Supporting Information

I_2 mediated synthesis of 5-substituted-3-methyl/benzyl-1,3,4-oxadiazol-2(*3H*)-ones via sequential condensation/oxidative cyclization and rearrangement

Shyam Sunder Patel,[a] Nisha Chandna,[a] Shreemoyee Kumar,[a] and Nidhi Jain*[a]

Department of Chemistry, Indian Institute of Technology, New Delhi-110016

*E-mail: njain@chemistry.iitd.ac.in

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Crystallographic Description:

Data Collection and Refinement Single-crystal X-ray data of compounds was collected on Bruker SMART CCD Diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å). Frames were collected at T = 298 K by ω, φ, and 2θ-rotations with full quadrant data collection strategy (four domains each with 600 frames) at 10s per frame with SMART. The measured intensities were reduced to F^2 and corrected for absorption with SADABS.[1] Structure solution, refinement, and data output were carried out with the SHELXTL package by direct methods.[2] Non-hydrogen atoms were refined anisotropically using the WinGX (version 1.80.05) program package.[3] All non-hydrogen atoms were refined anisotropically and hydrogen atoms were treated as riding atoms using SHELX default parameters. Molecular structures were drawn using ORTEP software shown in figure S1. Further information on the crystal structure determination (excluding structure factors) has been given as table S1 and also deposited in the Cambridge Crystallographic Data Centre as supplementary publications no. 1420804. Copies of the data can be obtained free of charge upon application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033. e-mail: deposit@ccdc.cam.ac.uk) or via internet.

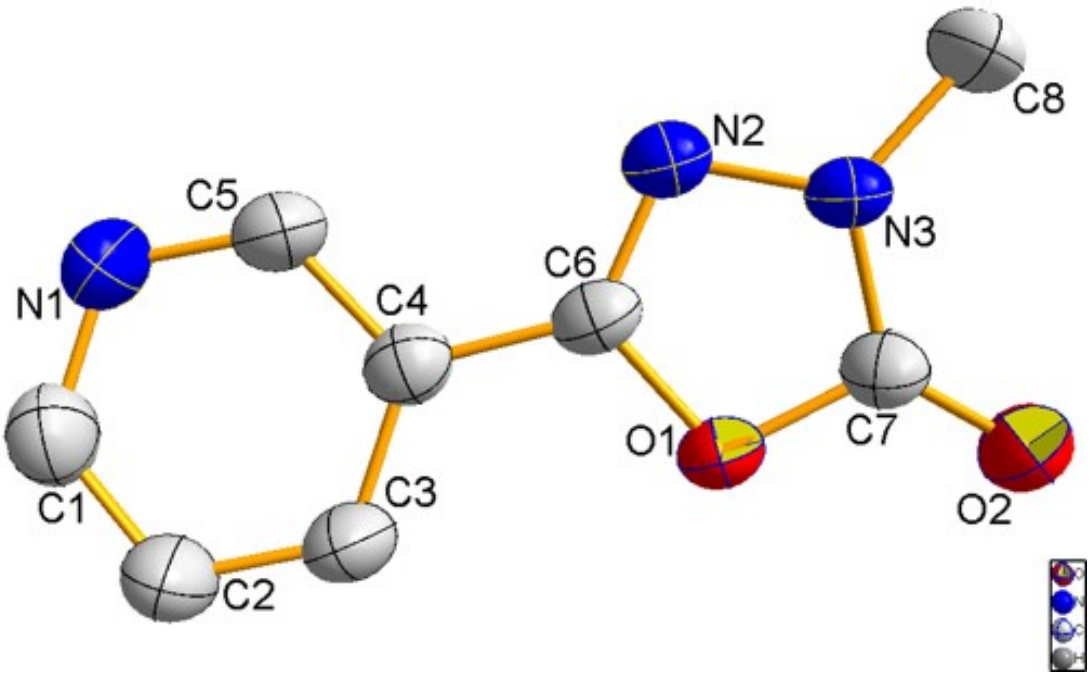


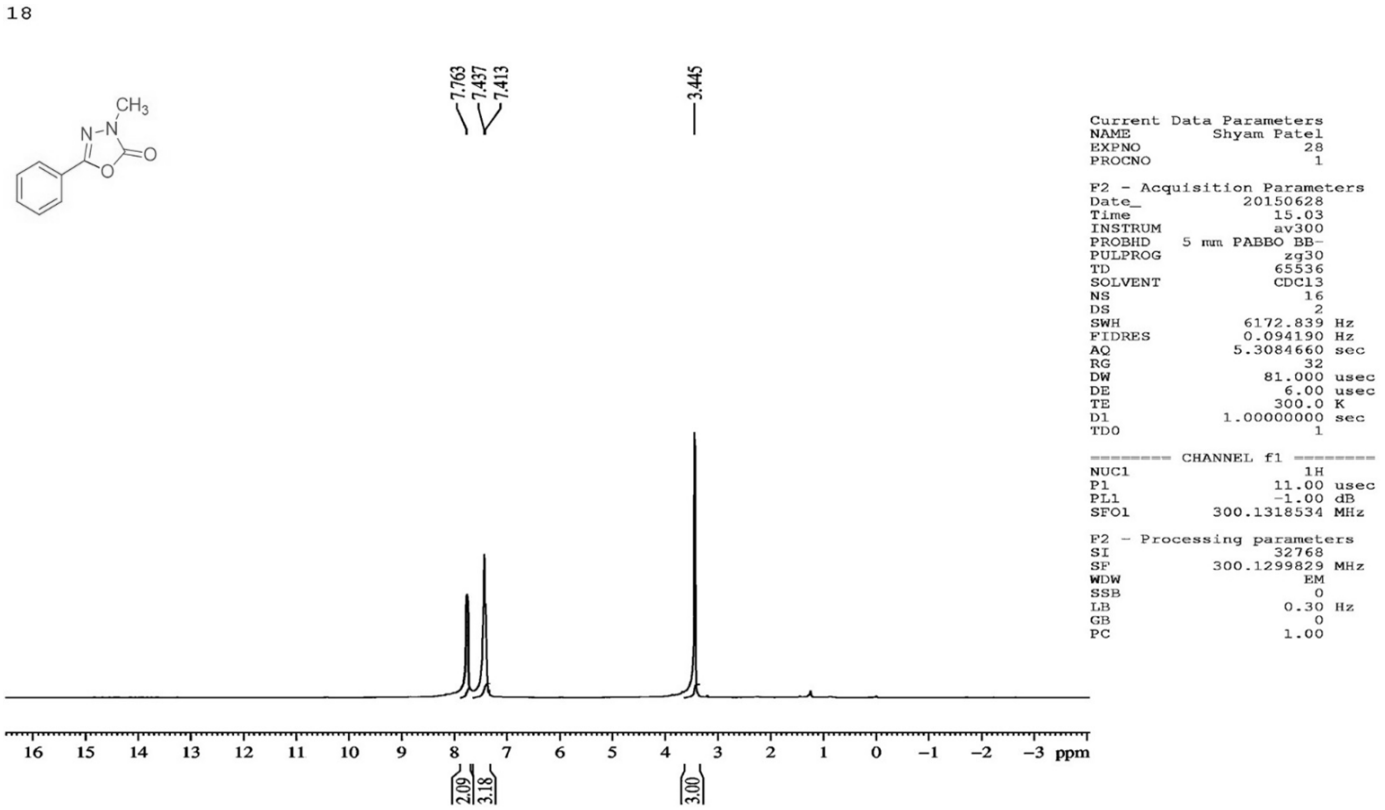
Fig. S1 ORTEP diagram of Compound **4q**

Crystallographic description of 3-methyl-5-(pyridin-3-yl)-1,3,4-oxadiazol-2(*3H*)-one (4q) (Table S1):

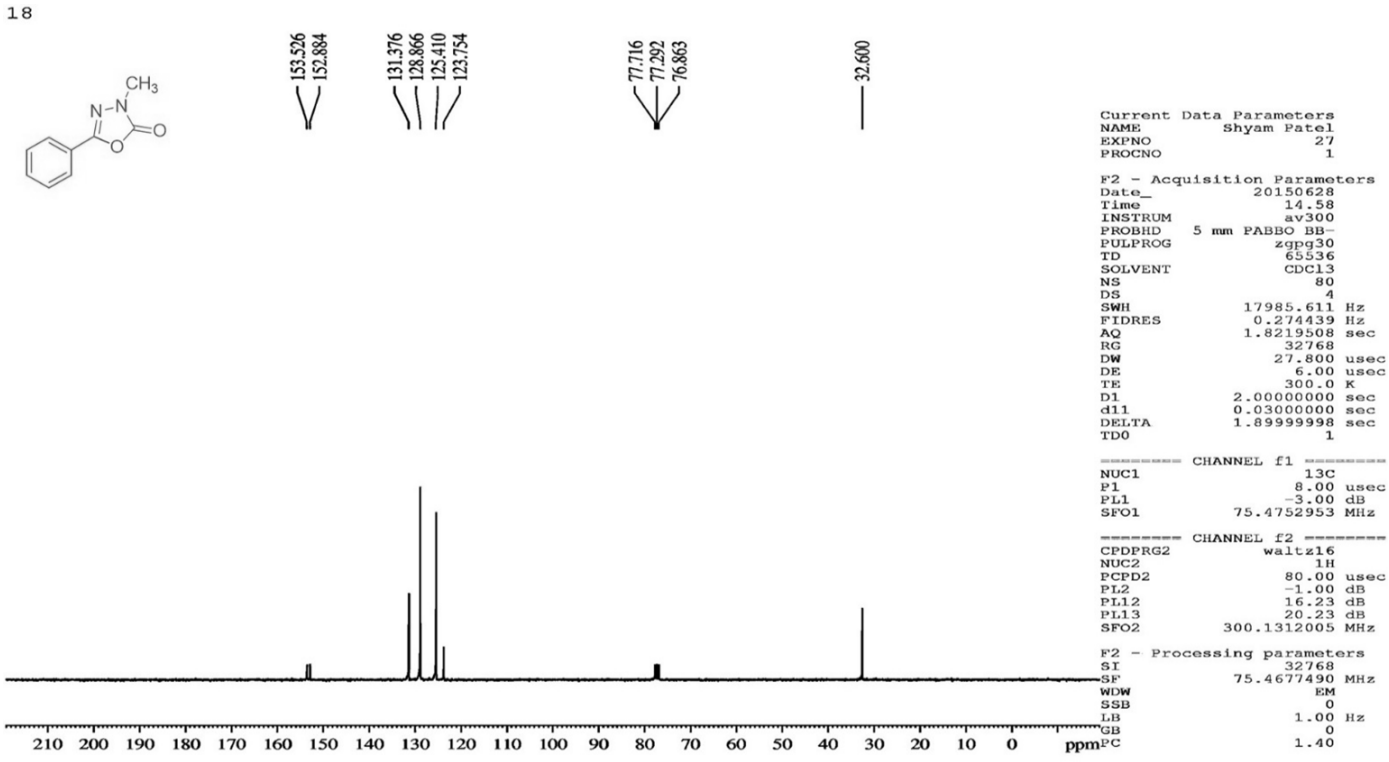
Identification code		
Empirical formula	$C_8H_7N_3O_2$	
Formula weight	177.17	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.7205(15) Å	a= 72.891(4)°
	b = 7.824(2) Å	b= 85.142(4)°
	c = 9.811(3) Å	g = 74.695(4)°
Volume	404.79(19) $Å^3$	
Z	2	
Density (calculated)	1.454 Mg/m^3	
Absorption coefficient	0.109 mm^{-1}	
F(000)	184.0	
Crystal size	0.53 x 0.34 x 0.13 mm^3	
Theta range for data collection	3.03 to 24.98°.	
Index ranges	-6<=h<=6, -9<=k<=9, -11<=l<=11	
Reflections collected	3825	
Independent reflections	1419 [R(int) = 0.0314]	
Completeness to theta = 24.98°	98.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1419 / 0 / 119	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1481	
R indices (all data)	R1 = 0.0745, wR2 = 0.1581	
Largest diff. peak and hole	0.287 and -0.174 $e.Å^{-3}$	

