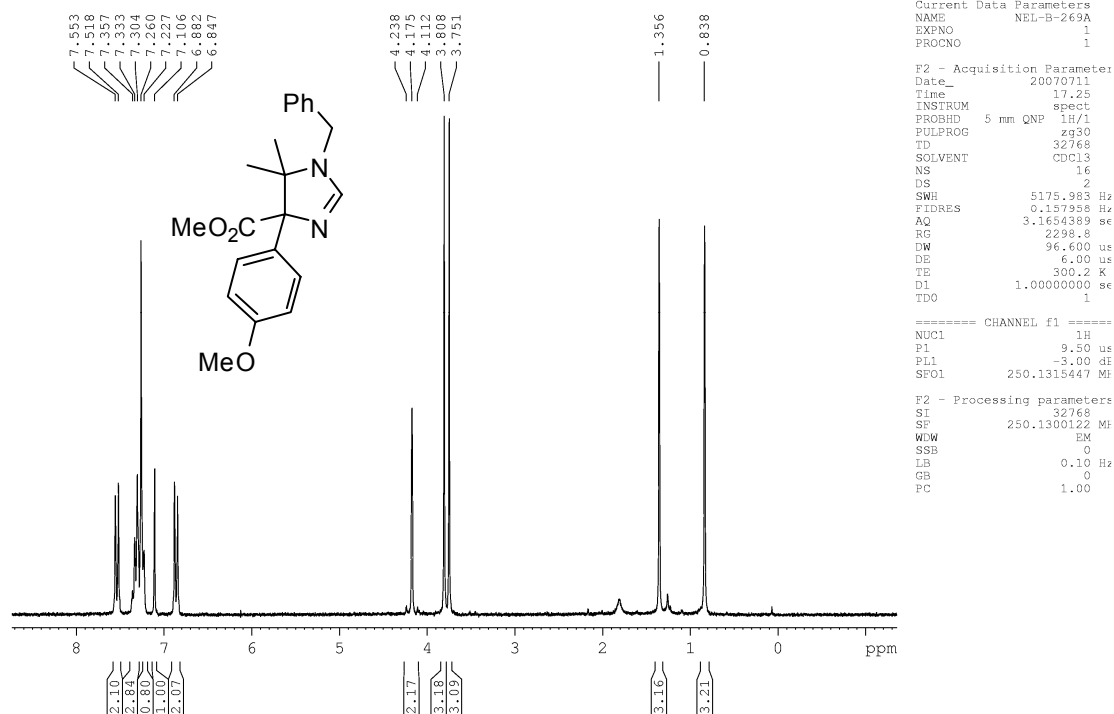


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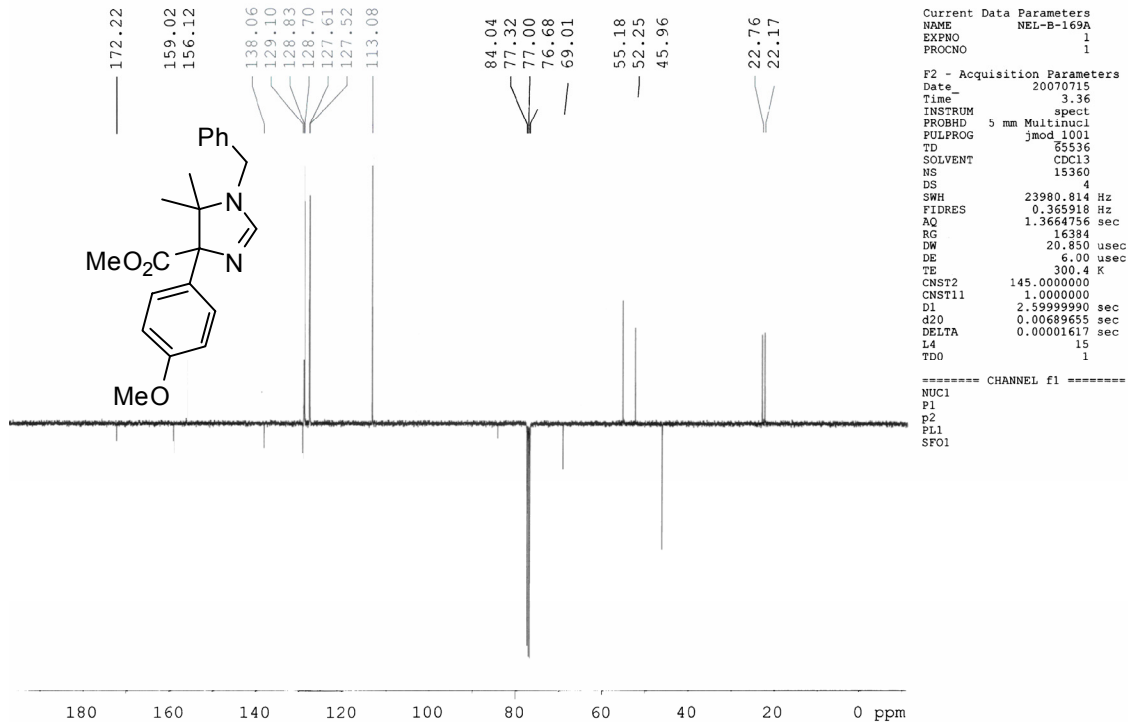


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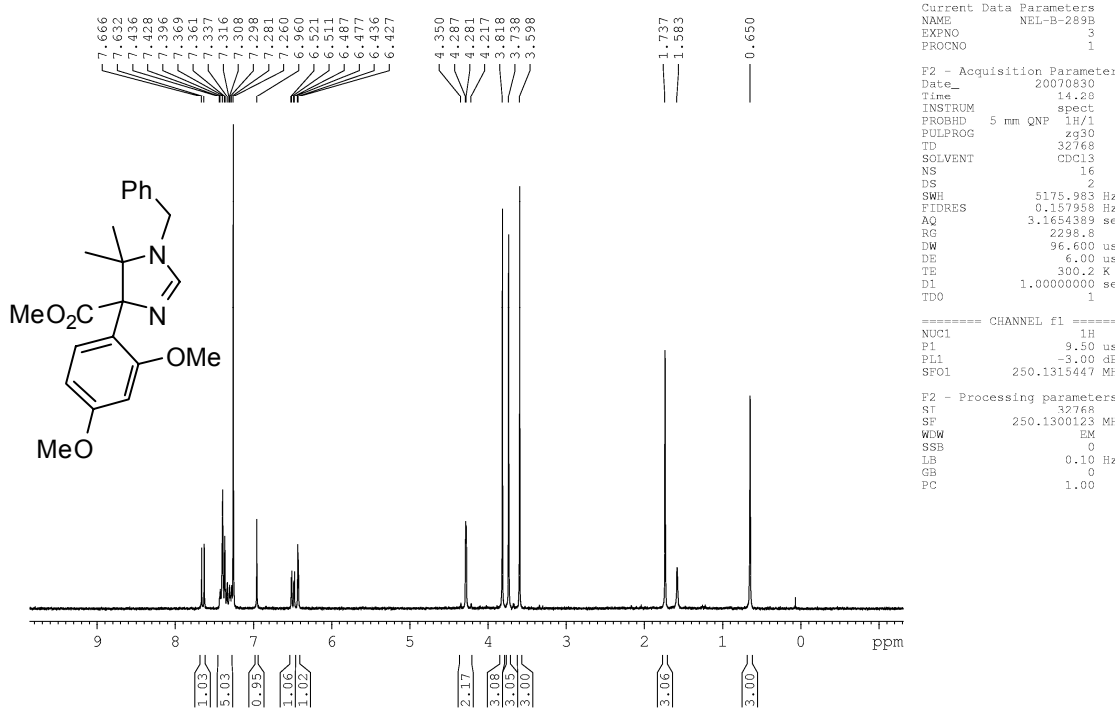


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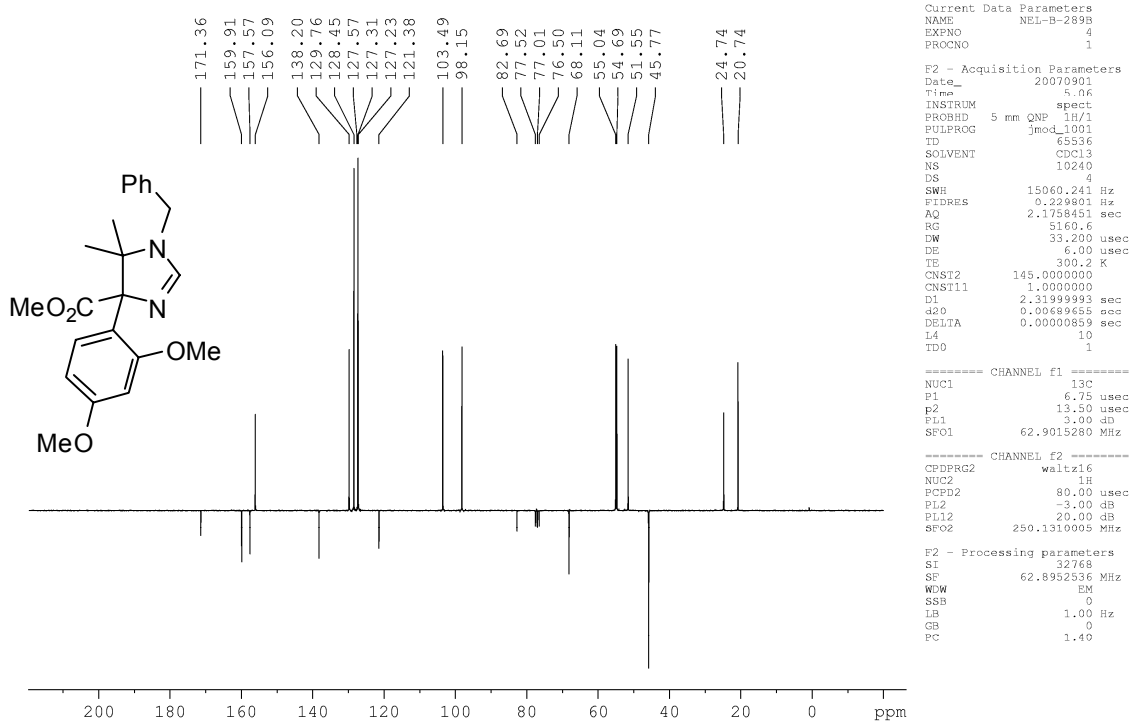


Methyl 1-benzyl-4-(2,4-dimethoxyphenyl)-5,5-dimethyl-4,5-dihydro-1H-imidazole-4-carboxylate (4j):

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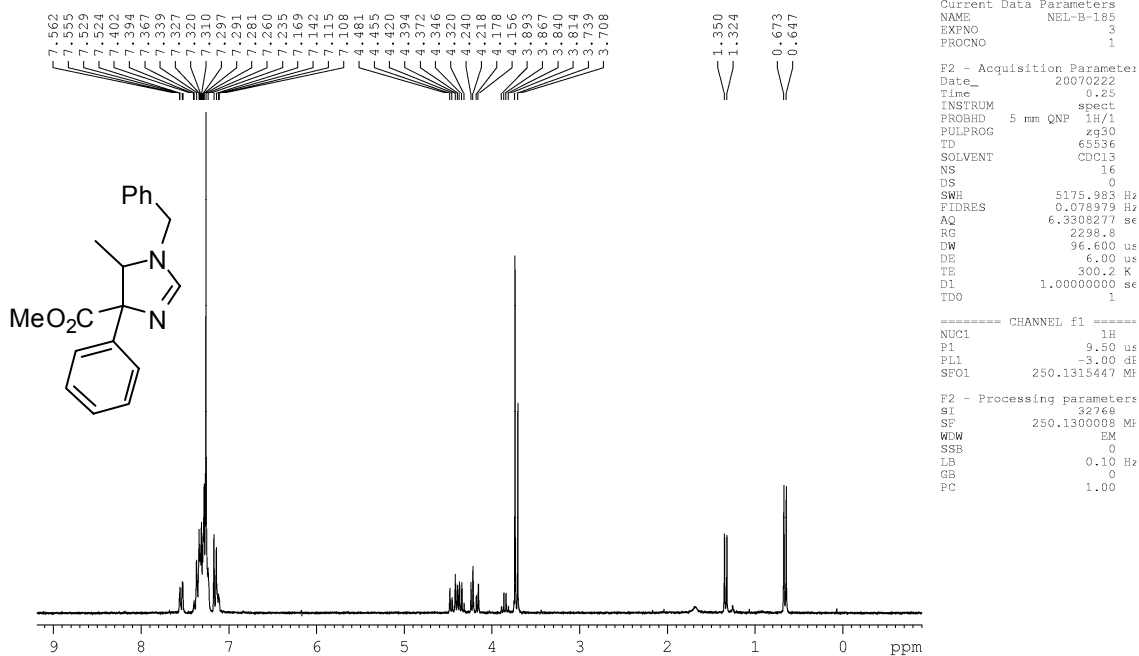