^{1}HNMR and ^{13}CNMR Spectra of synthesized compounds

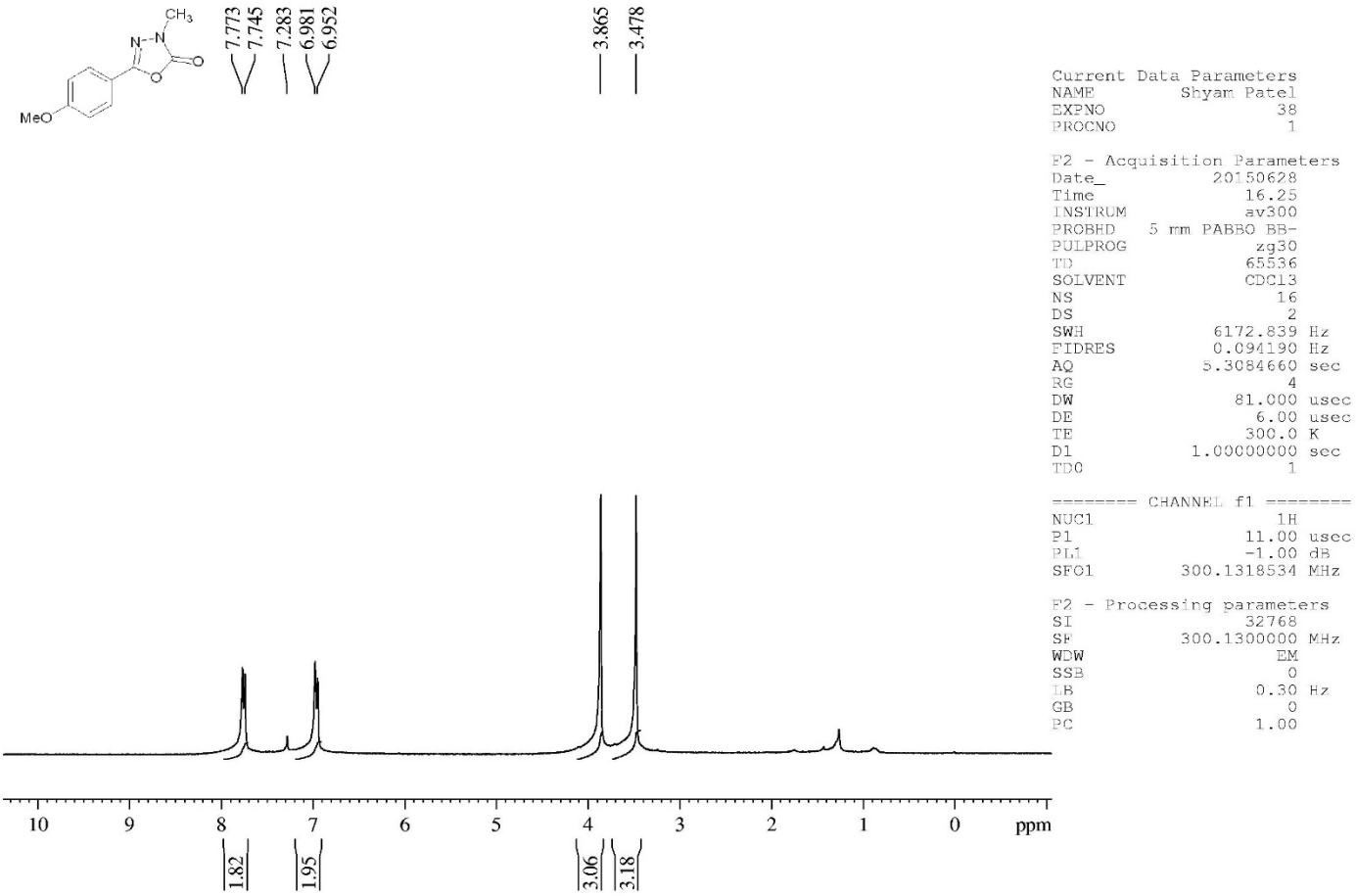
3-methyl-5-phenyl-1,3,4-oxadiazol-2(*3H*)-one (4a):



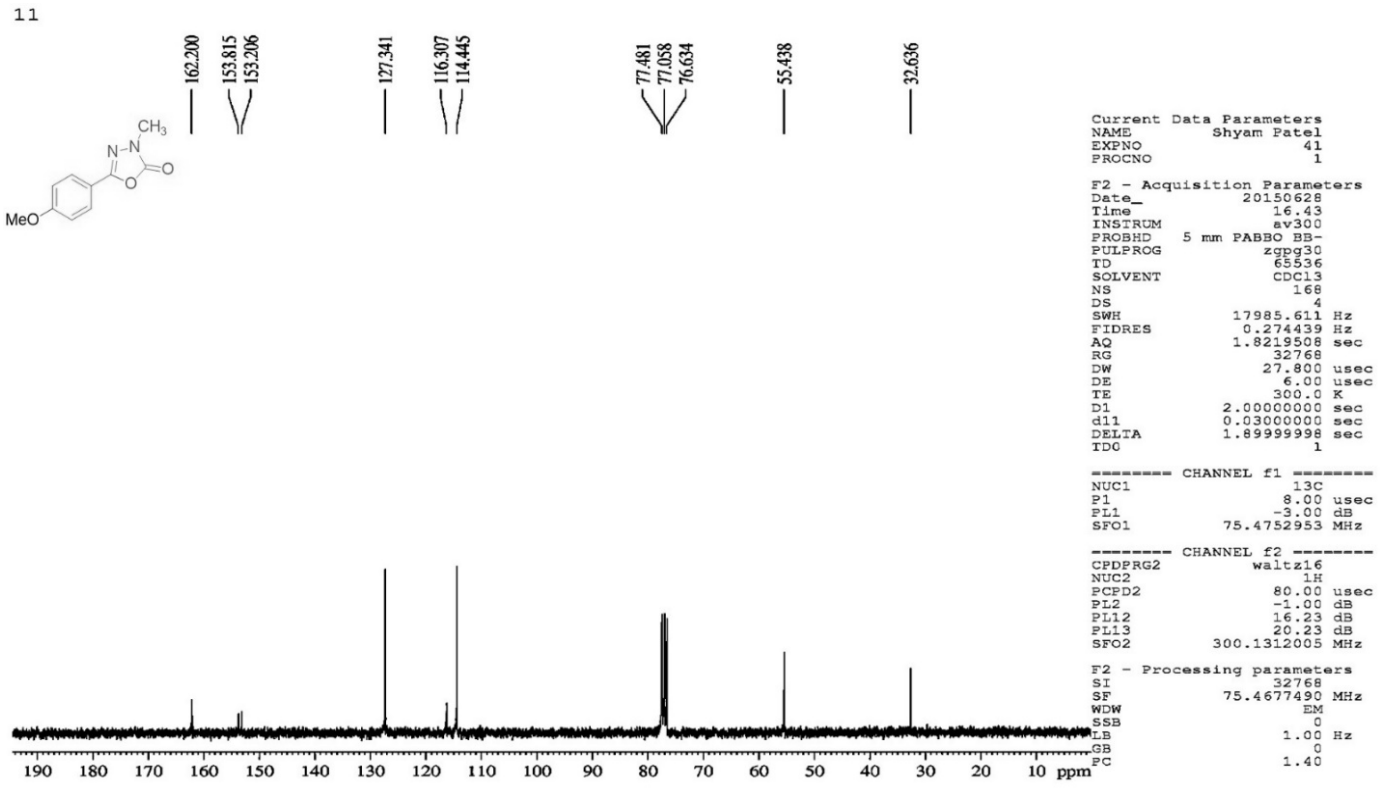
3-methyl-5-phenyl-1,3,4-oxadiazol-2(*3H*)-one (4a):



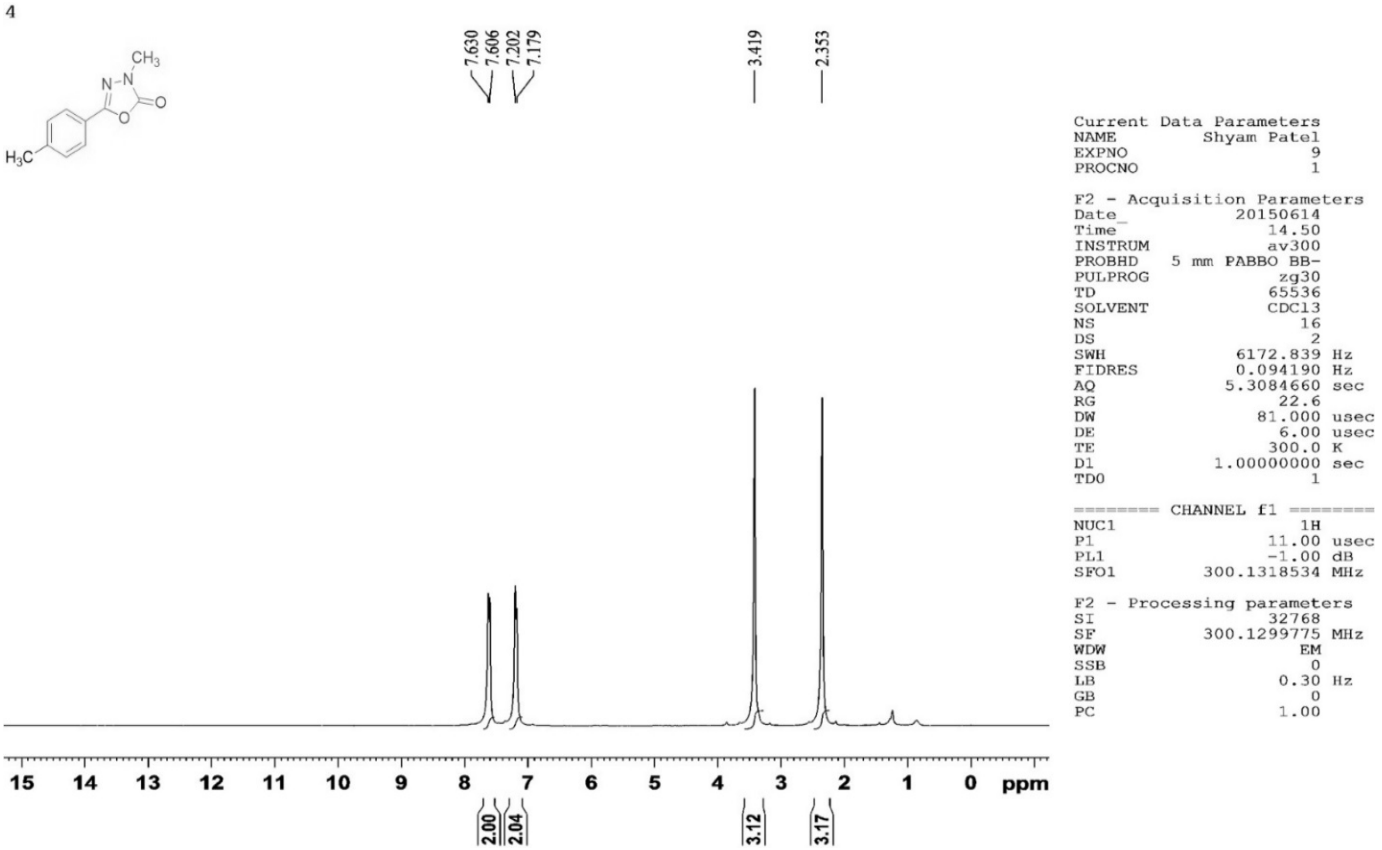
5-(4-methoxyphenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4b):



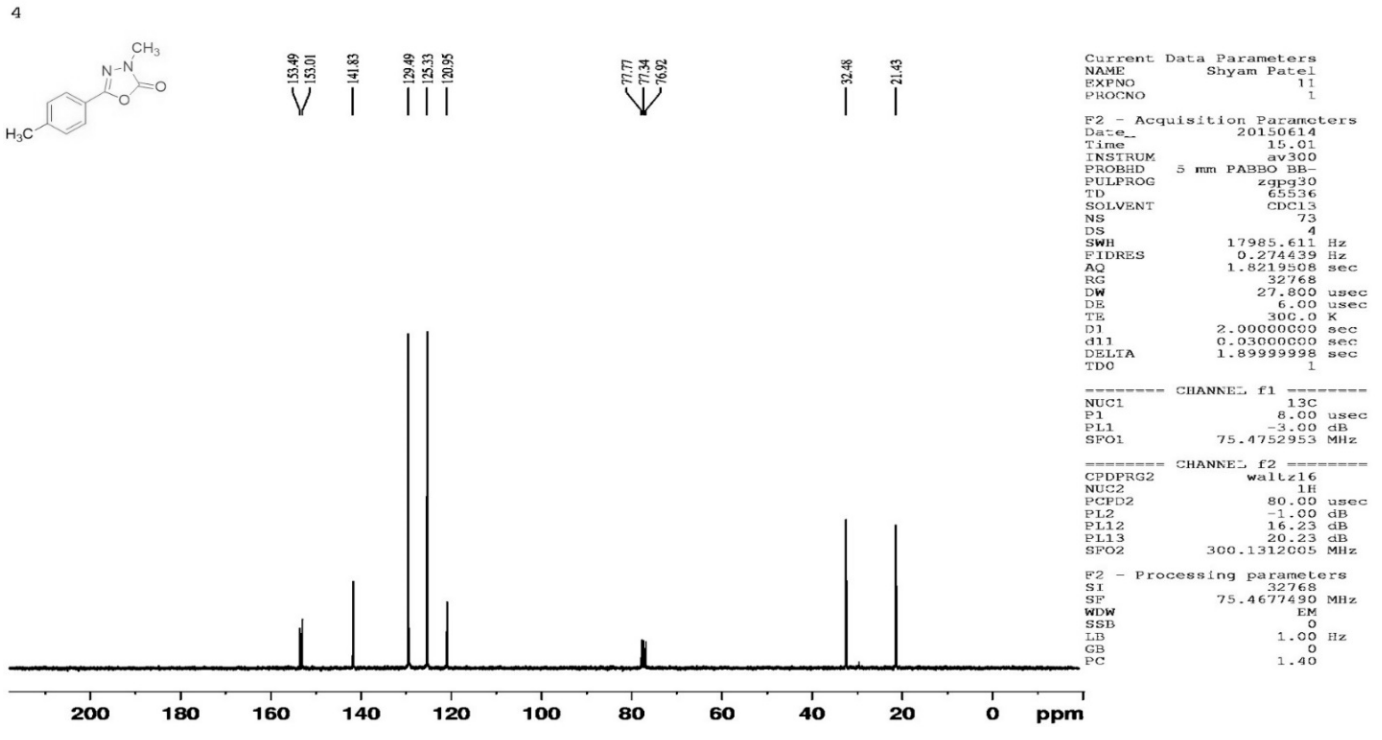
5-(4-methoxyphenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4b):



3-methyl-5-(p-tolyl)-1,3,4-oxadiazol-2(*3H*)-one (4c):



3-methyl-5-(p-tolyl)-1,3,4-oxadiazol-2(*3H*)-one (4c):