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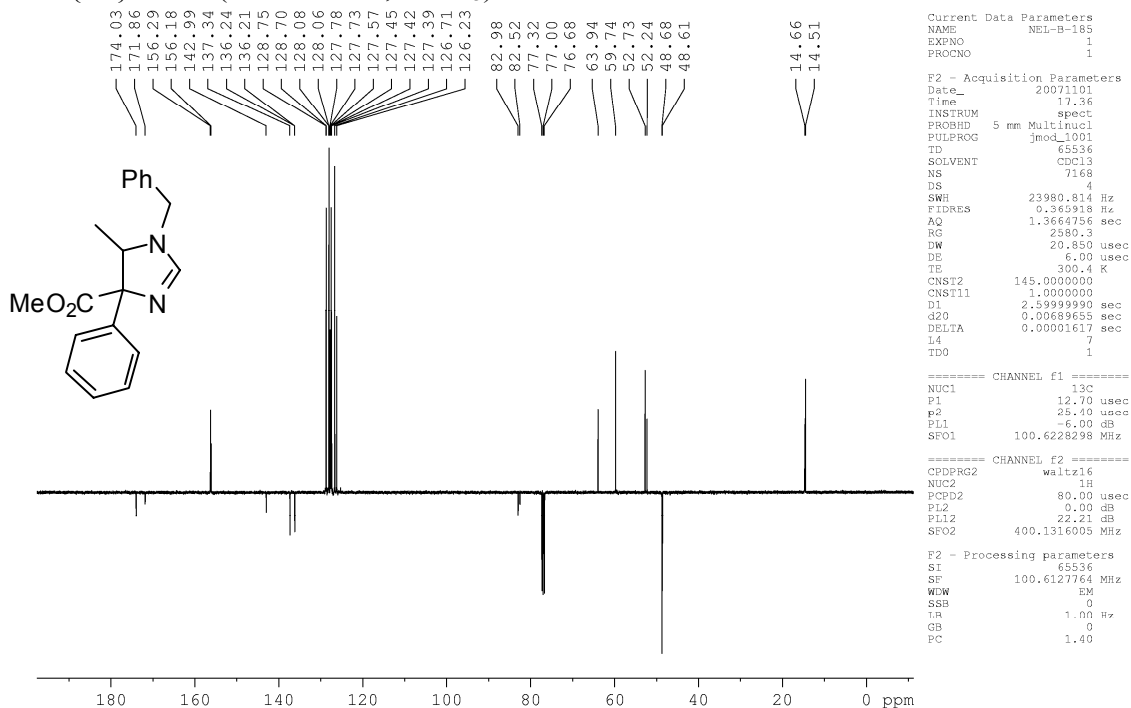


Methyl 1-benzyl-5-methyl-4-phenyl-4,5-dihydro-1H-imidazole-4-carboxylate (4k):

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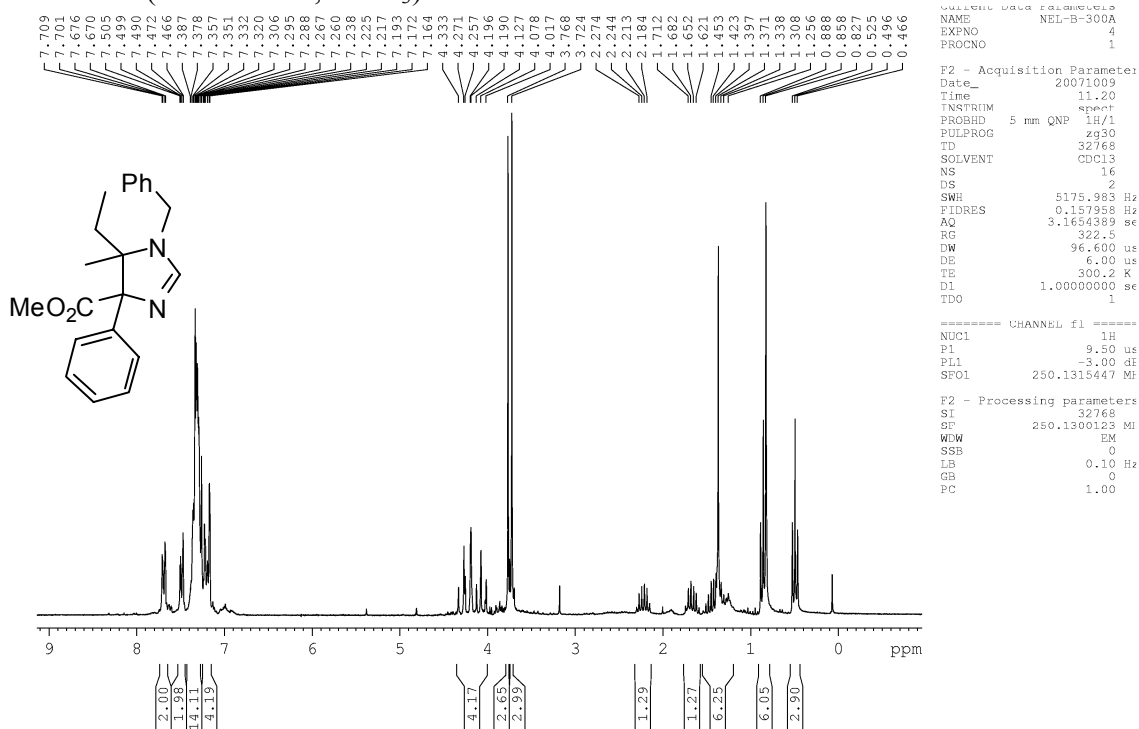
¹³C{¹H} NMR (100.62 MHz, CDCl₃)



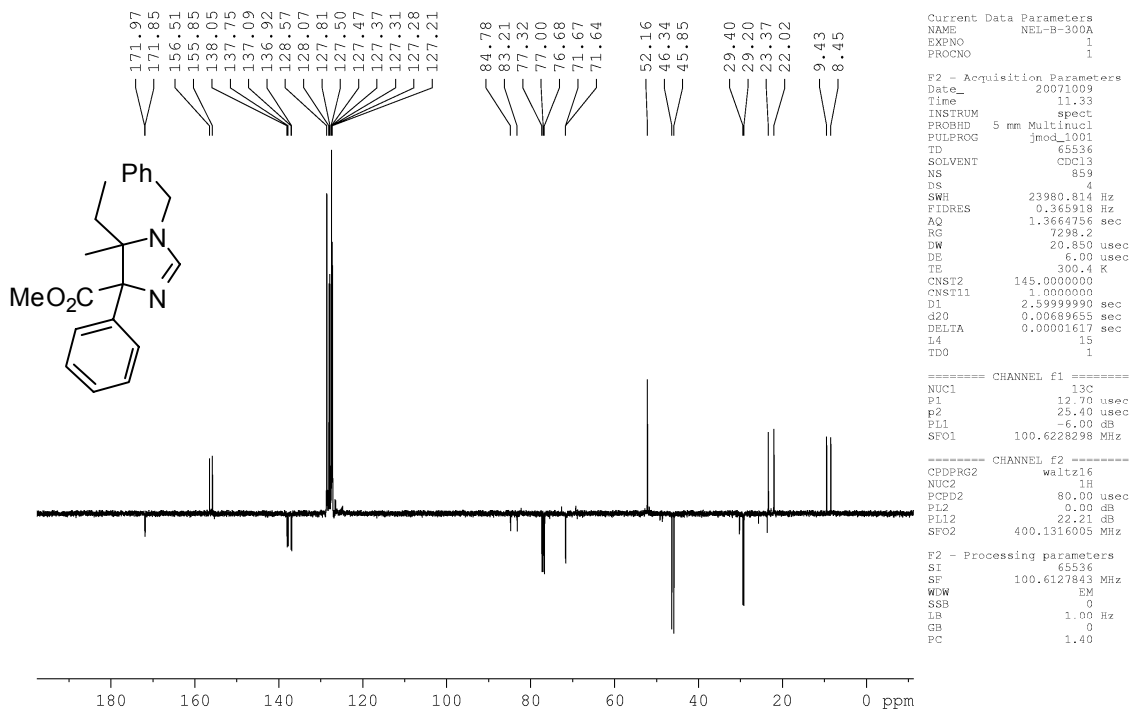
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(4l):

^1H NMR (250.13 MHz, CDCl_3)

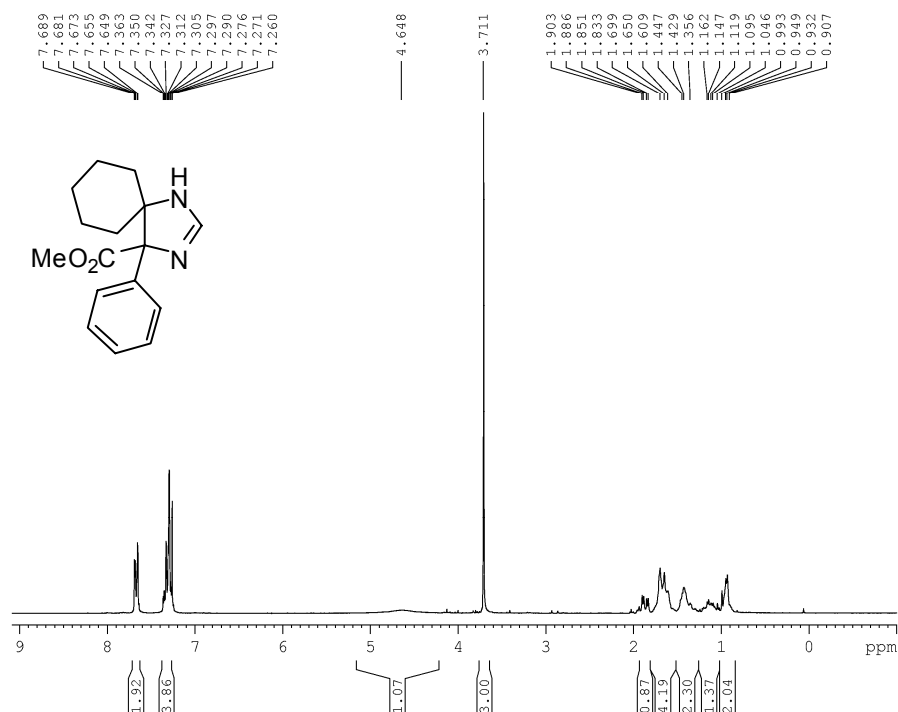


$^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl_3)



Methyl 4-phenyl-1,3-diazaspiro[4.5]dec-2-ene-4-carboxylate (4n):

^1H NMR (250.13 MHz, CDCl_3)



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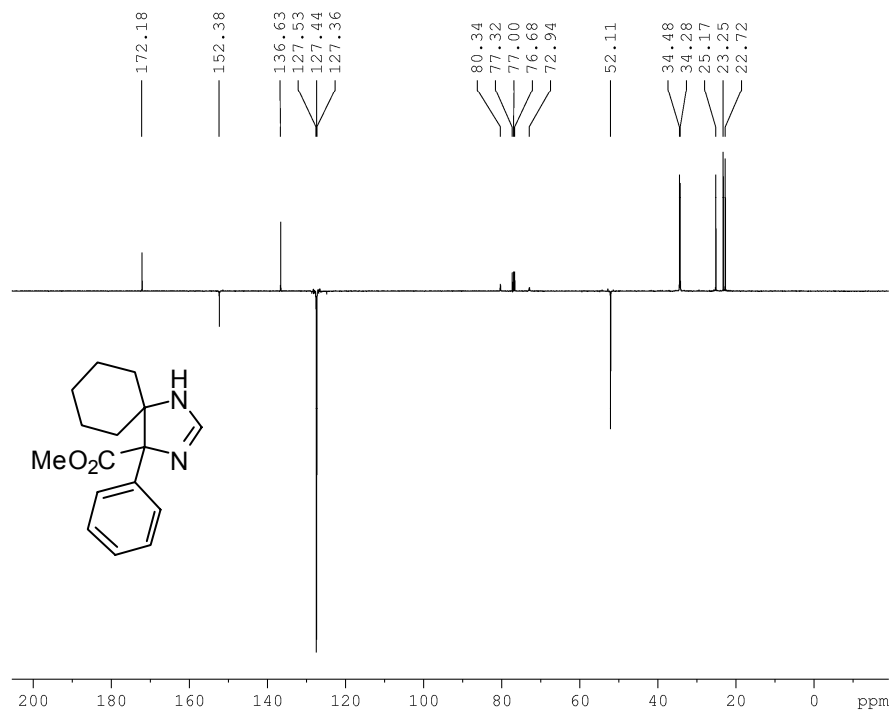
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FIDRES 0.157958 Hz
AQ 3.1654389 sec
RG 256
DW 96.600 us
DE 6.00 us
TE 300.2 K
D1 1.00000000 sec
TDO 1

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SFO1 250.1315447 MHz

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$^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl_3)



Current Data Parameters

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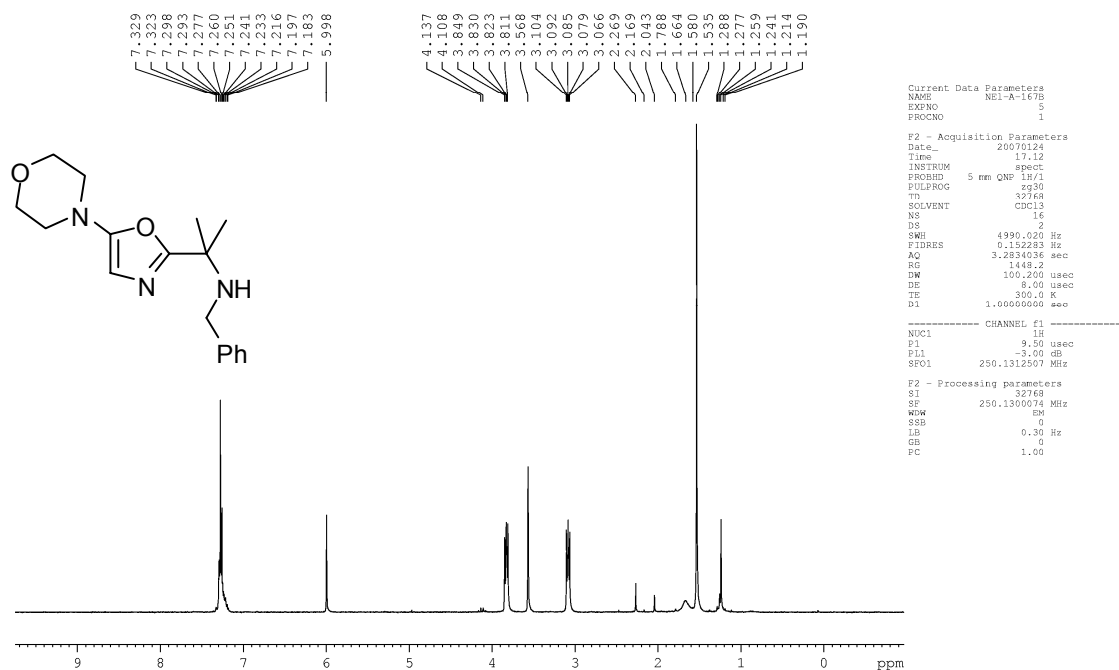
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FIDRES 0.365918 Hz
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DW 20.850 usec
DE 6.00 usec
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CNST11 1.0000000
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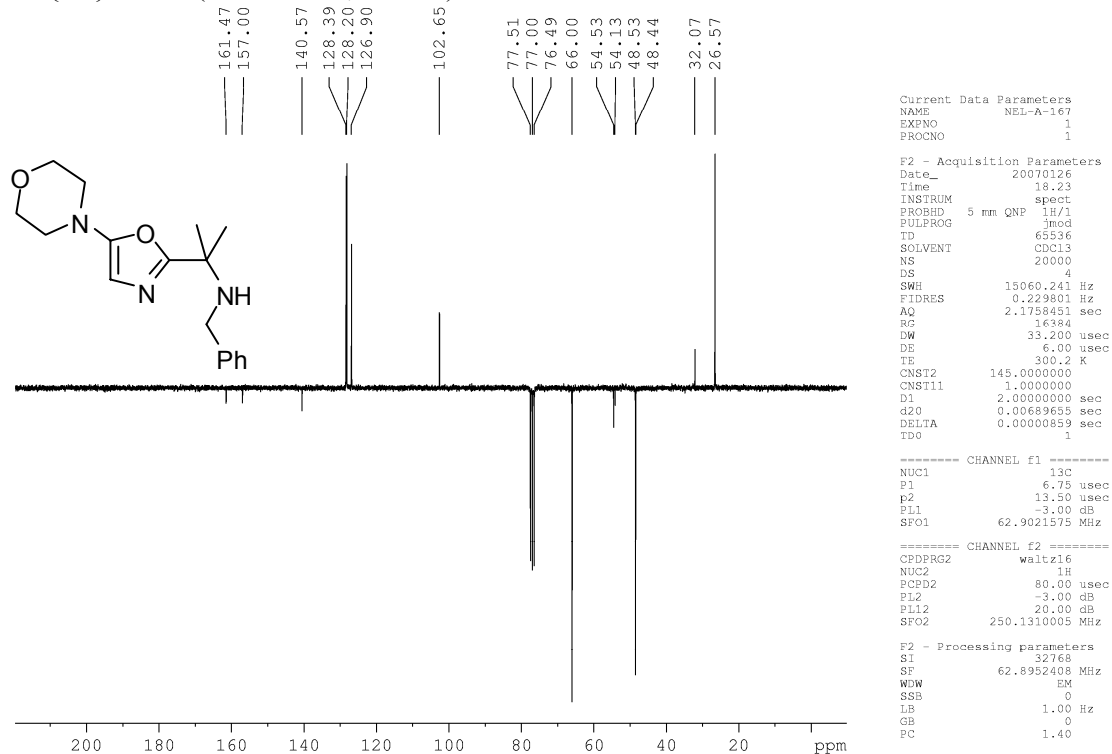
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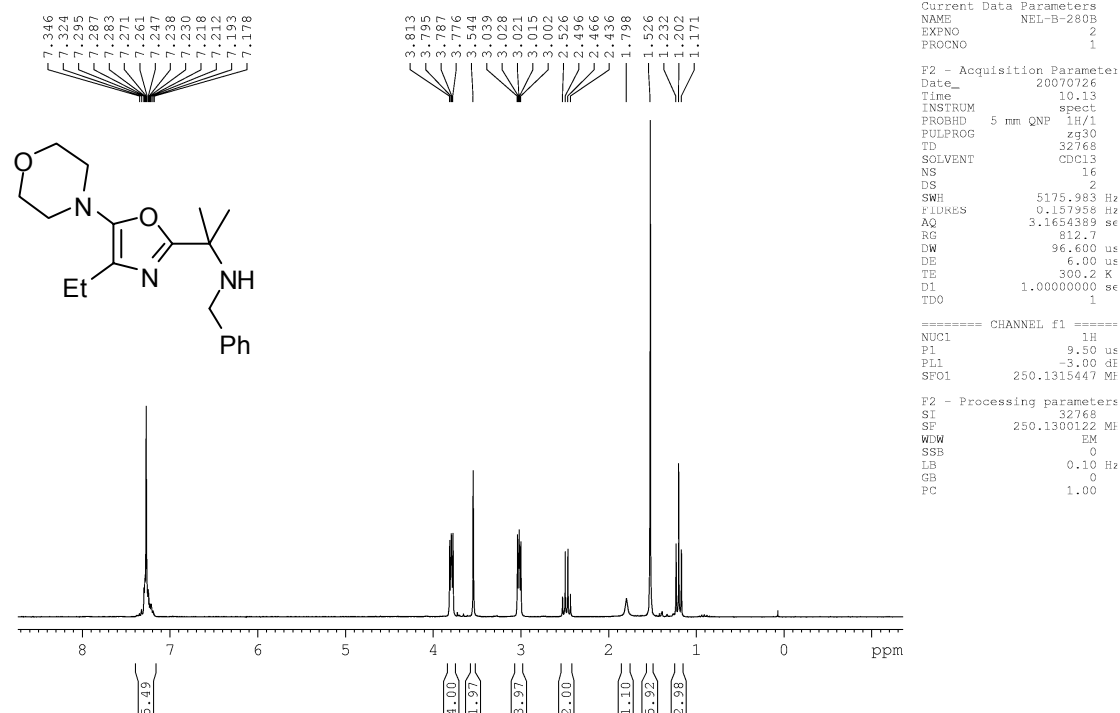
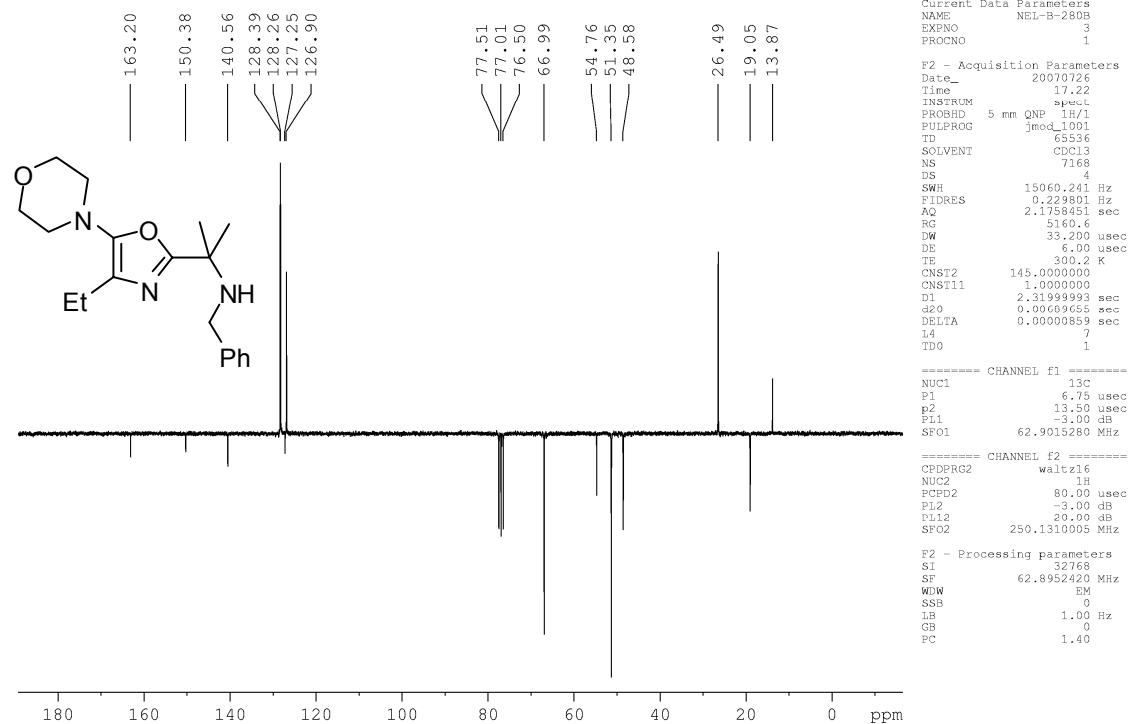
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N-benzyl-2-(5-morpholinooxazol-2-yl)propan-2-amine (5a):
¹H NMR (250.13 MHz, CDCl₃)



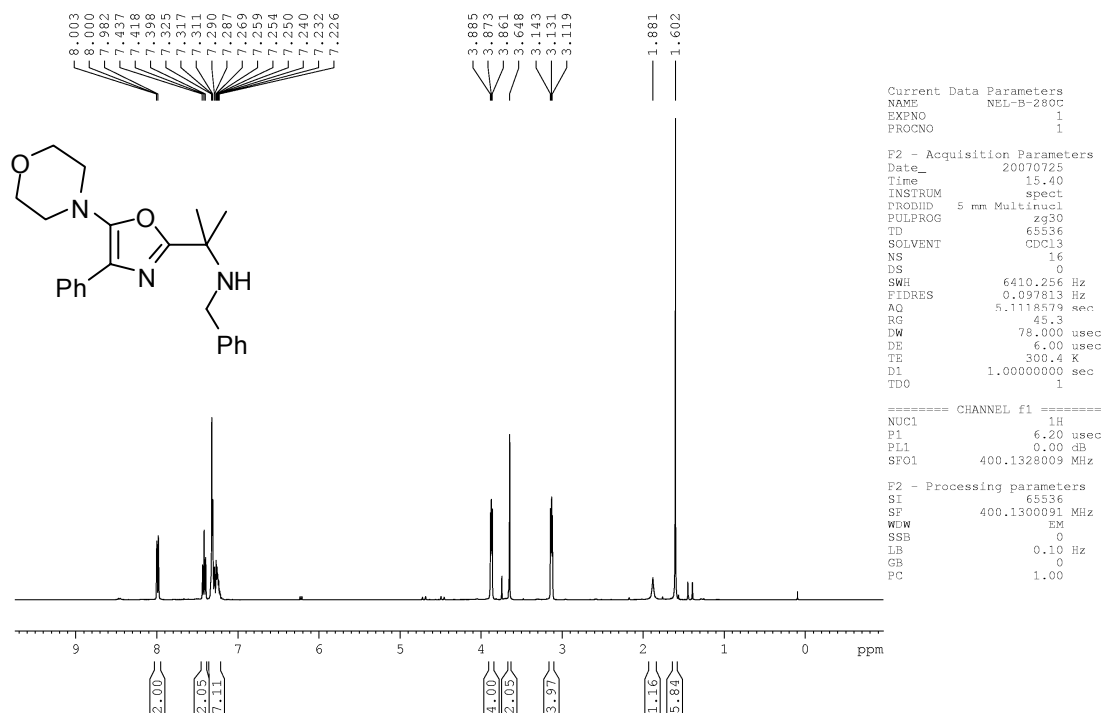
¹³C{¹H} NMR (62.90 MHz, CDCl₃)