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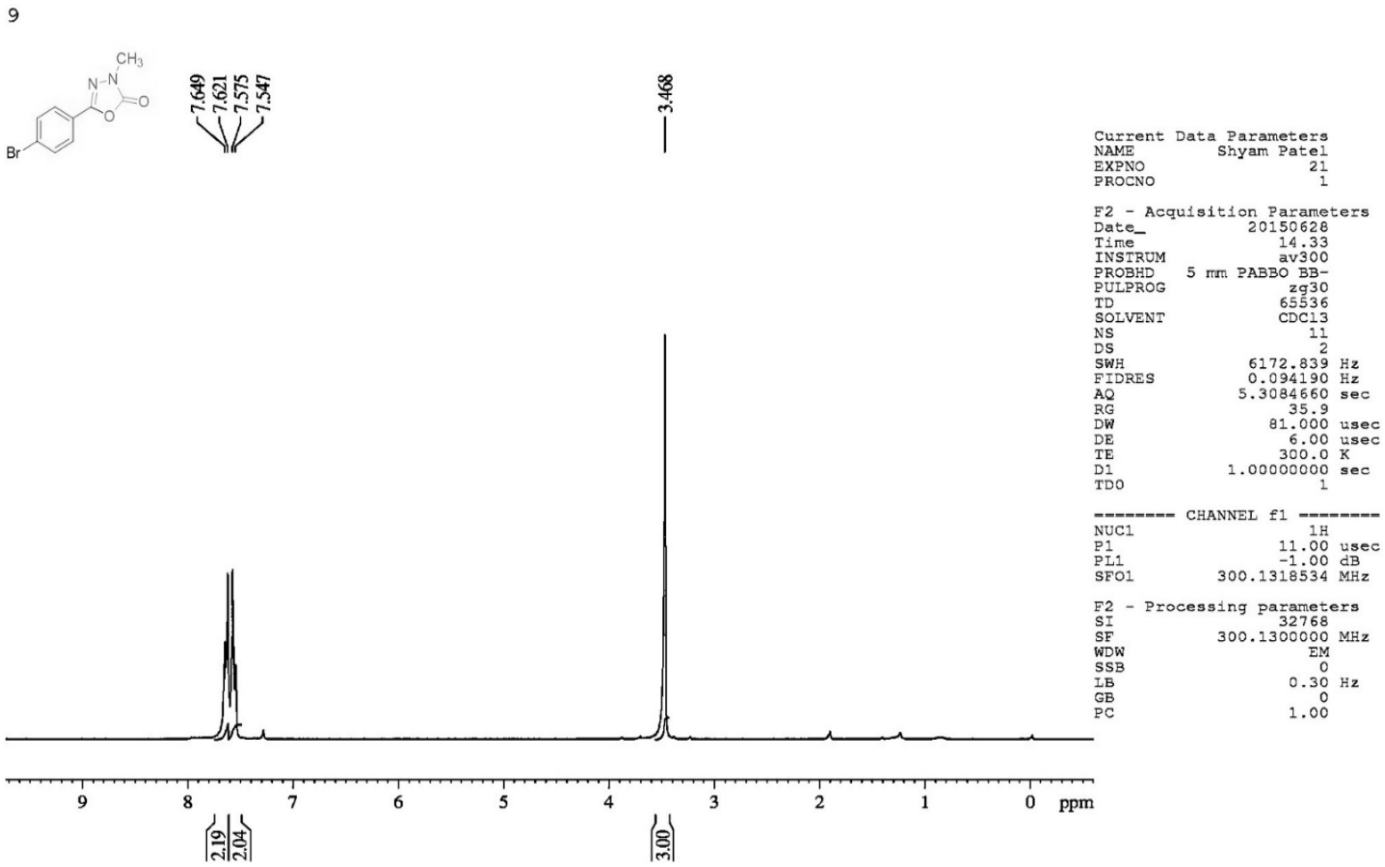
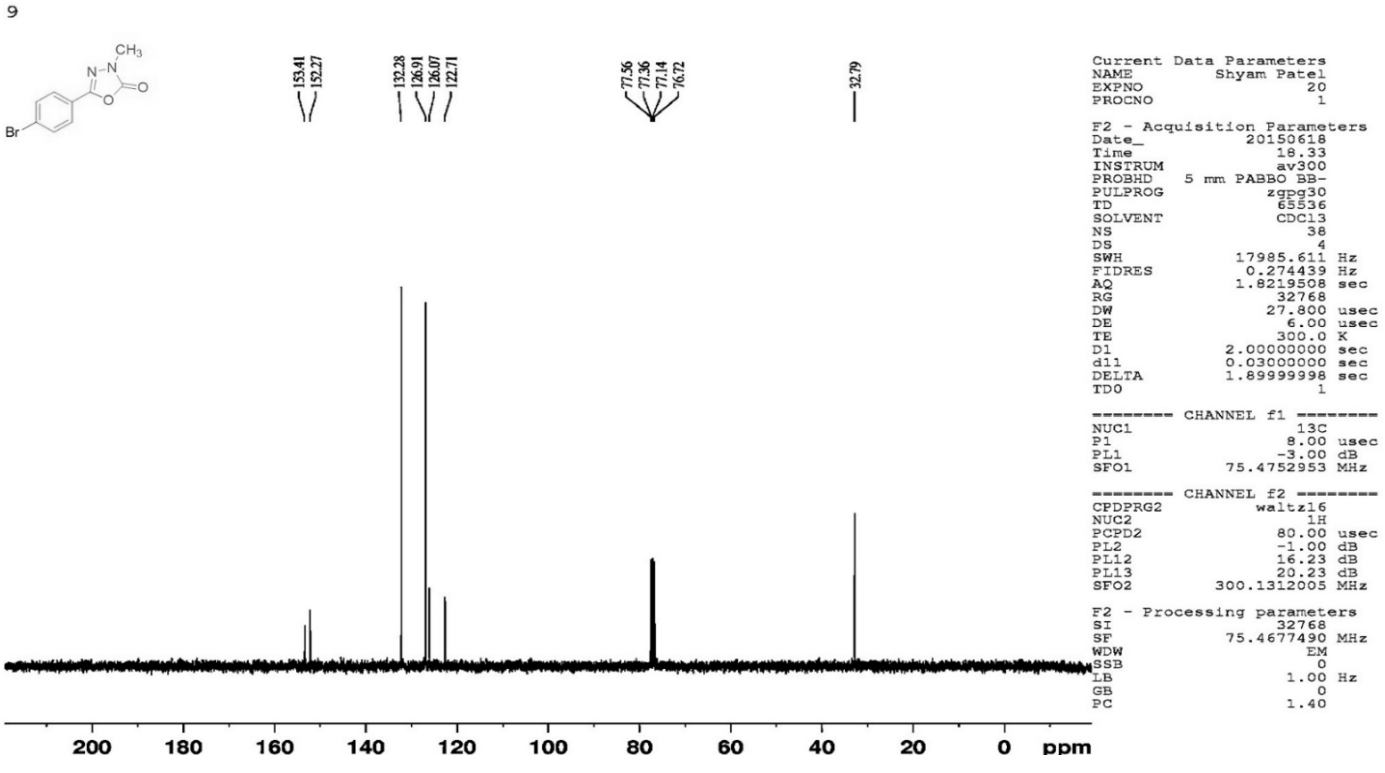


5-(4-bromophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4d):



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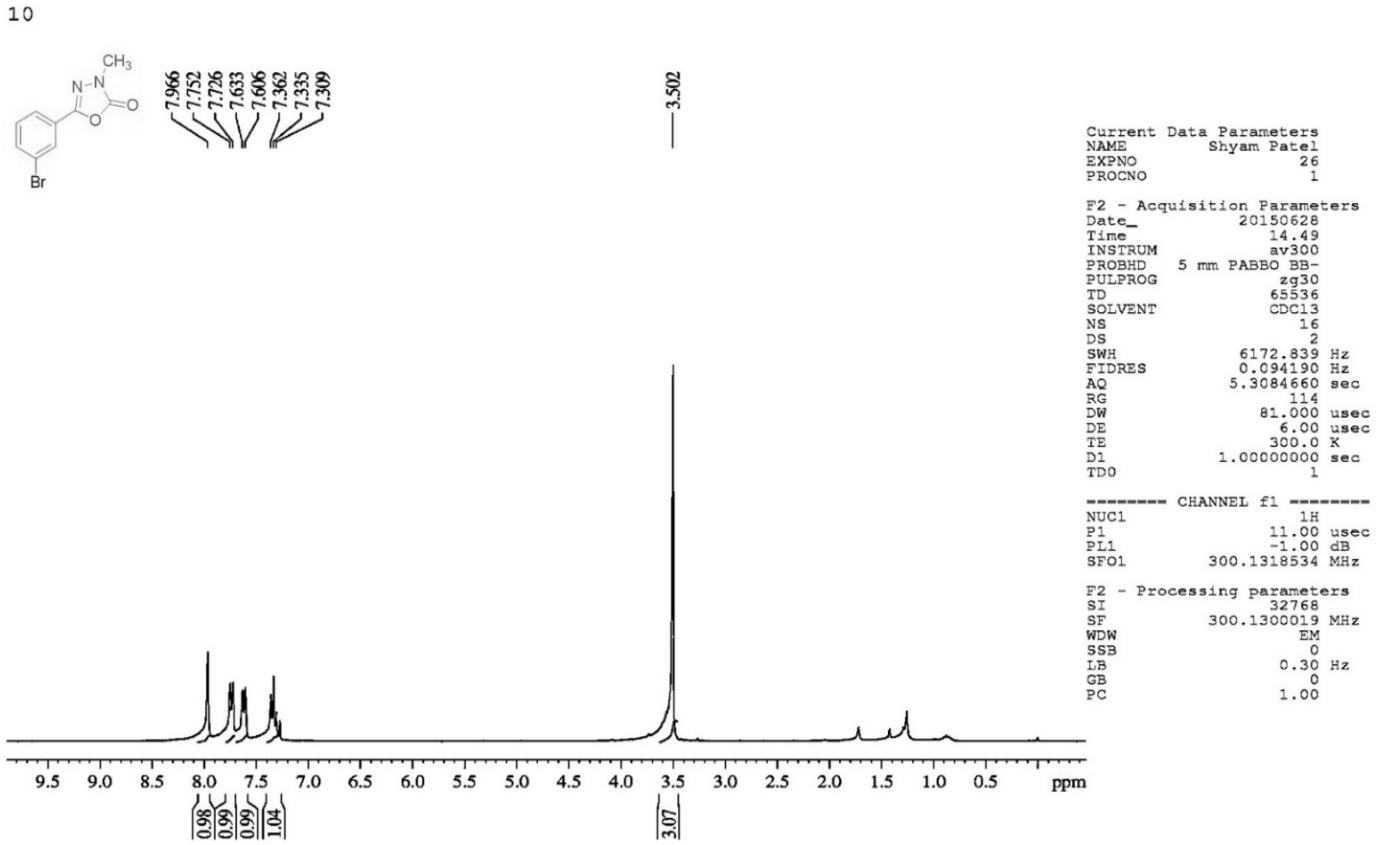
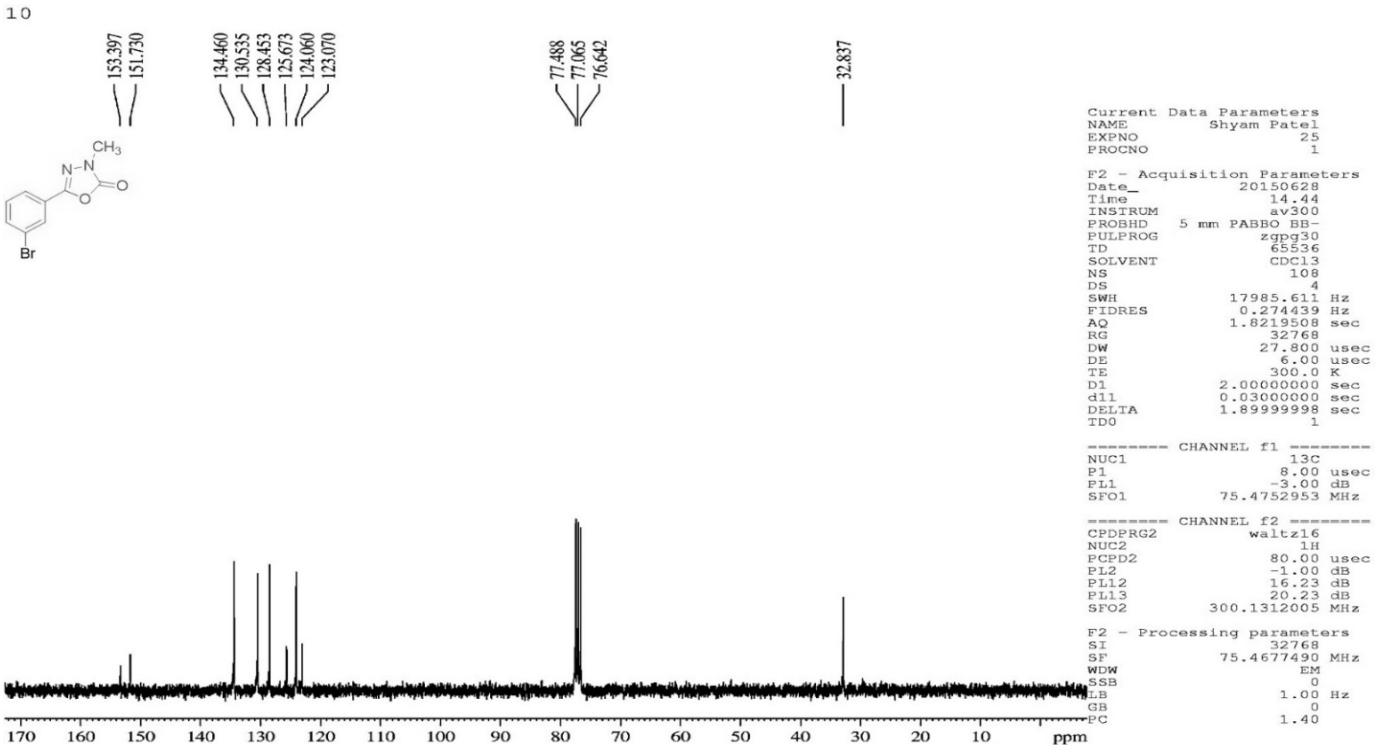
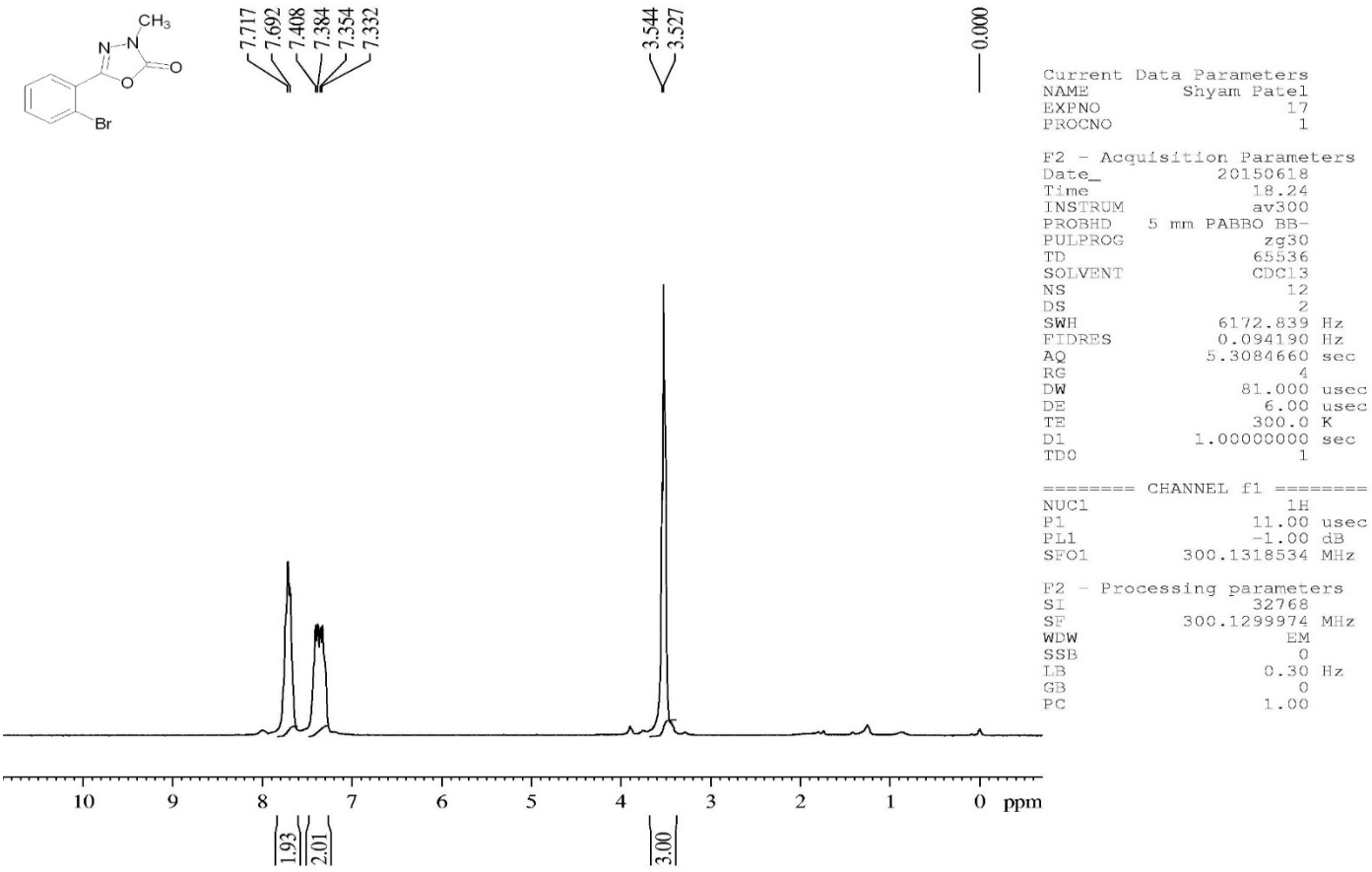