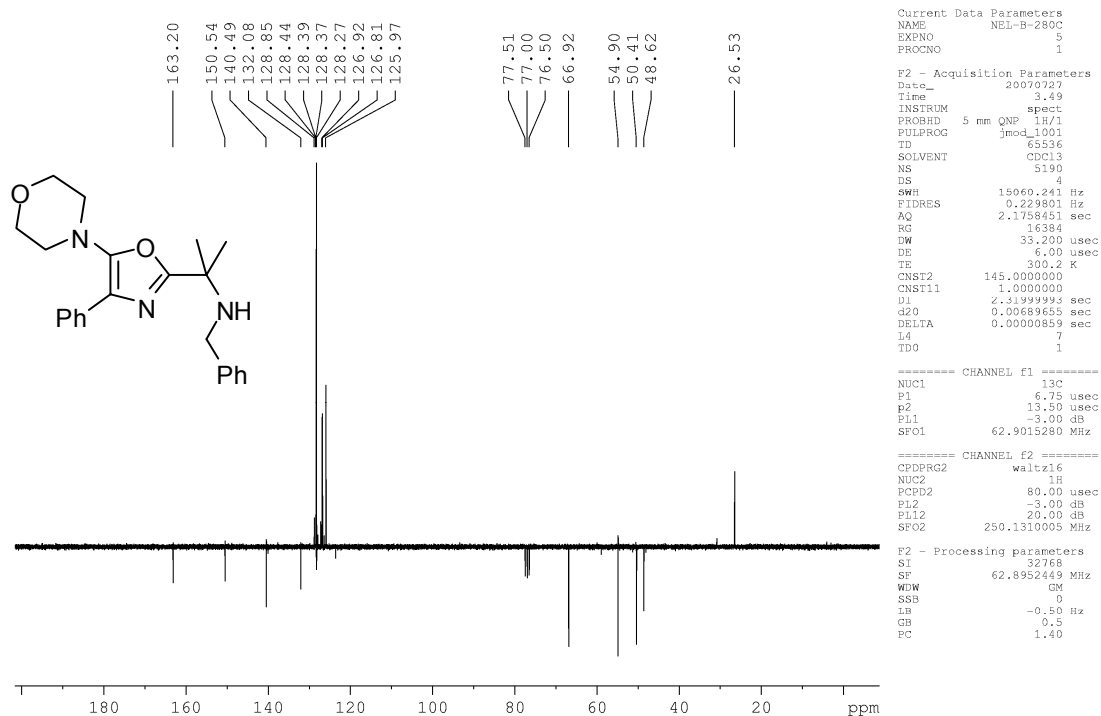
¹H NMR (250.13 MHz, CDCl₃) $^{13}\text{C}\{^1\text{H}\}$ NMR (62.90 MHz, CDCl_3)

N-benzyl-2-(5-morpholino-4-phenyloxazol-2-yl)propan-2-amine (5c):

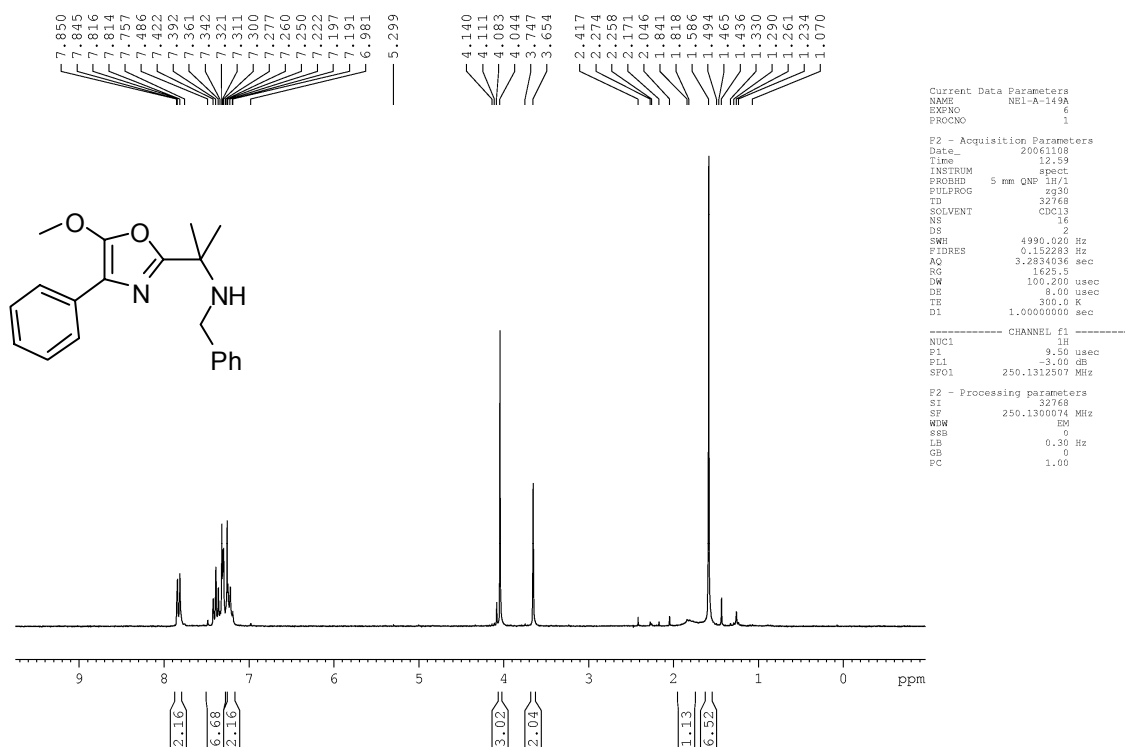
¹H NMR (400.13 MHz, CDCl₃)



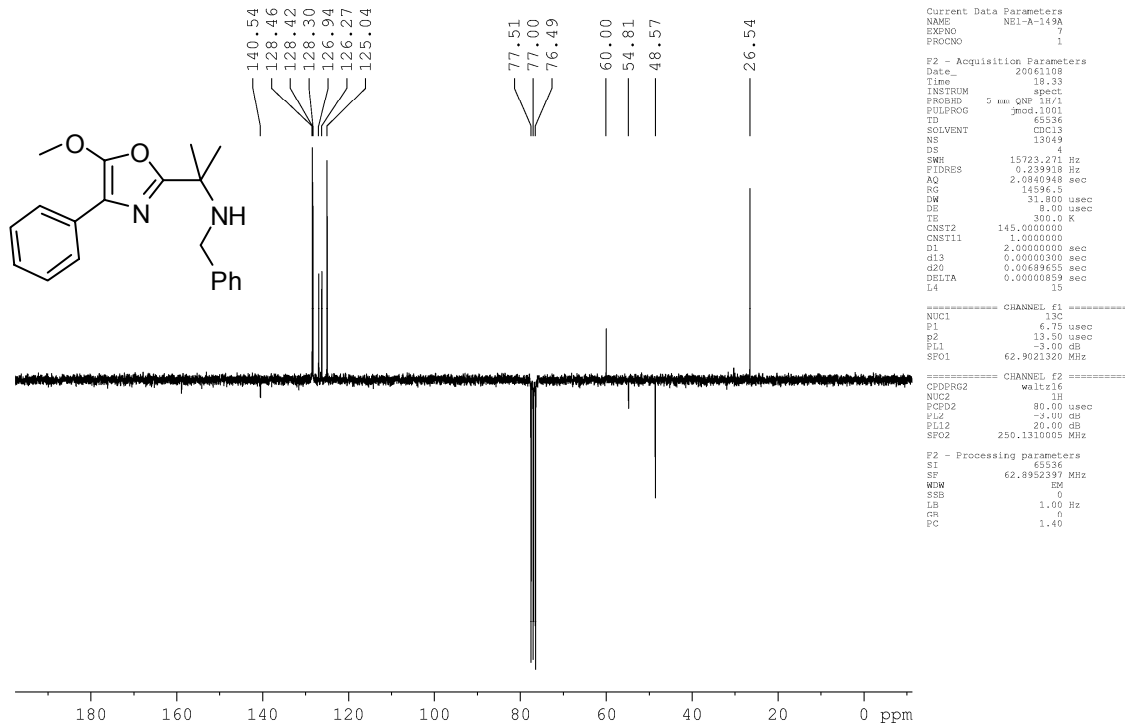
¹³C{¹H} NMR (62.90 MHz, CDCl₃)



N-benzyl-2-(5-methoxy-4-phenyloxazol-2-yl)propan-2-amine (5d):
¹H NMR (250.13 MHz, CDCl₃)

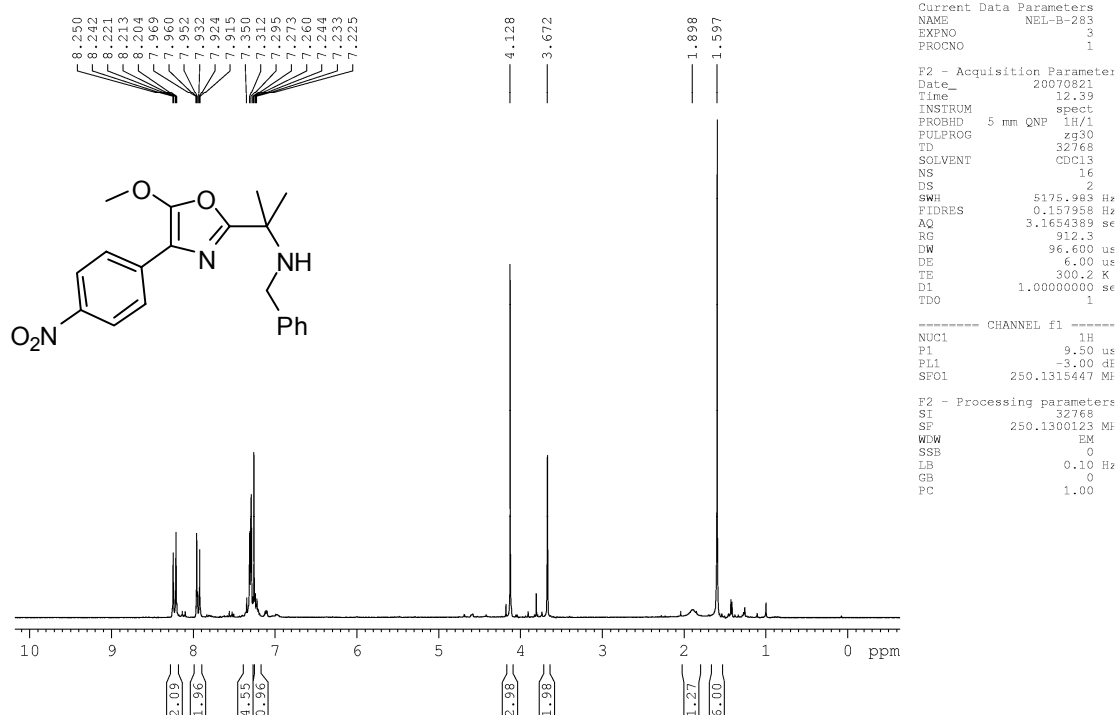


¹³C{¹H} NMR (100.62 MHz, CDCl₃)