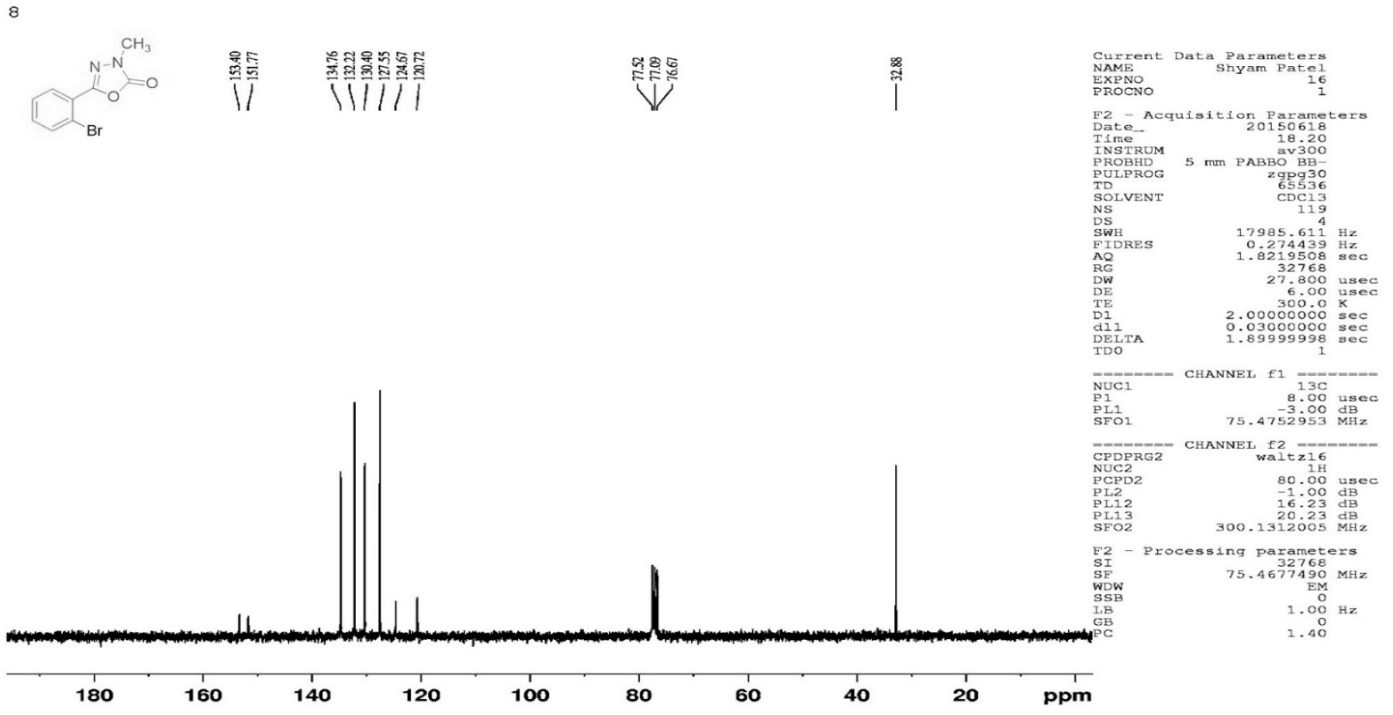
5-(3-bromophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4e):



5-(2-bromophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4f):



5-(2-bromophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4f):



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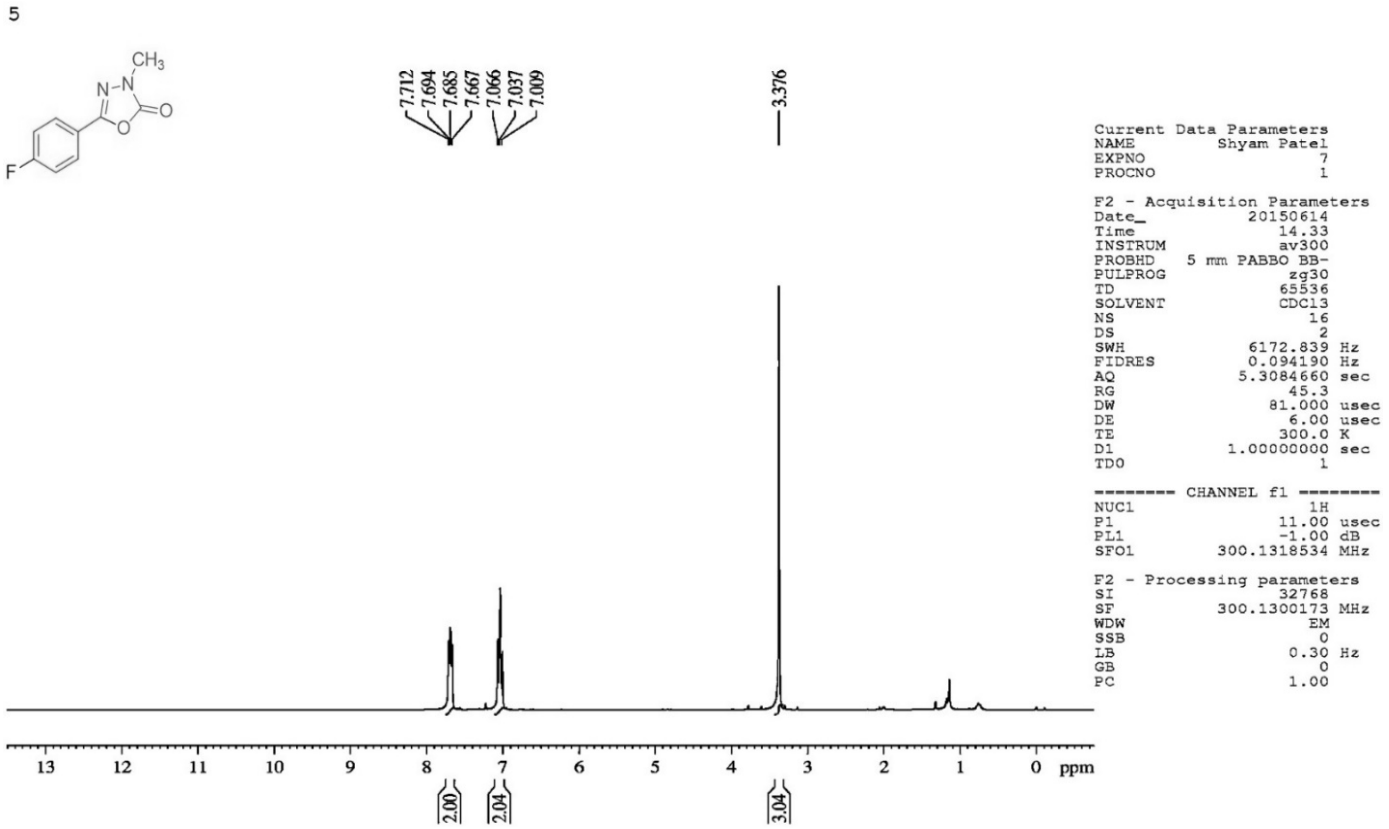
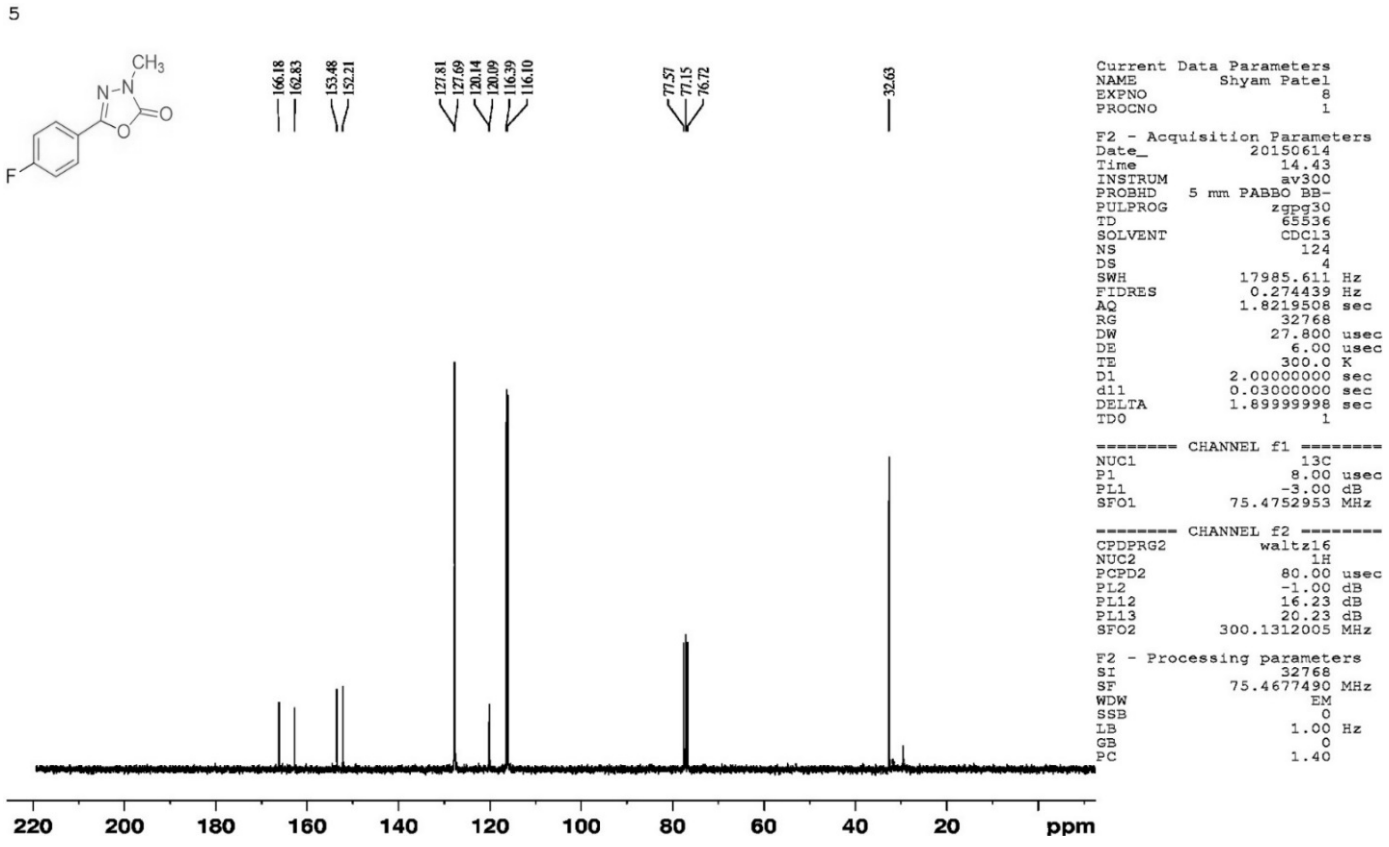
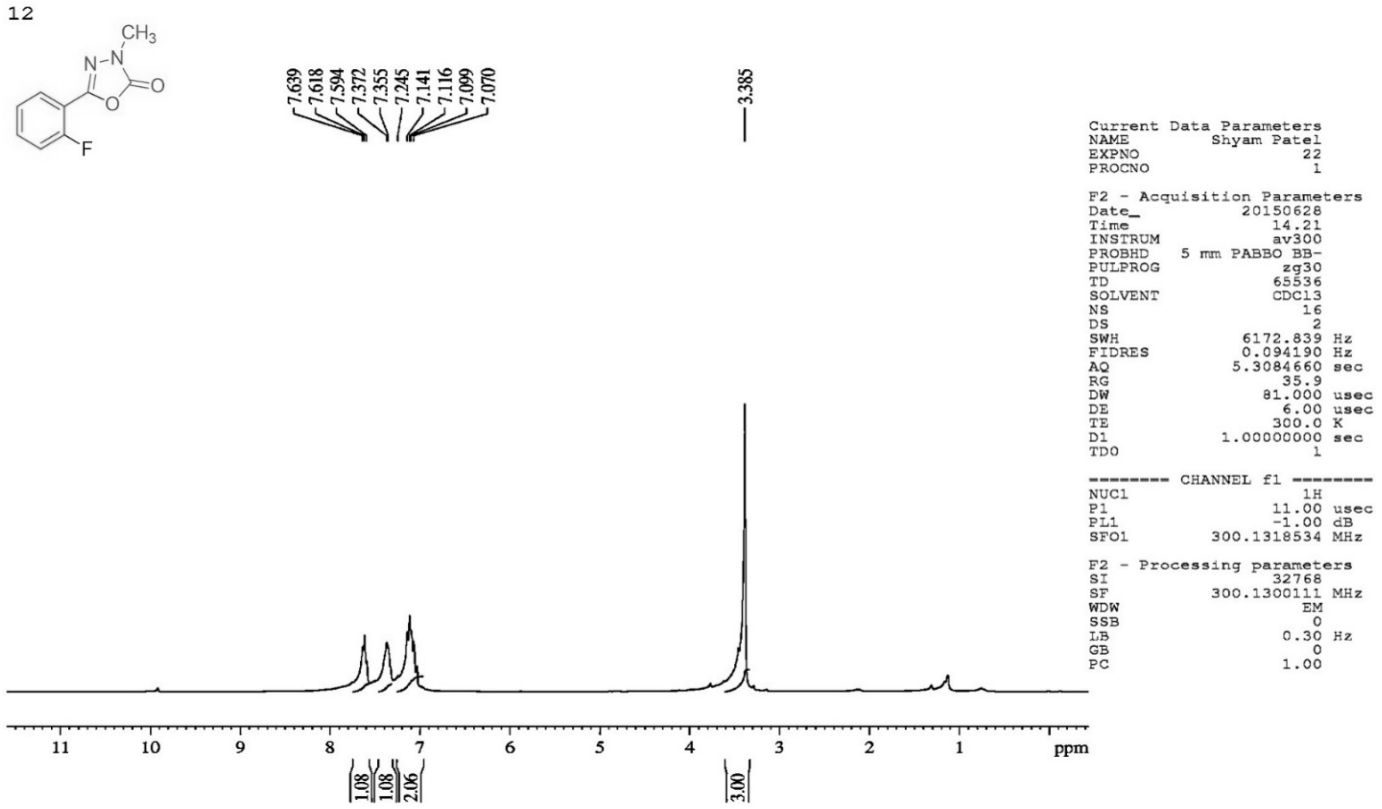