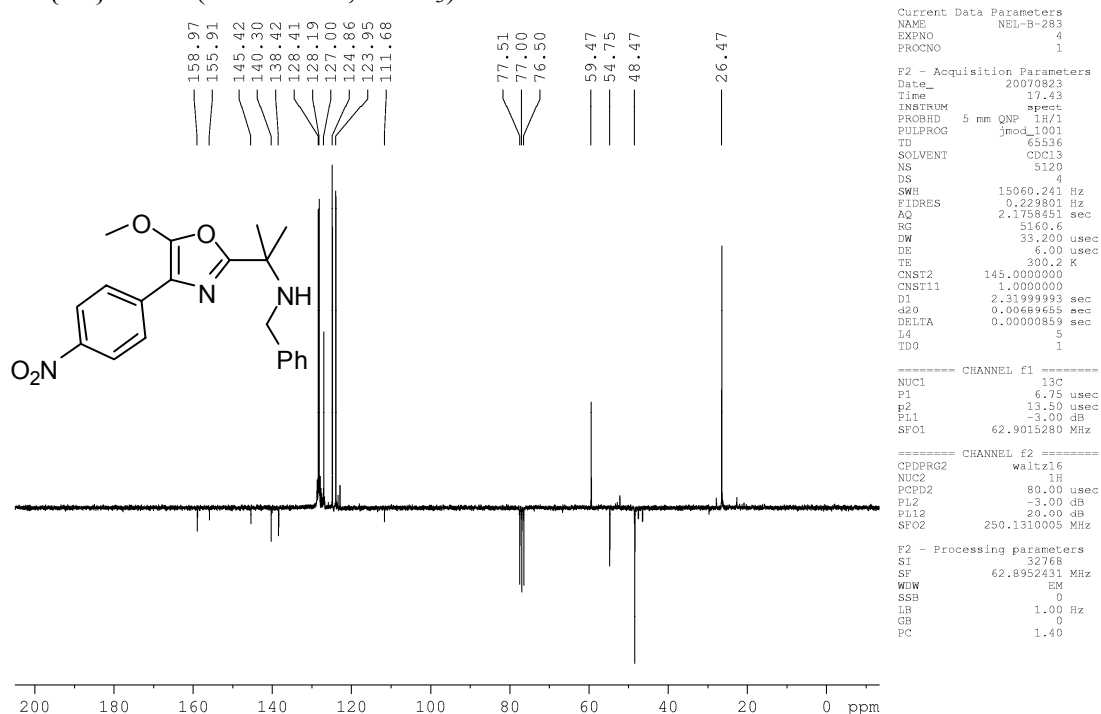


N-benzyl-2-(5-methoxy-4-(4-nitrophenyl)oxazol-2-yl)propan-2-amine (5c):

¹H NMR (250.13 MHz, CDCl₃)

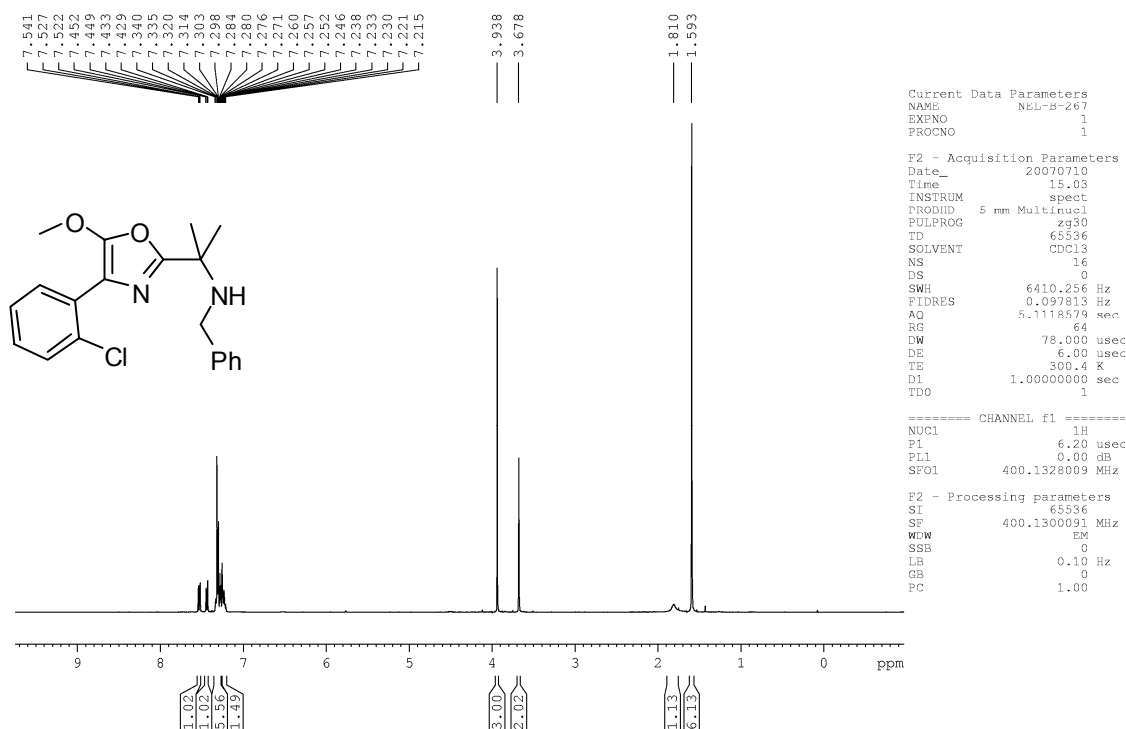


¹³C{¹H} NMR (62.90 MHz, CDCl₃)

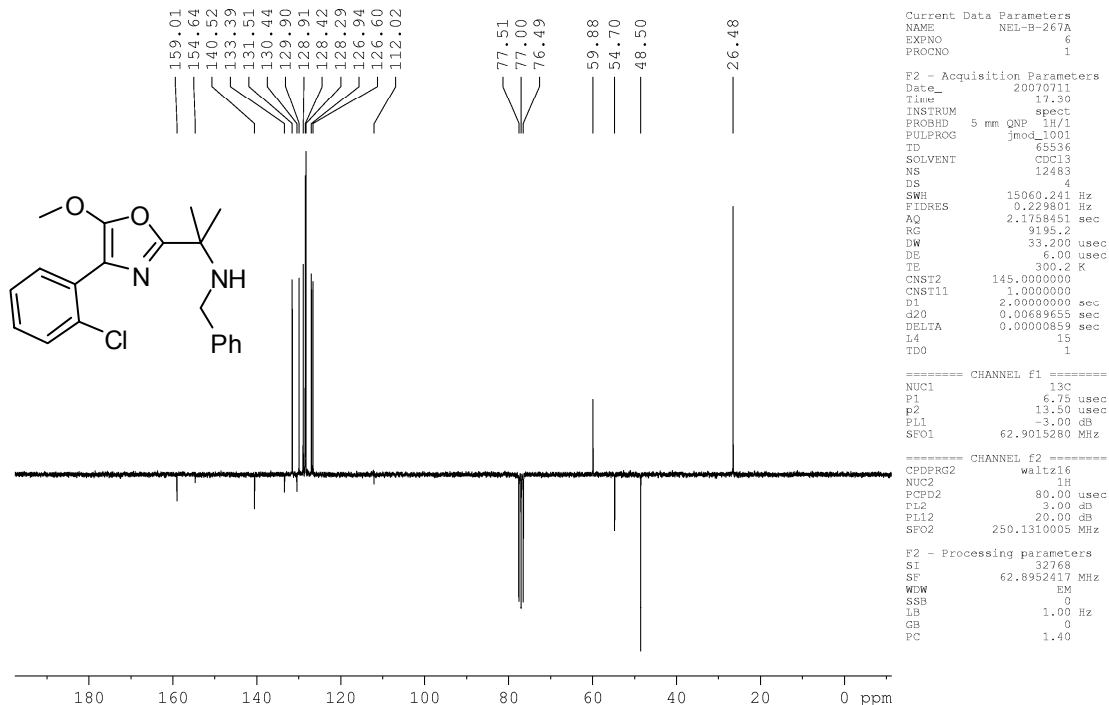


N-benzyl-2-(4-(2-chlorophenyl)-5-methoxyoxazol-2-yl)propan-2-amine (5f):

¹H NMR (400.13 MHz, CDCl₃)

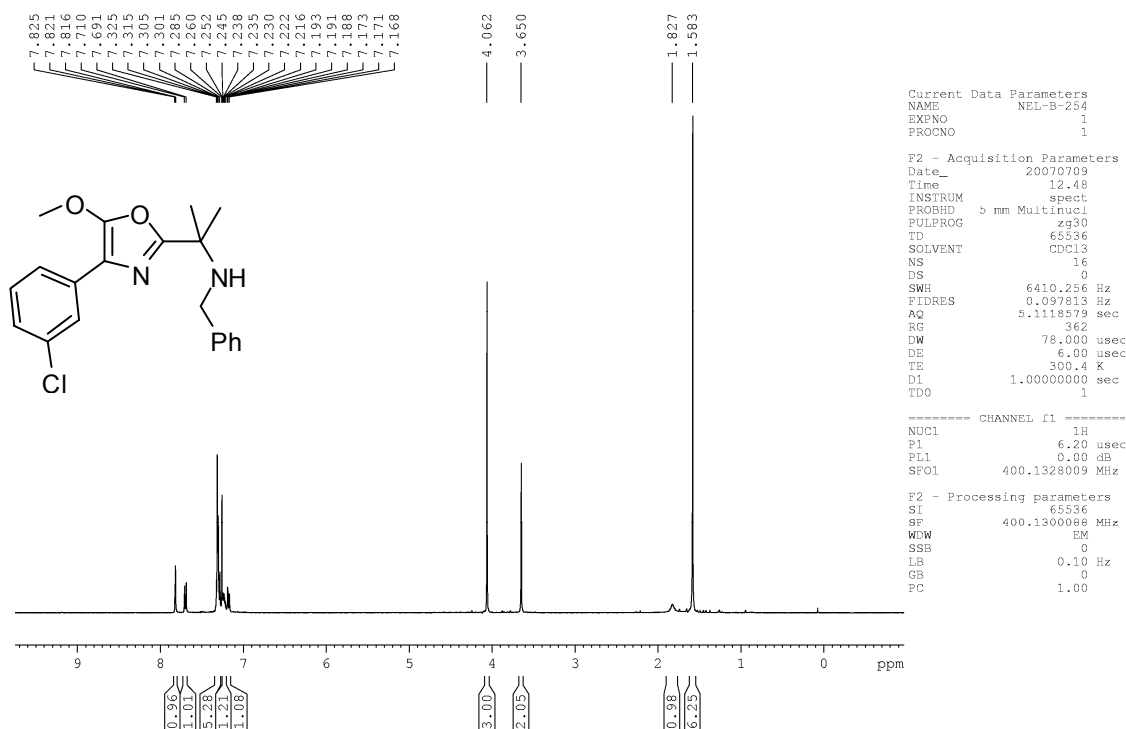


¹³C{¹H} NMR (62.90 MHz, CDCl₃)

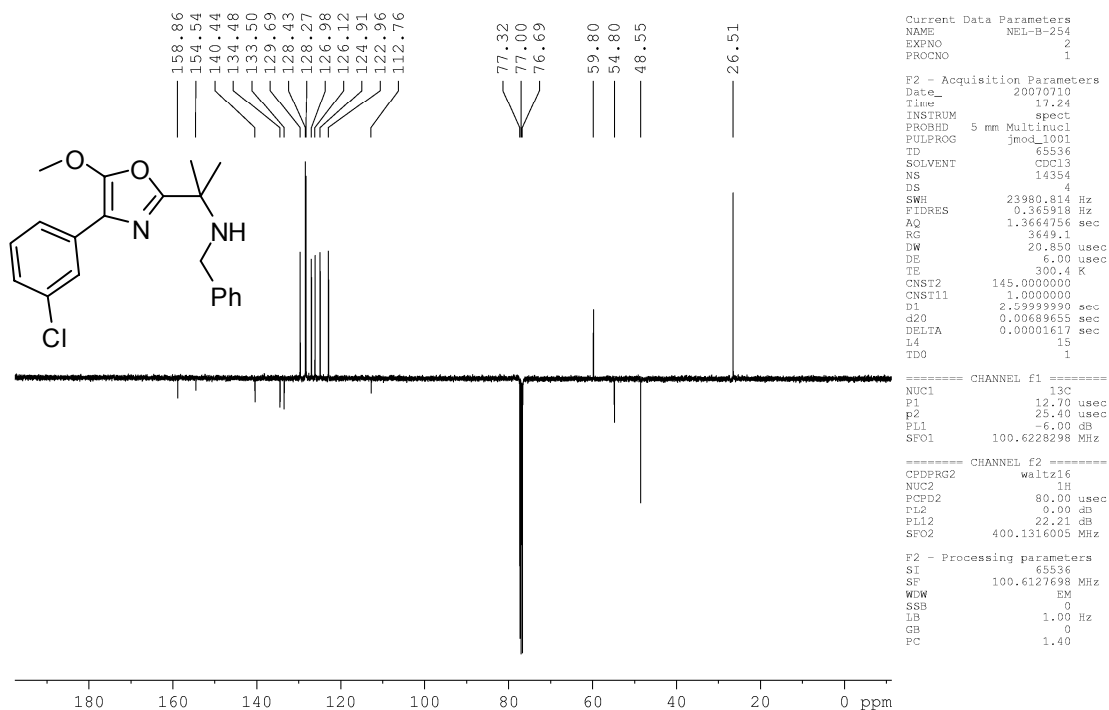


N-benzyl-2-(4-(3-chlorophenyl)-5-methoxyoxazol-2-yl)propan-2-amine (5g):

¹H NMR (400.13 MHz, CDCl₃)