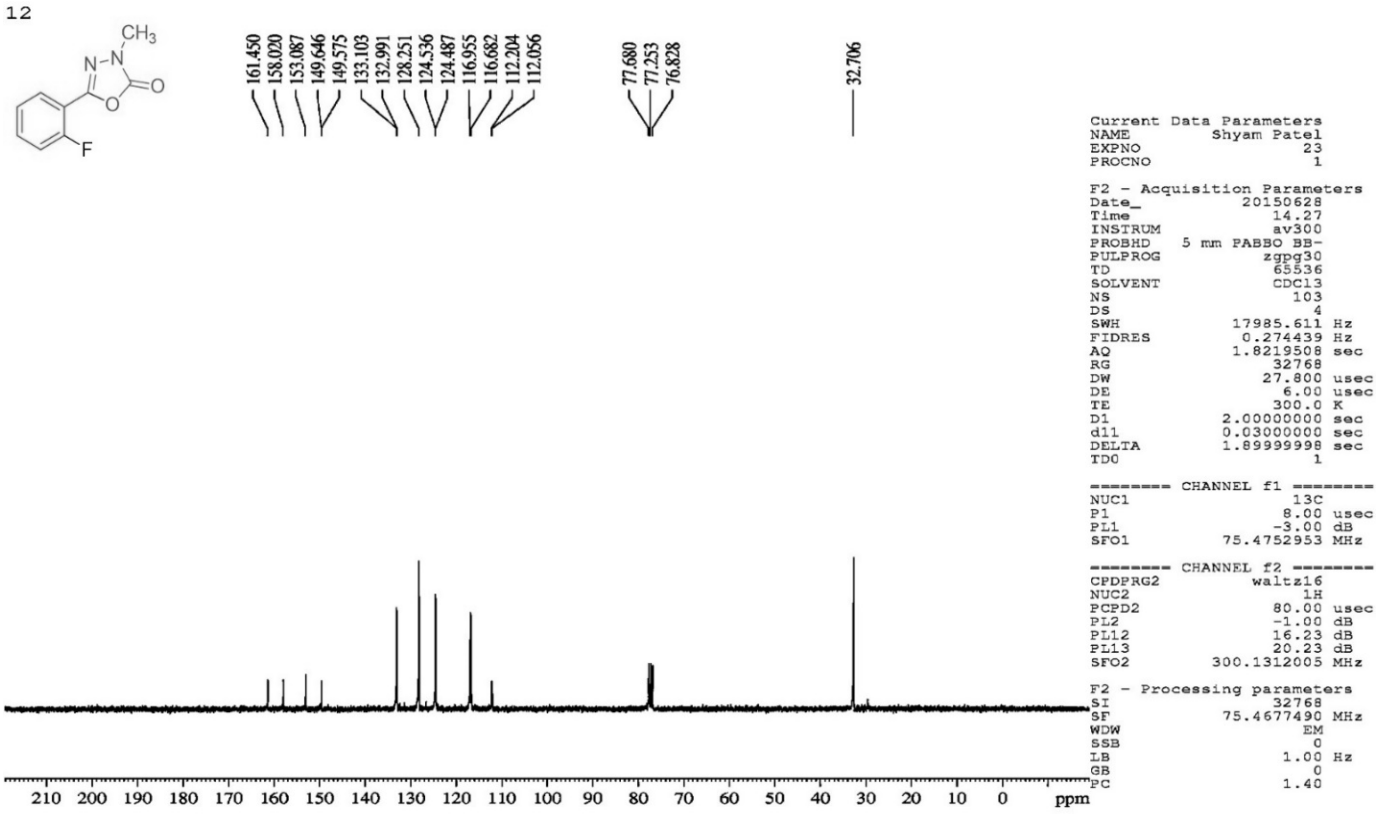
5-(4-fluorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4g):



5-(2-fluorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4h):



5-(2-fluorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4h):



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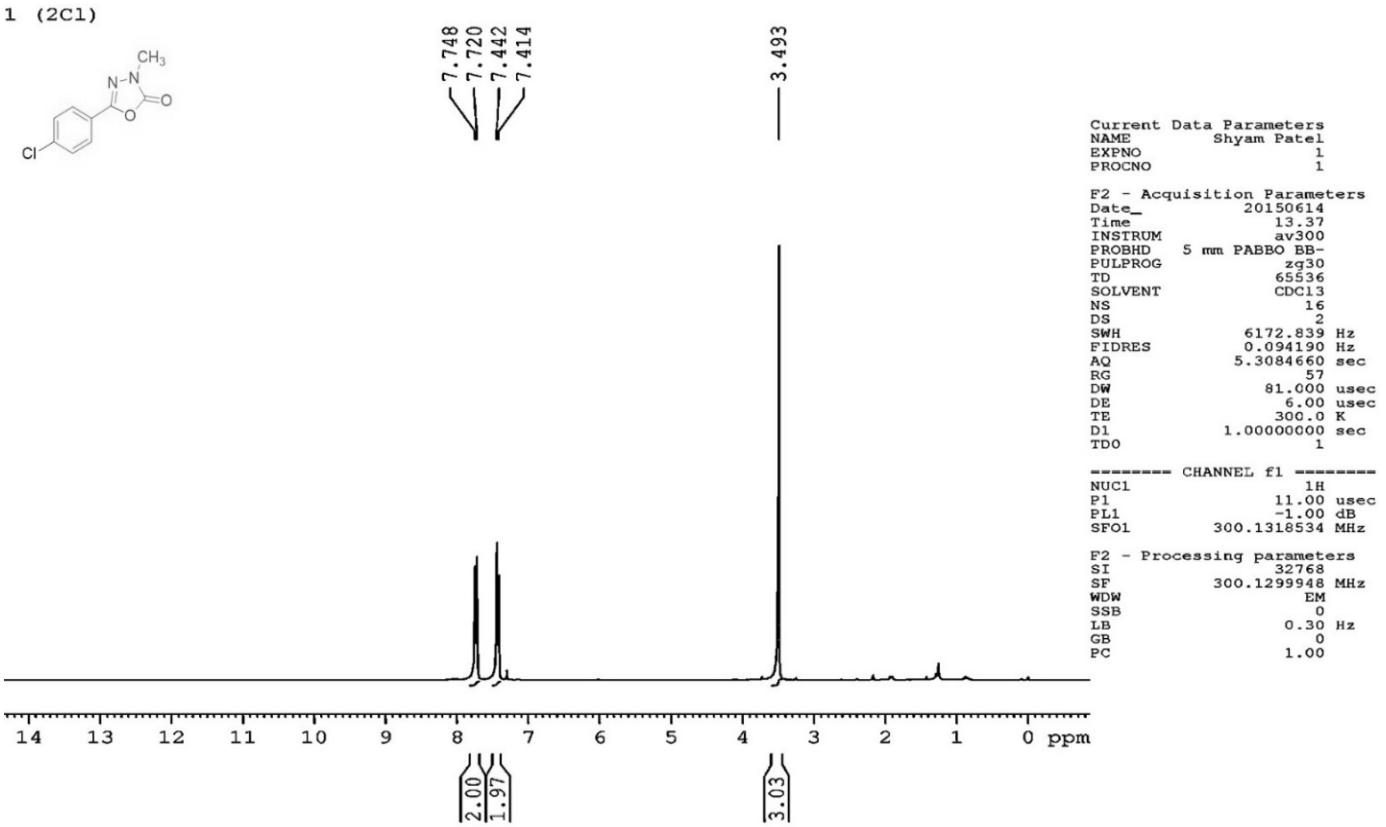
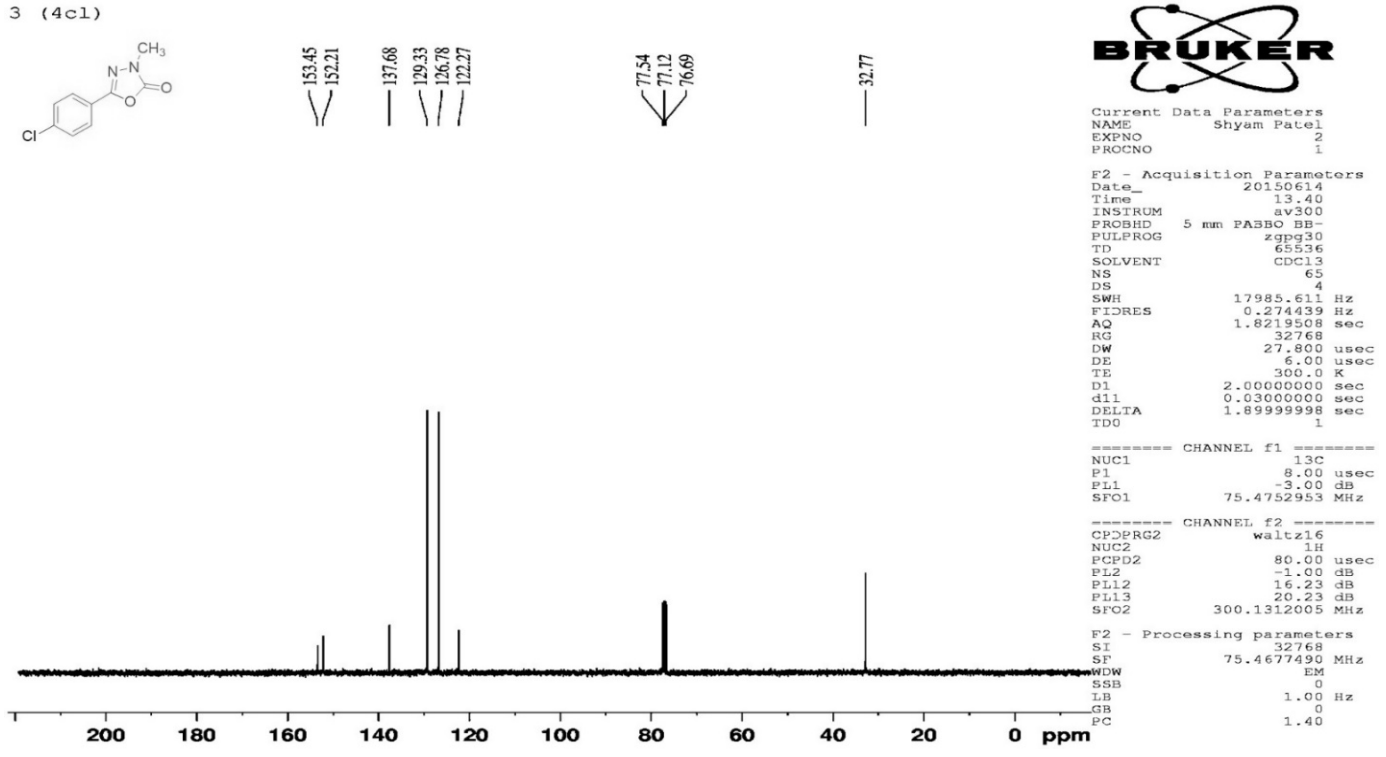
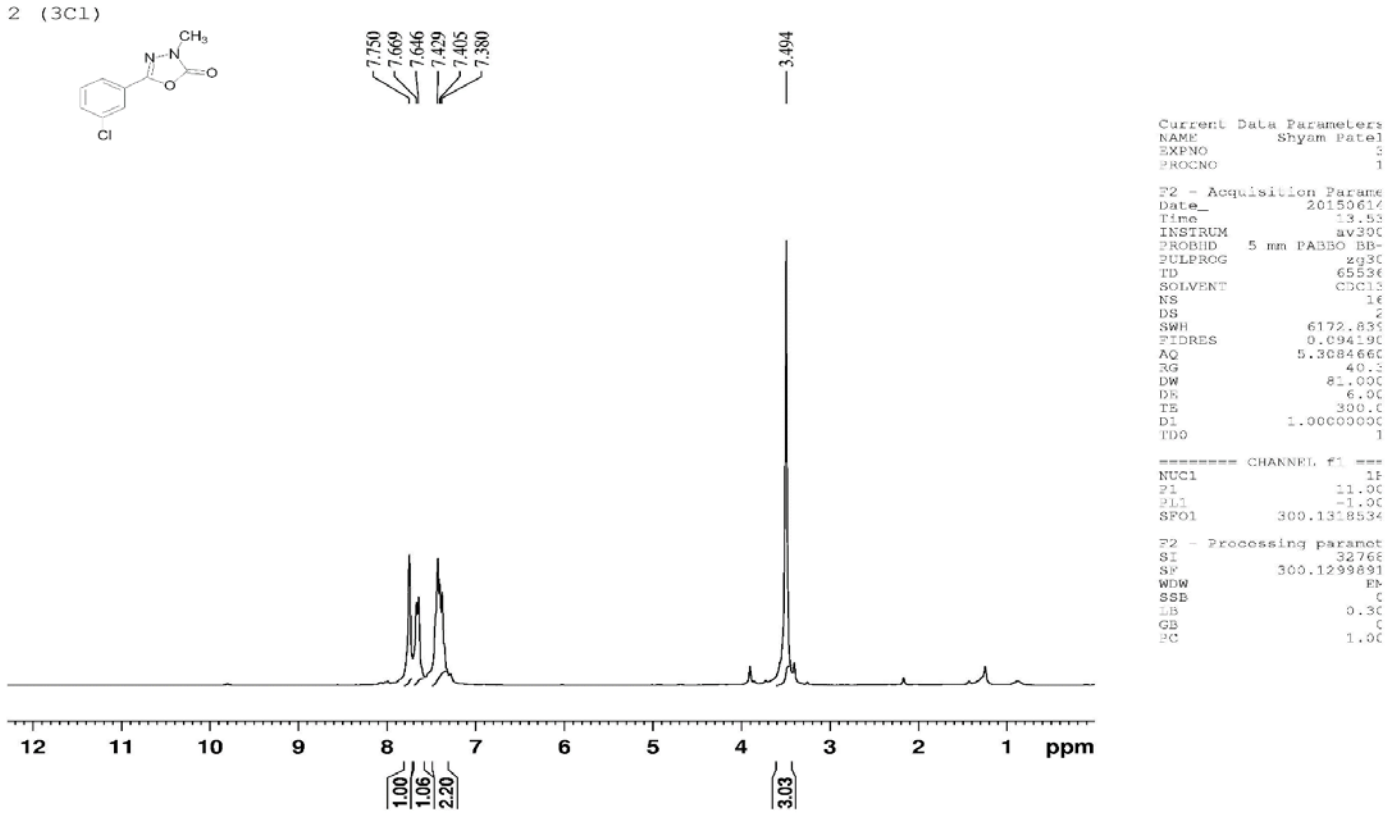


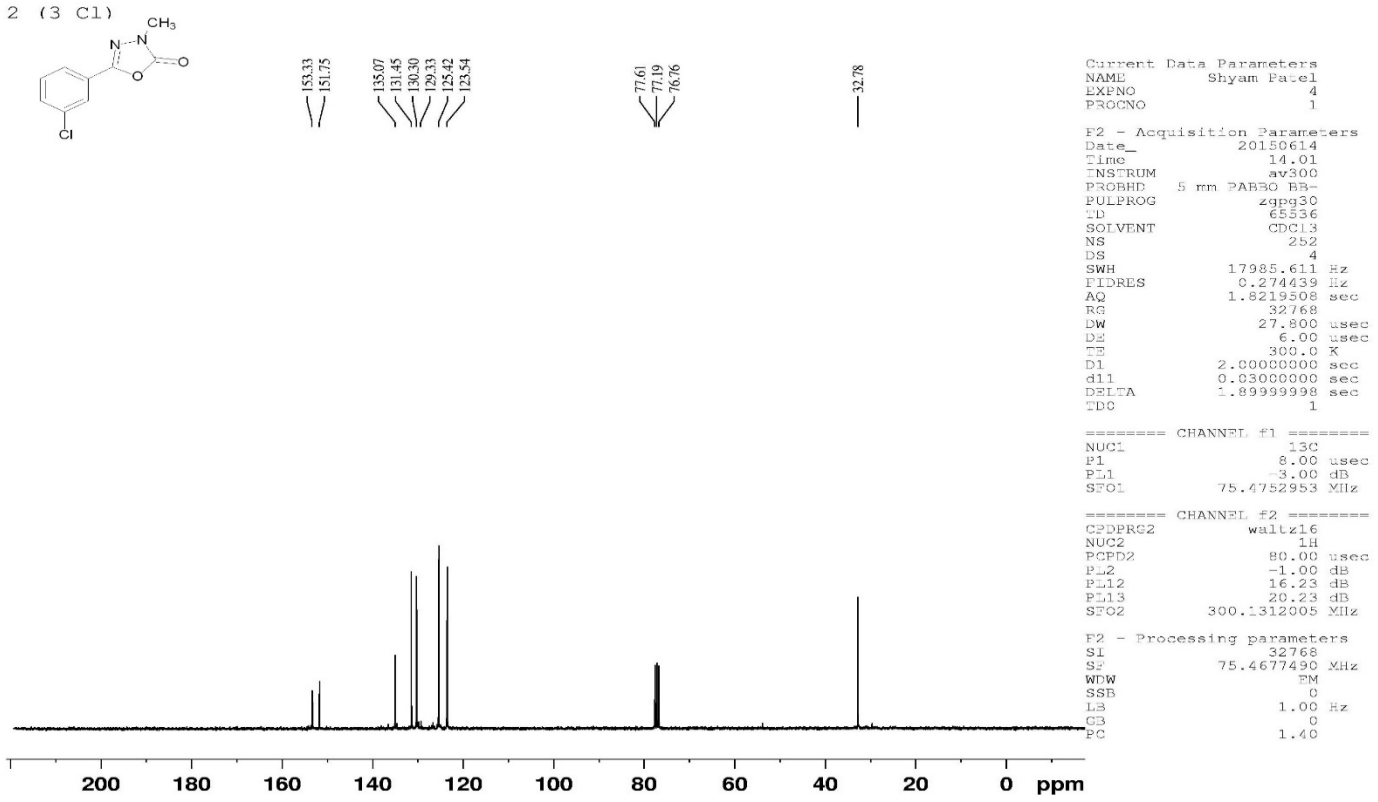
5-(4-chlorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4i):



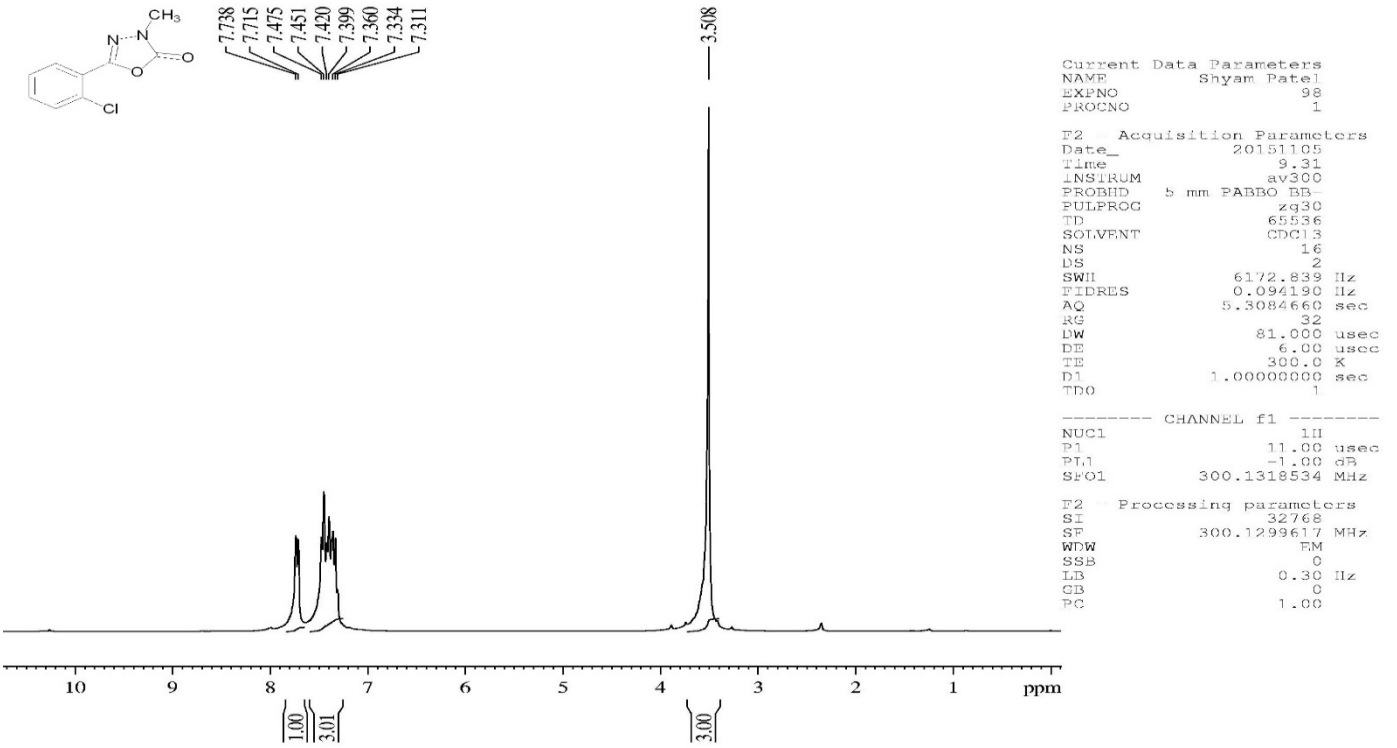
5-(3-chlorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4j):



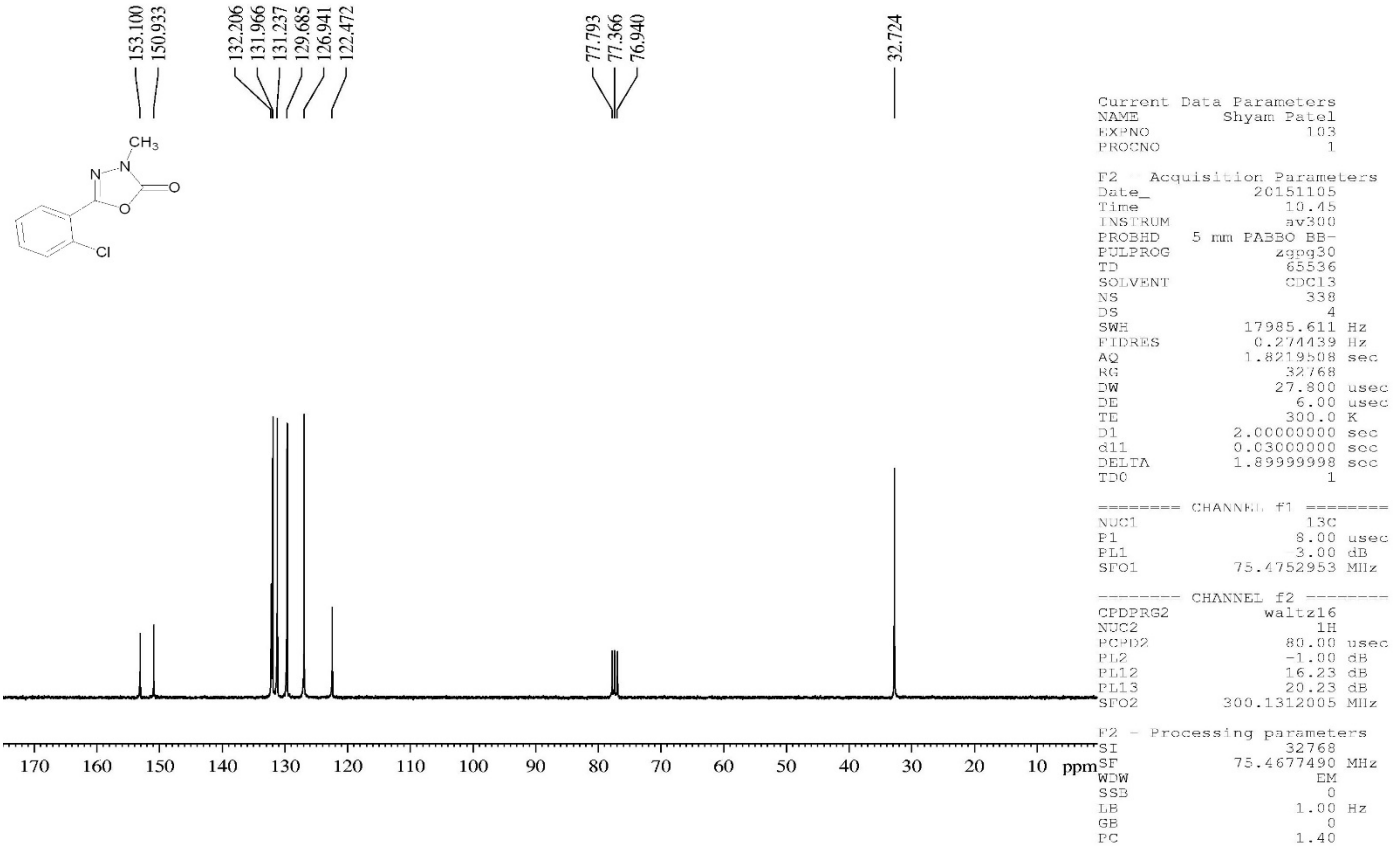
5-(3-chlorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4j):