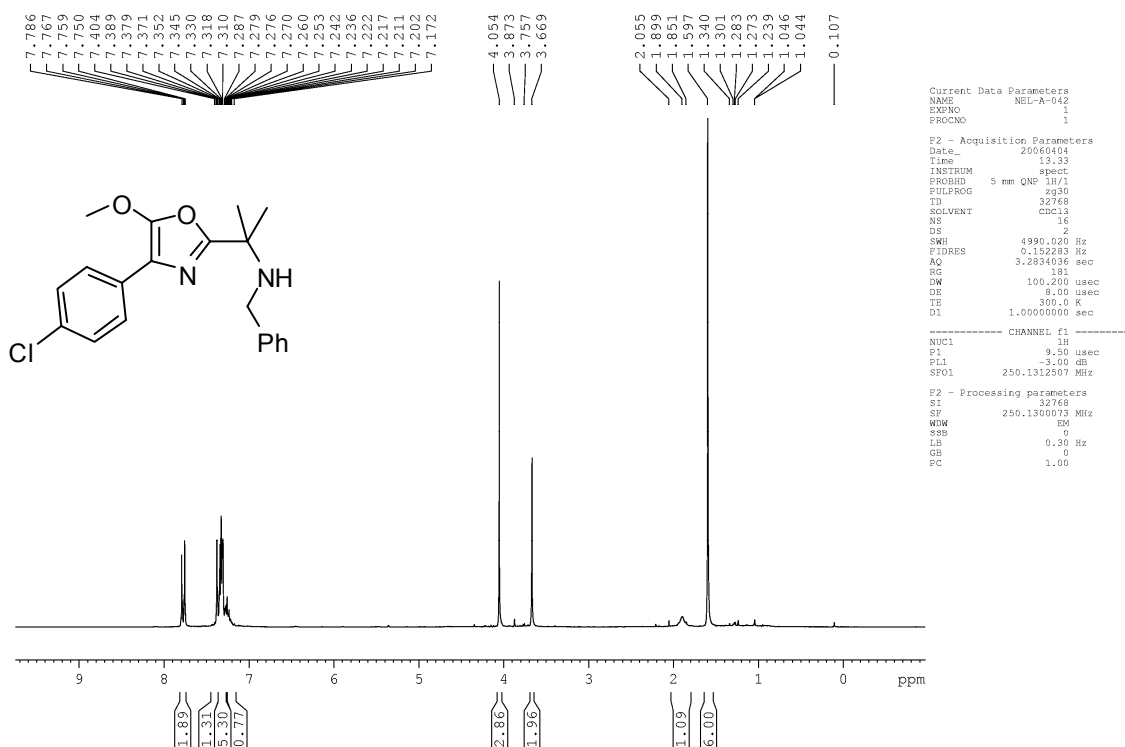


¹³C{¹H} NMR (100.62 MHz, CDCl₃)

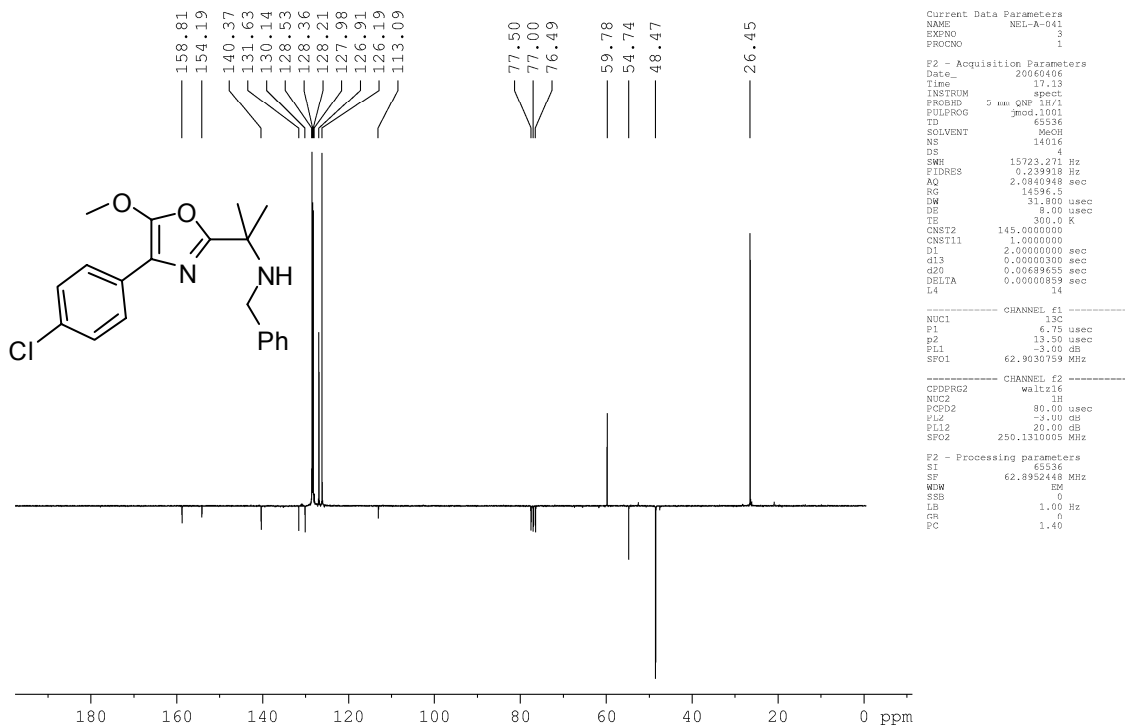


N-benzyl-2-(4-(4-chlorophenyl)-5-methoxyoxazol-2-yl)propan-2-amine (5h):

¹H NMR (250.13 MHz, CDCl₃)

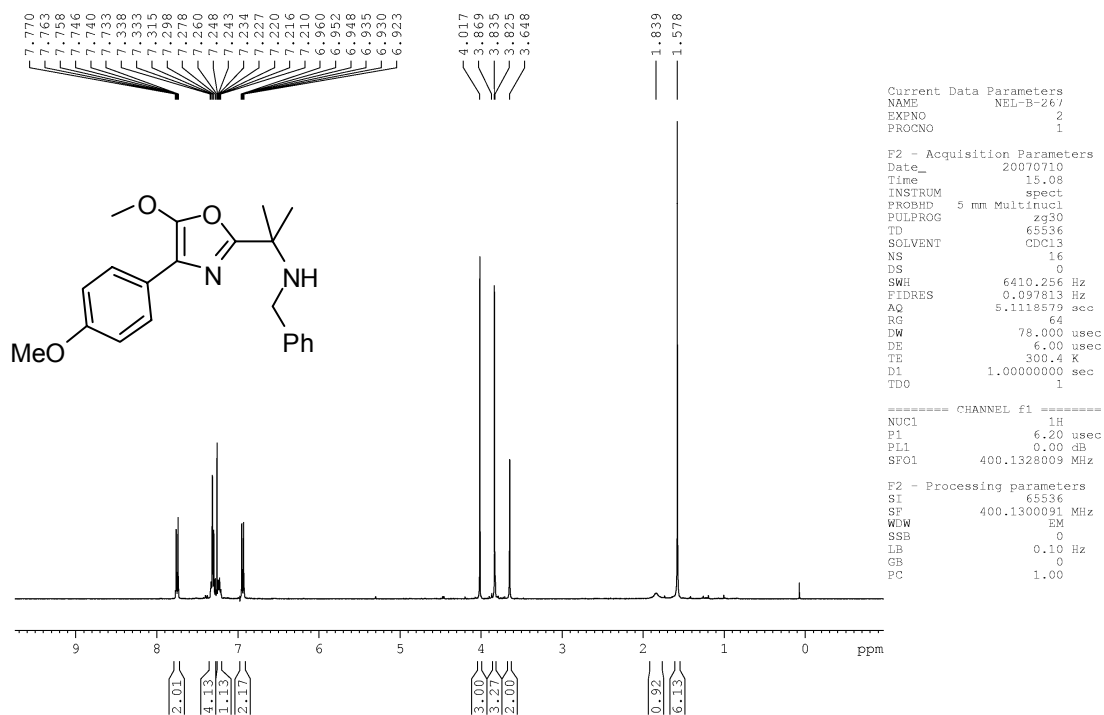


¹³C{¹H} NMR (62.90 MHz, CDCl₃)

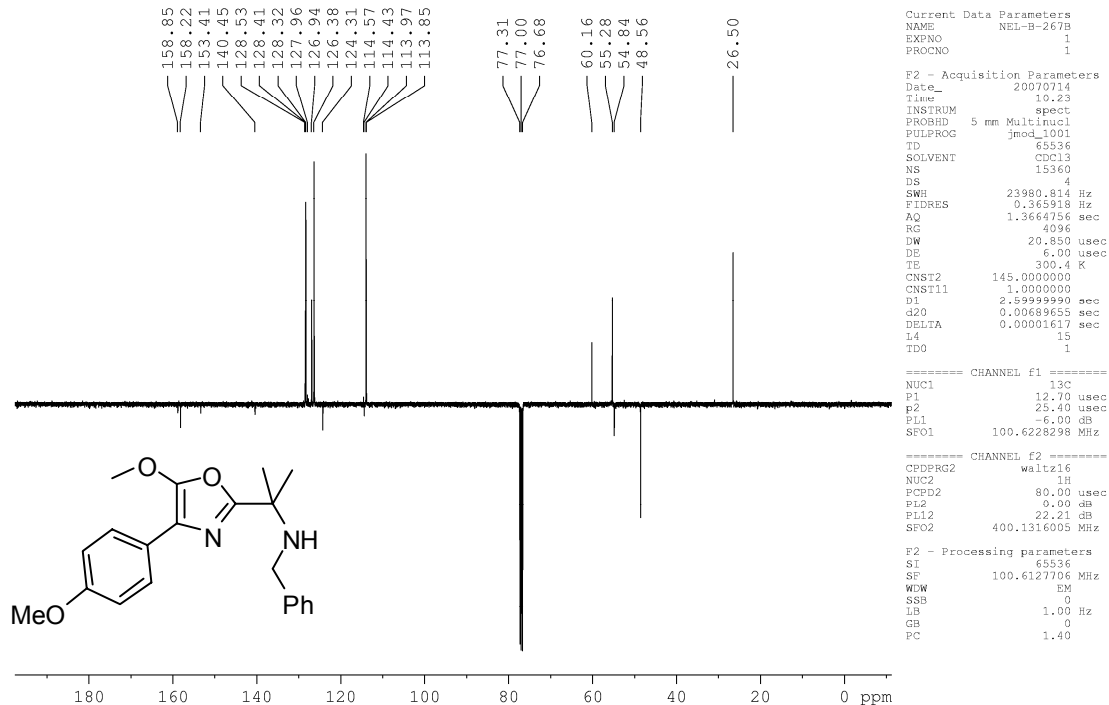


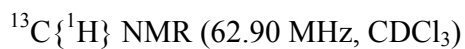
N-benzyl-2-(4-(4-methoxyphenyl)-5-methoxyoxazol-2-yl)propan-2-amine (5i):

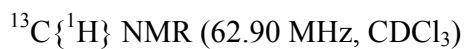
¹H NMR (400.13 MHz, CDCl₃)

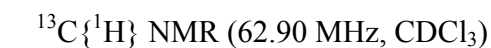


¹³C{¹H} NMR (100.62 MHz, CDCl₃)



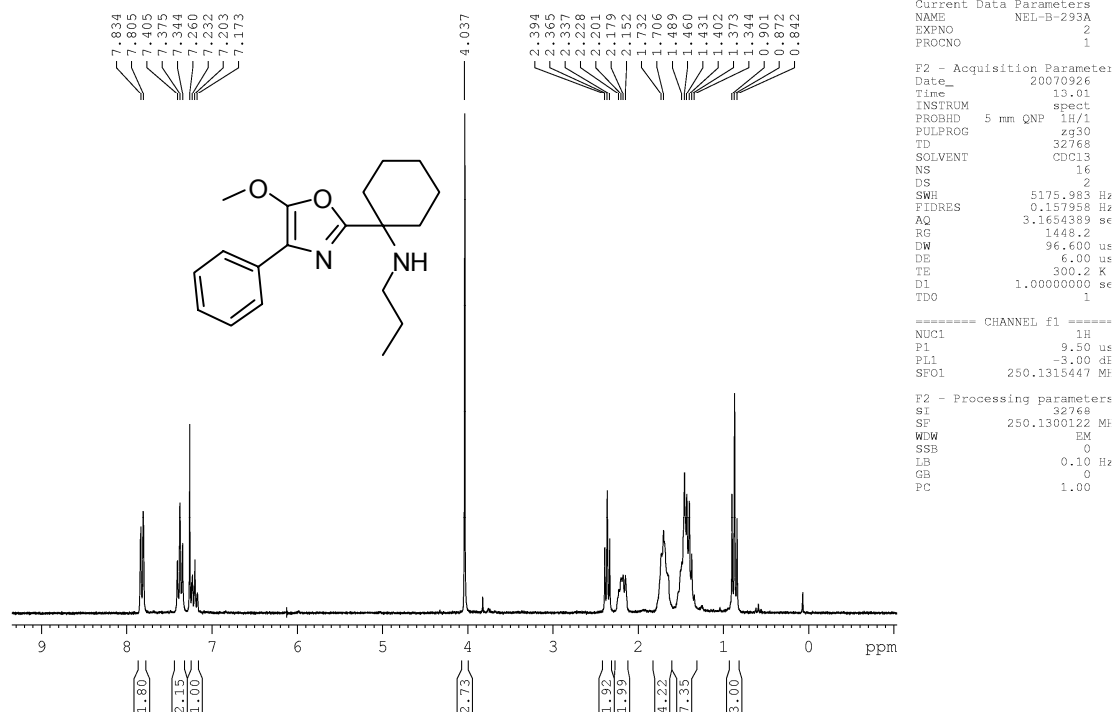
¹H NMR (250.13 MHz, CDCl₃)

¹H NMR (250.13 MHz, CDCl₃)

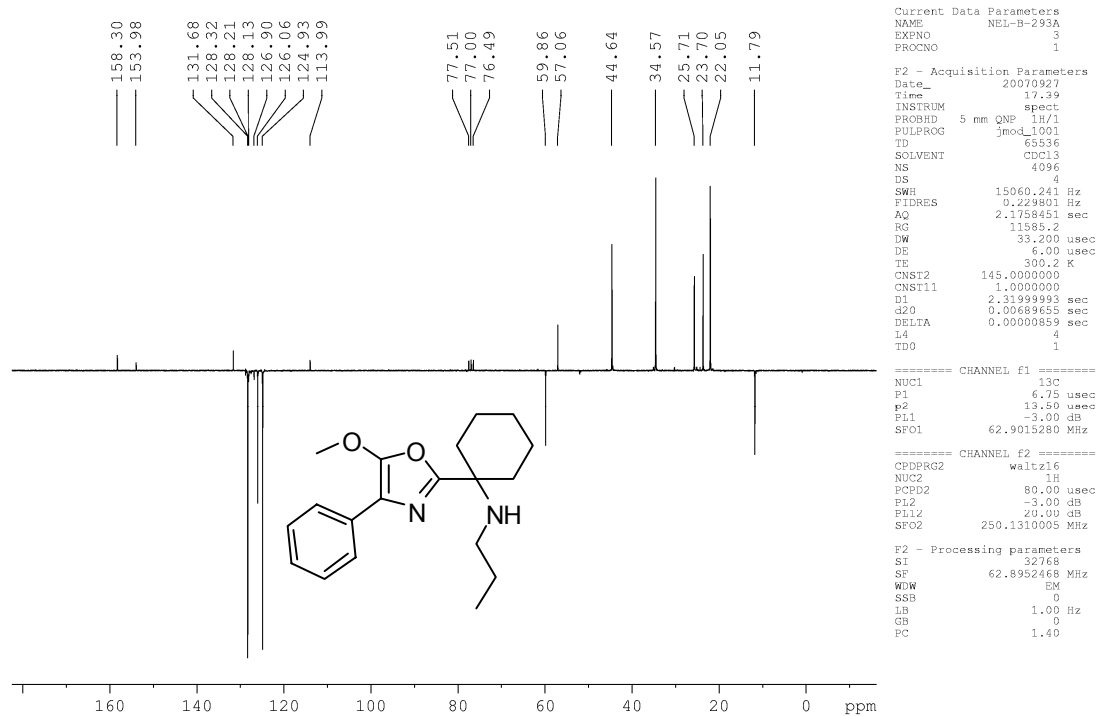
¹H NMR (250.13 MHz, CDCl₃)

1-(5-methoxy-4-phenyloxazol-2-yl)-N-propylcyclohexanamine (5o):

^1H NMR (250.13 MHz, CDCl_3)

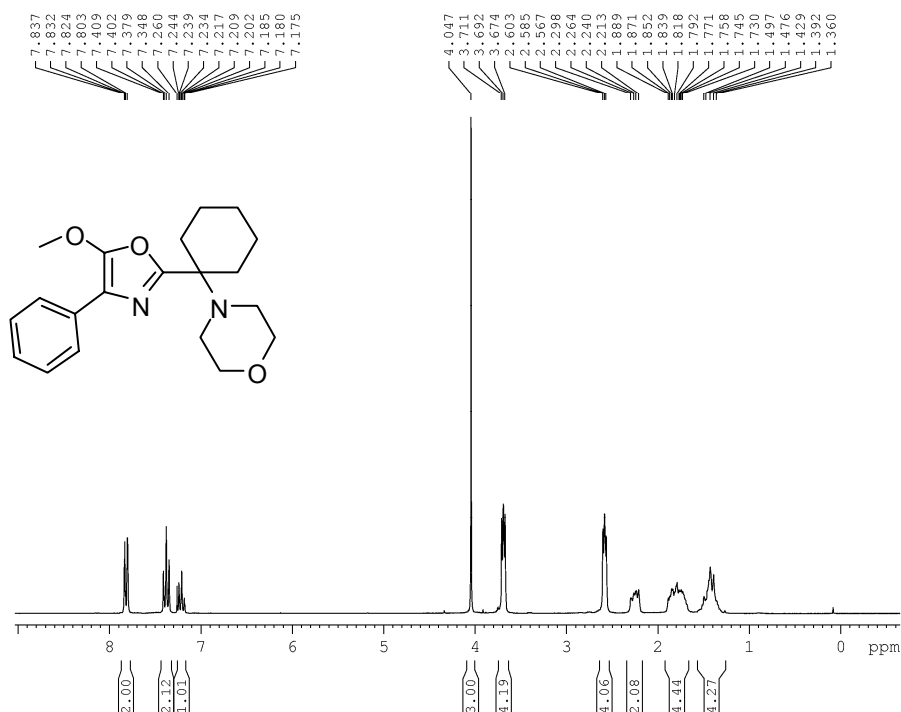


$^{13}\text{C}\{^1\text{H}\}$ NMR (62.90 MHz, CDCl_3)



4-(1-(5-methoxy-4-phenyloxazol-2-yl)cyclohexyl)morpholine (5p):

¹H NMR (250.13 MHz, CDCl₃)



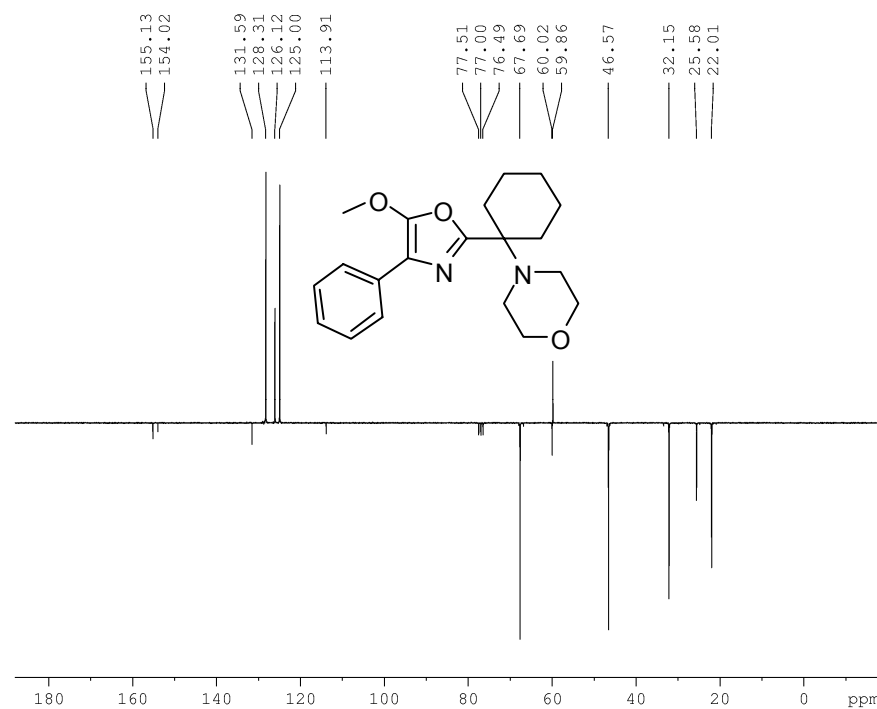
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Current Data Parameters
NAME      NEL-B-295D
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters:
Date_     20070927
Time      11.12
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        5175.983 Hz
FIDRES     0.157958 Hz
AQ         3.1654389 sec
RG         203.2
DW         96.600 us
DE         6.00 us
TE         300.2 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.50 us
PL1        -3.00 dB
SFO1       250.1315447 MHz