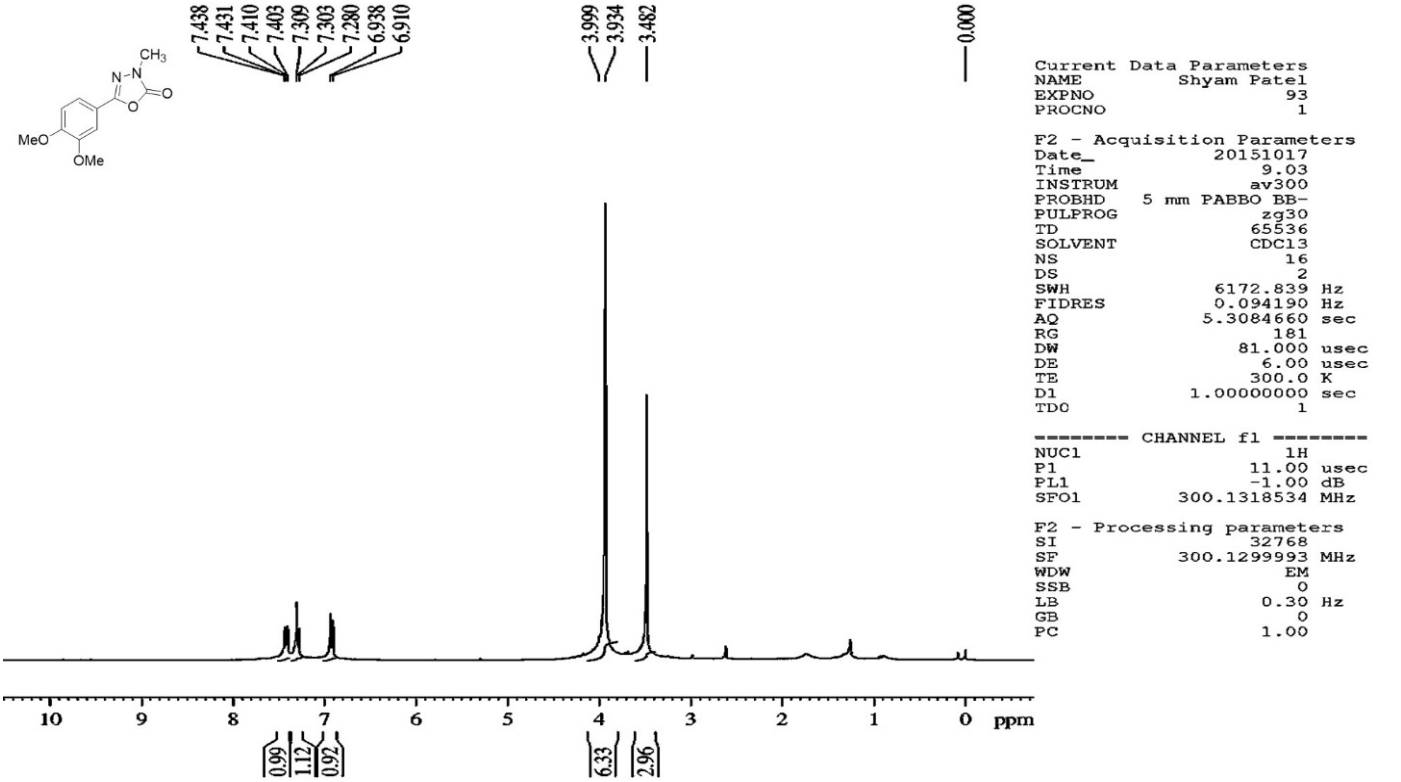
5-(2-chlorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4k):



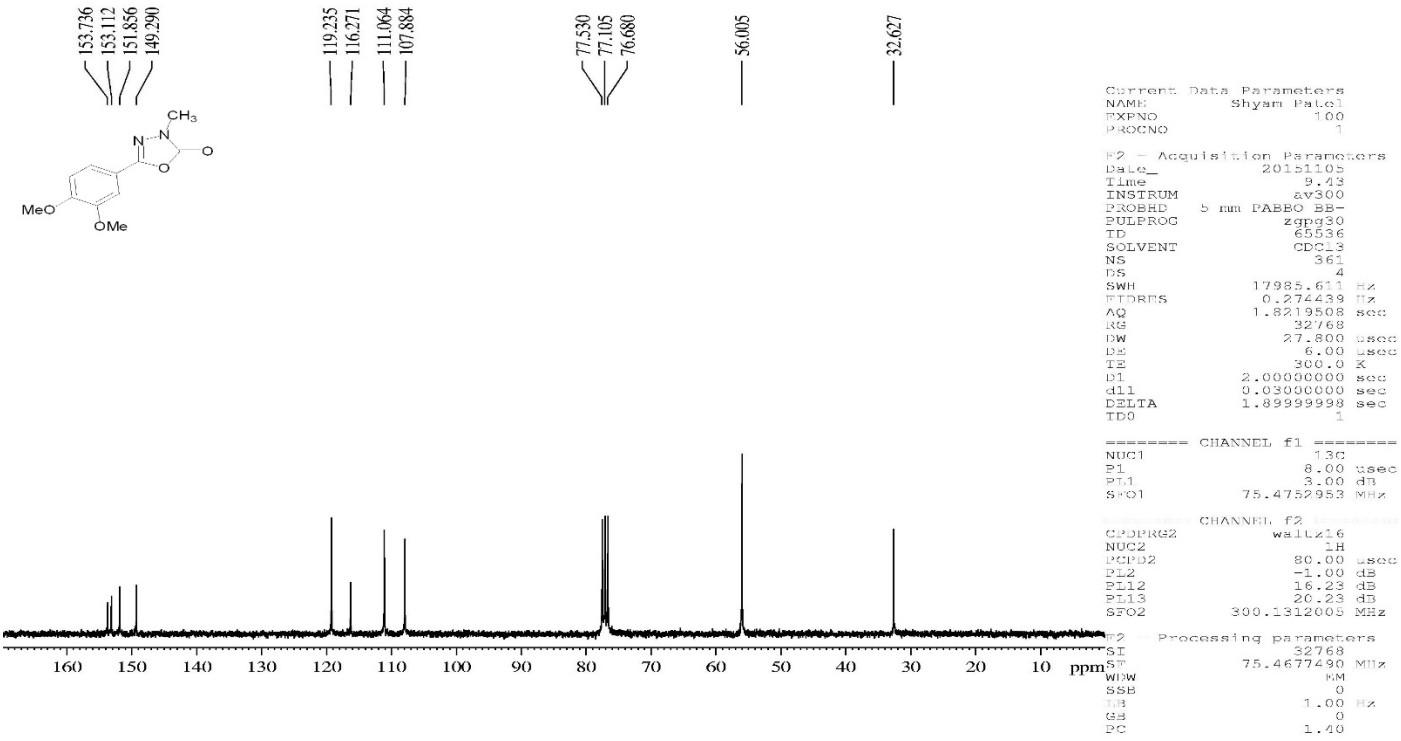
5-(2-chlorophenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4k):



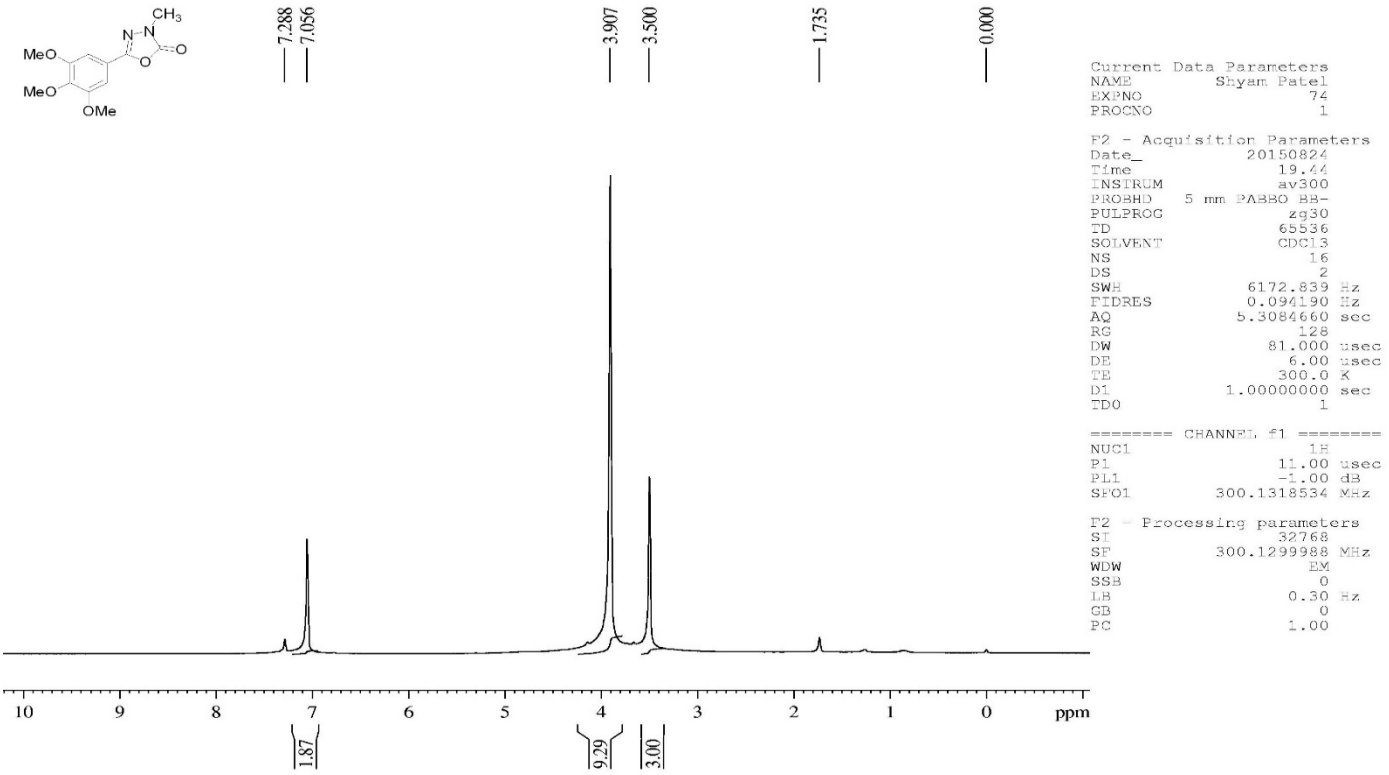
5-(3,4-dimethoxyphenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4l):



5-(3,4-dimethoxyphenyl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4l):



3-methyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(*3H*)-one (4m):

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DS                     2
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AQ            5.3084660 sec
RG                   128
DW              81.000 usec
DE               6.00 usec
TE              300.0 K
D1            1.00000000 sec
TD0                    1

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P1                11.00 usec
PL1               -1.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
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SF           300.1299988 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
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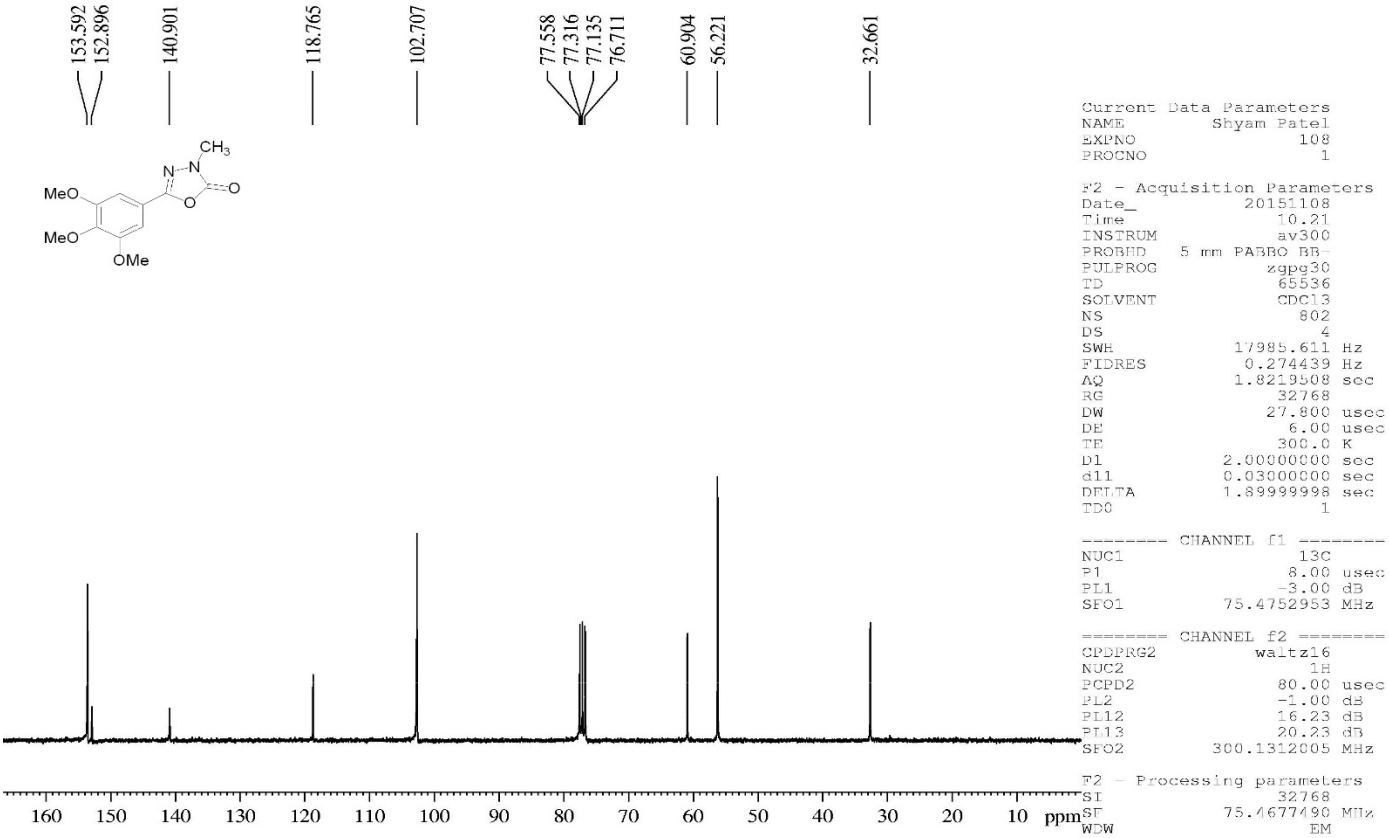
3-methyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(*3H*)-one (4m):