F2 - Processing parameters:
SI         32768
SF         250.1300123 MHz
WDW        EM
SSB        0
LB         0.10 Hz
GB         0
PC         1.00
```

¹³C{¹H} NMR (62.90 MHz, CDCl₃)



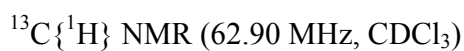
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Current Data Parameters
NAME      NEL-B-295D
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters:
Date_     20070928
Time      8.29
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   jmod1001
TD         65536
SOLVENT   CDCl3
NS         3072
DS         4
SWH        15060.241 Hz
FIDRES     0.229801 Hz
AQ         2.1758451 sec
RG         16384
DW         33.200 usec
DE         6.00 usec
TE         300.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.31999993 sec
g20        0.00689655 sec
DELTA     0.00000859 sec
L4         6
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         6.75 usec
p2         13.50 usec
PL1        -3.00 dB
SFO1       62.9015280 MHz

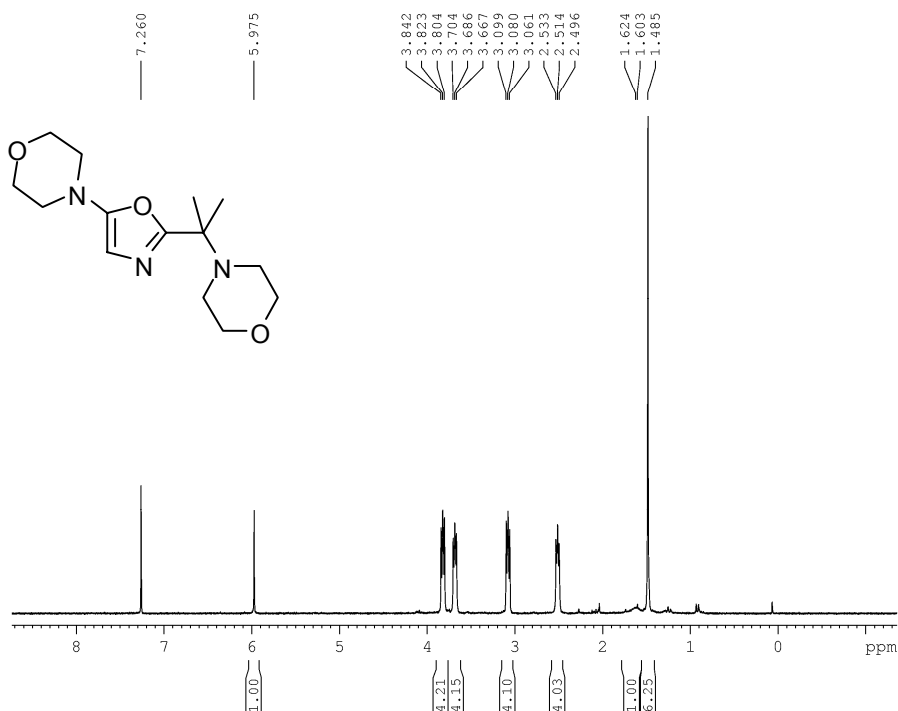
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -3.00 dB
PL12       20.00 dB
SFO2       250.1310005 MHz

F2 - Processing parameters:
SI         32768
SF         62.8952484 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

¹H NMR (250.13 MHz, CDCl₃)

4-(2-(5-morpholinooxazol-2-yl)propan-2-yl)morpholine (6):

¹H NMR (250.13 MHz, CDCl₃)



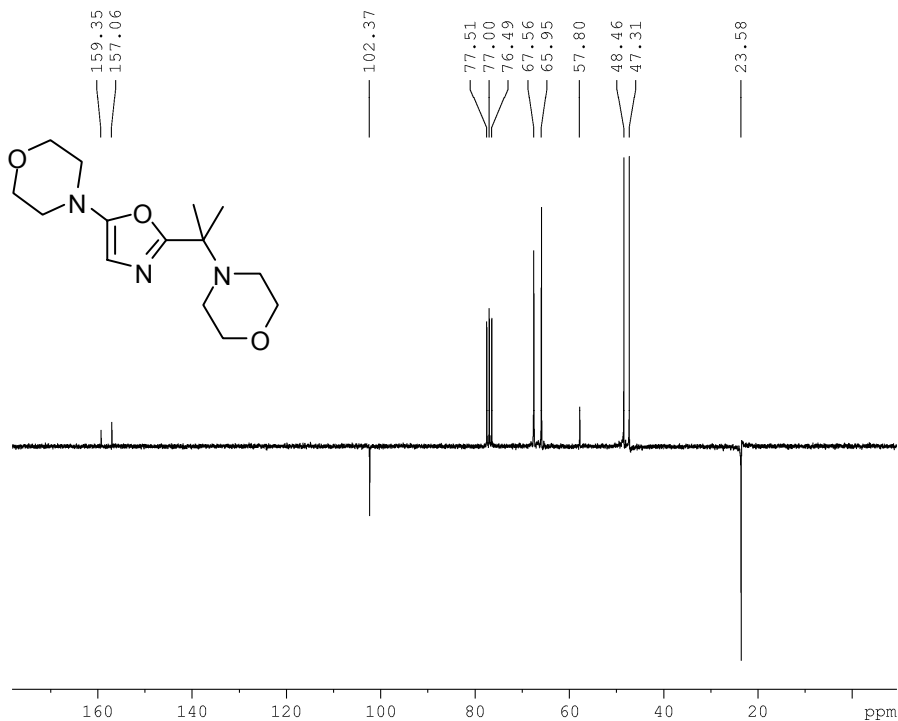
Current Data Parameters
NAME NEL-B-279
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070719
Time 15.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5175.983 Hz
FIDRES 0.157958 Hz
AQ 3.1654389 sec
RG 4096
DW 96.600 us
DE 6.00 us
TE 300.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 us
PL1 -3.00 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1300124 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (62.90 MHz, CDCl₃)



Current Data Parameters
NAME NEL-B-279
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070724
Time 17.31
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG jmod1001
TD 65536
SOLVENT CDCl3
NS 12275
DS 4
SWH 15060.241 Hz
FIDRES 0.229801 Hz
AQ 2.1758451 sec
RG 16384
DW 33.200 usec
DE 6.00 usec
TE 300.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.31999993 sec
d20 0.00609655 sec
DELTA 0.00000859 sec
L4 14
TD0 1

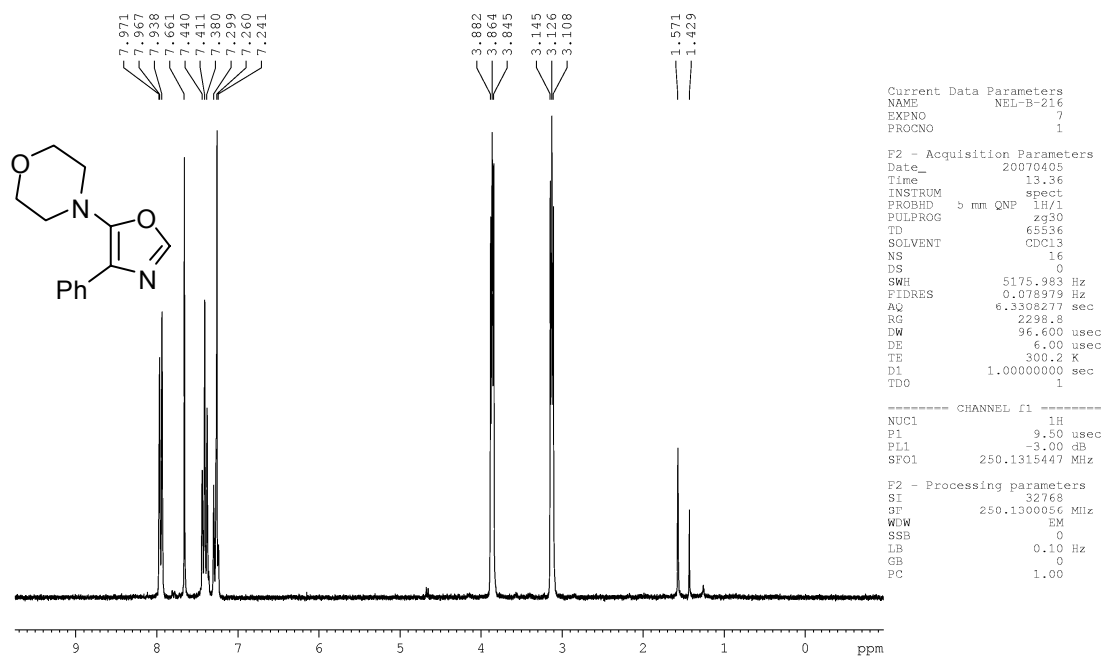
===== CHANNEL f1 =====
NUC1 13C
P1 6.75 usec
p2 13.50 usec
PL1 -3.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 20.00 dB
SFO2 250.1310005 MHz

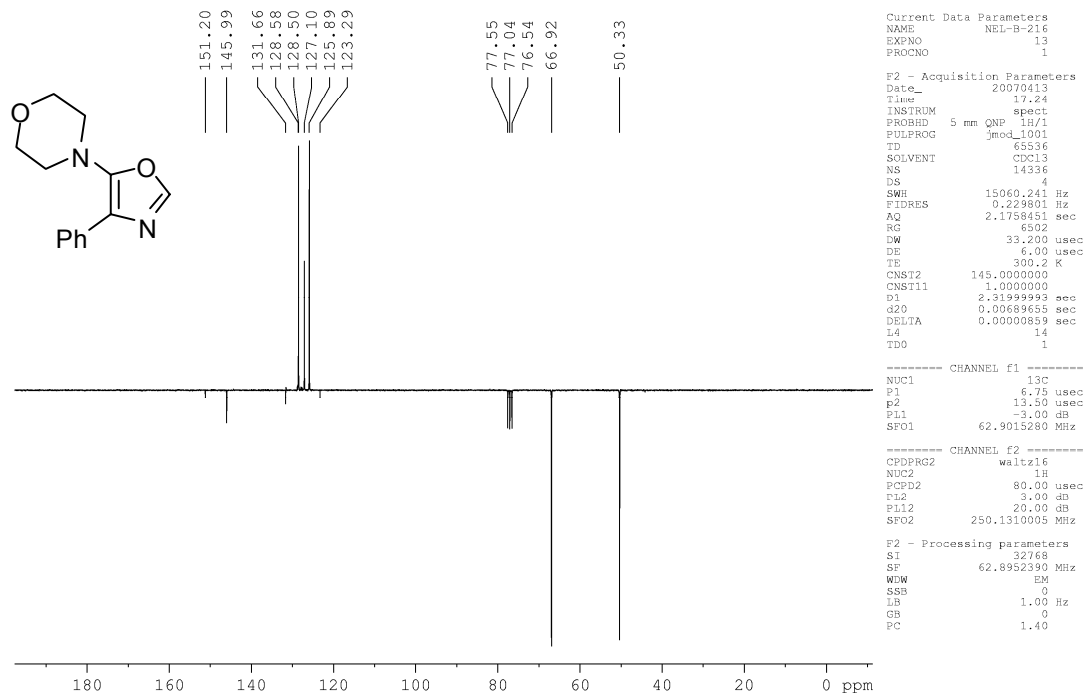
F2 - Processing parameters
SI 32768
SF 62.8952418 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-(4-phenyloxazol-5-yl)morpholine (7):

¹H NMR (250.13 MHz, CDCl₃)

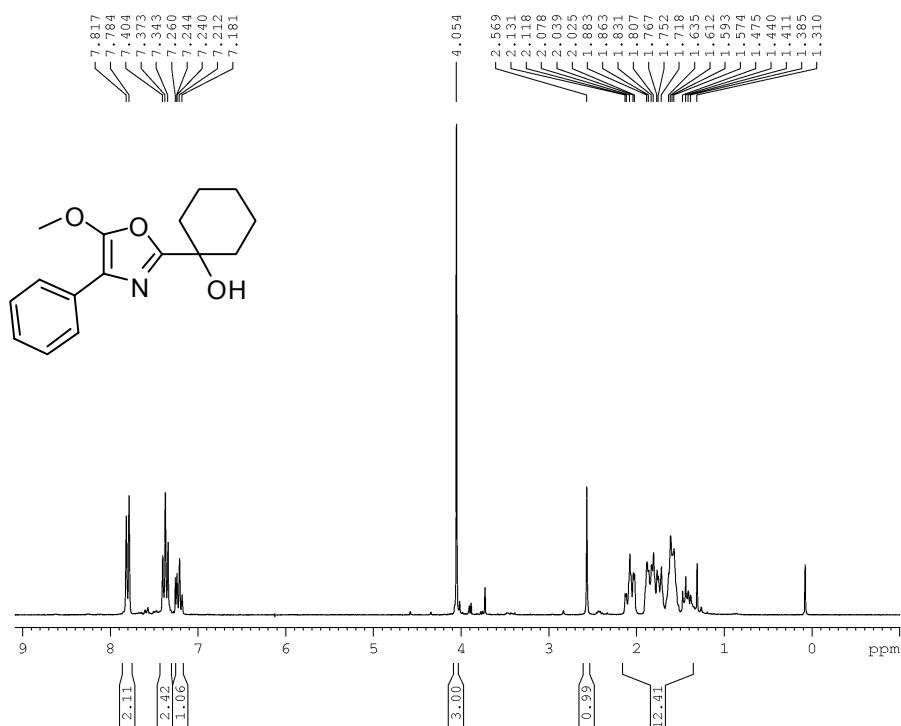


¹³C{¹H} NMR (62.90 MHz, CDCl₃)



1-(5-methoxy-4-phenyloxazol-2-yl)cyclohexanol (8):

¹H NMR (250.13 MHz, CDCl₃)



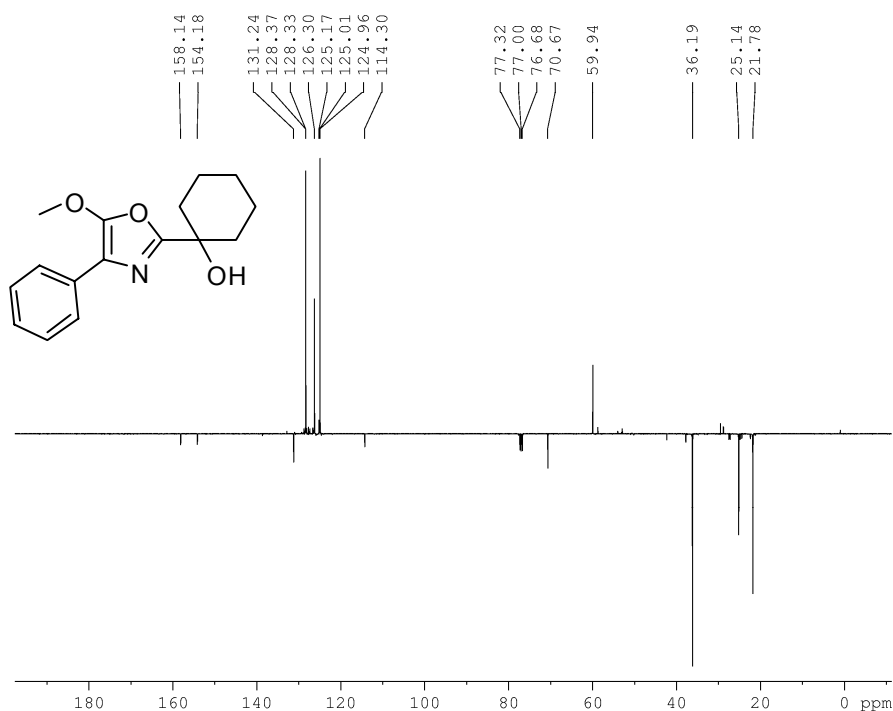
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Current Data Parameters
NAME      NEL-B-295C
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20071001
Time      13.20
INSTRUM   spect
PROBHD    5 mm QNP
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        5175.983 Hz
FIDRES     0.157958 Hz
AQ         3.1654389 sec
RG         362
DW         96.600 us
DE         6.00 us
TE         300.2 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.50 us
PL1        -3.00 dB
SFO1       250.1315447 MHz

F2 - Processing parameters
SI         32768
SF         250.1300122 MHz
WDW        EM
SSB        0
LB         0.10 Hz
GB         0
PC         1.00
```

¹³C{¹H} NMR (62.90 MHz, CDCl₃)



```
Current Data Parameters
NAME      NEL-B-295C
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20071001
Time      16.16
INSTRUM   spect
PROBHD    5 mm Multinuc1
PULPROG   jmod_1001
TD         65536
SOLVENT   CDCl3
NS         15360
DS         4
SWH        23980.814 Hz
FIDRES     0.365918 Hz
AQ         1.3664756 sec
RG         7298.2
DW         20.850 usec
DE         6.00 usec
TE         300.4 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.599999990 sec
d20       0.00689655 sec
DELTA     0.00001617 sec
L4         15
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         12.70 usec
p2         25.40 usec
PL1        -6.00 dB
SFO1       100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.00 dB
PL12       22.21 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         65536
SF         100.6127766 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```