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SOLVENT            CDCl3
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TE              300.0 K
D1            2.00000000 sec
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TD0                    1

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PL1               -3.00 dB
SFO1         75.4752953 MHz

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CPDPRG2          waltz16
NUC2                  1H
PCPD2            80.00 usec
PL2               -1.00 dB
PL12              16.23 dB
PL13              20.23 dB
SFO2         300.1312005 MHz

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SI                 32768
SF           75.4677490 MHz
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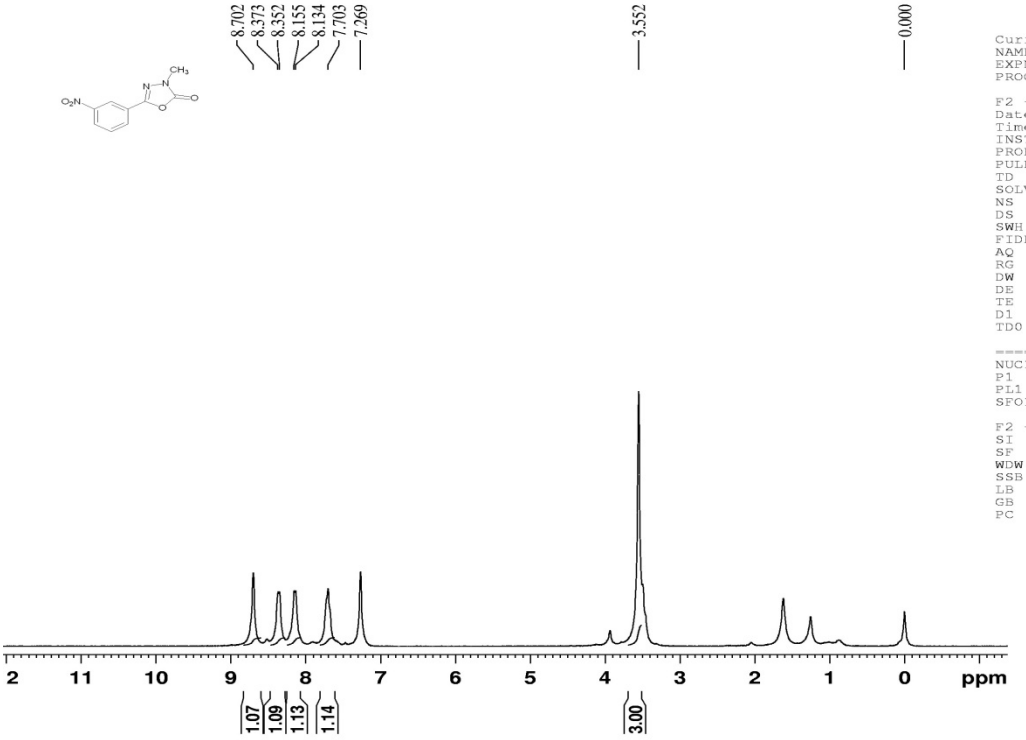
3-methyl-5-(3-nitrophenyl)-1,3,4-oxadiazol-2(*3*H)-one (4n):

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TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                    362
DW                 81.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.00 usec
PL1                -1.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300044 MHz
WDW                    EM
SSB                     0
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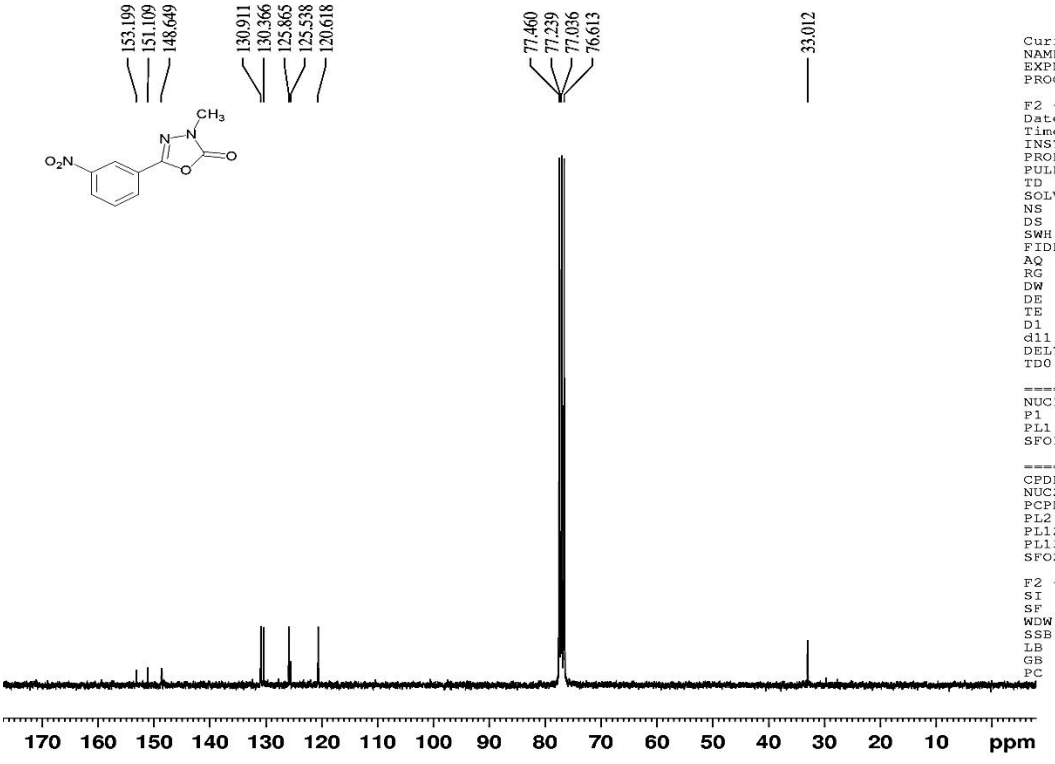
3-methyl-5-(3-nitrophenyl)-1,3,4-oxadiazol-2(*3*H)-one (4n):

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SOLVENT             CDCl3
NS                   3017
DS                      4
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FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                    32768
DW                 27.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.00 usec
PL1                -3.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.23 dB
PL13               20.23 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                  32768
SF            75.4677490 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
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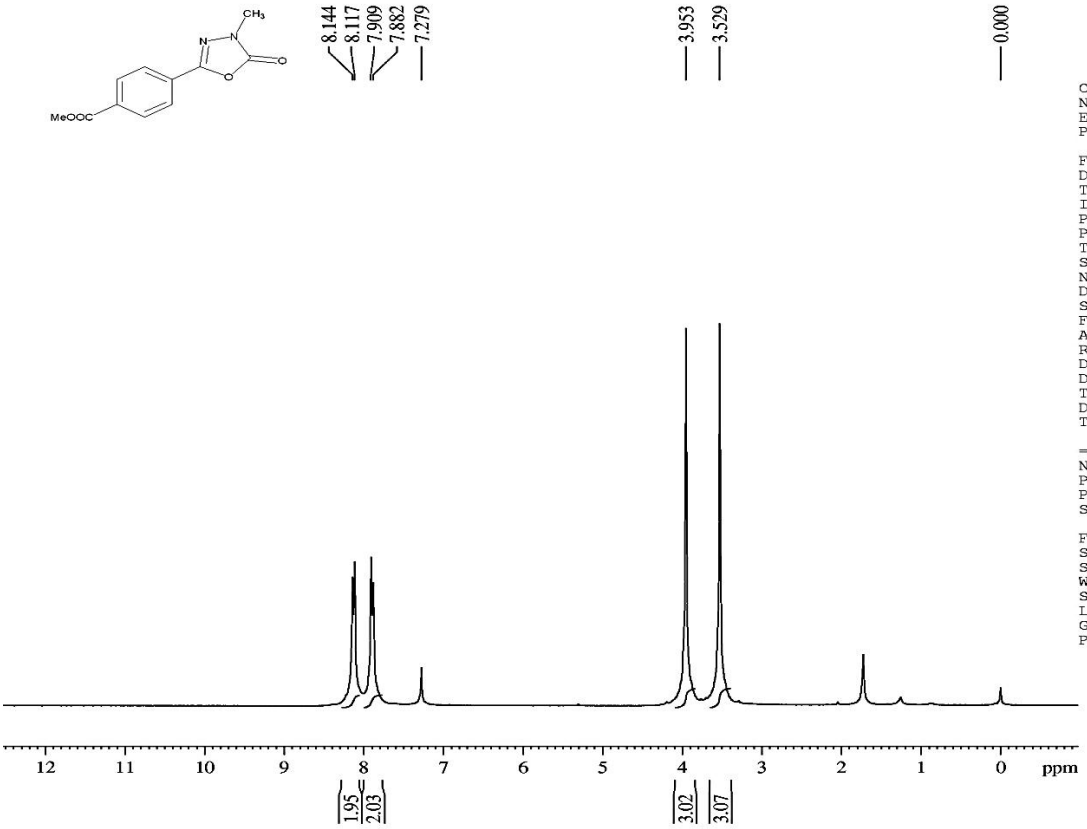
Methyl 4-(4-methyl-5-oxo-4,5-dihydro-1,3,4-oxadiazol-2-yl) benzoate(4o):

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NS                   16
DS                    2
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FIDRES        0.094190 Hz
AQ            5.3084660 sec
RG                  256
DW               81.000 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1              11.00 usec
PL1             -1.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
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SF          300.1300008 MHz
WDW                   EM
SSB                    0
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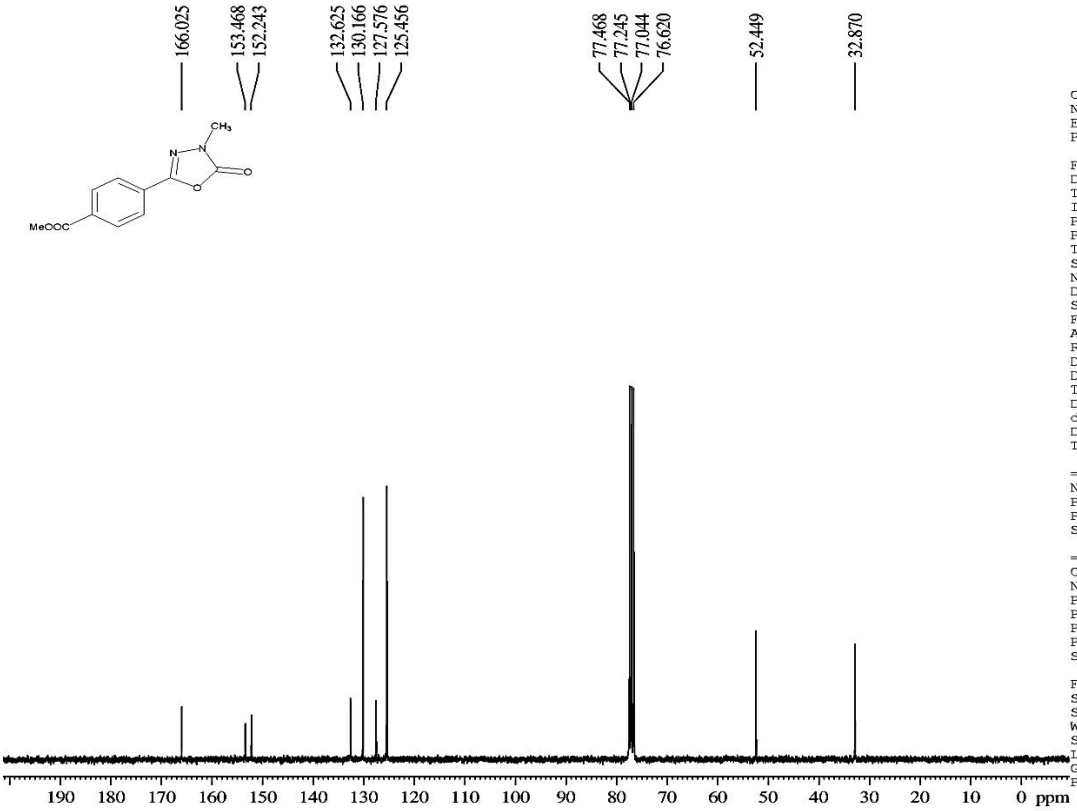
Methyl 4-(4-methyl-5-oxo-4,5-dihydro-1,3,4-oxadiazol-2-yl) benzoate(4o):

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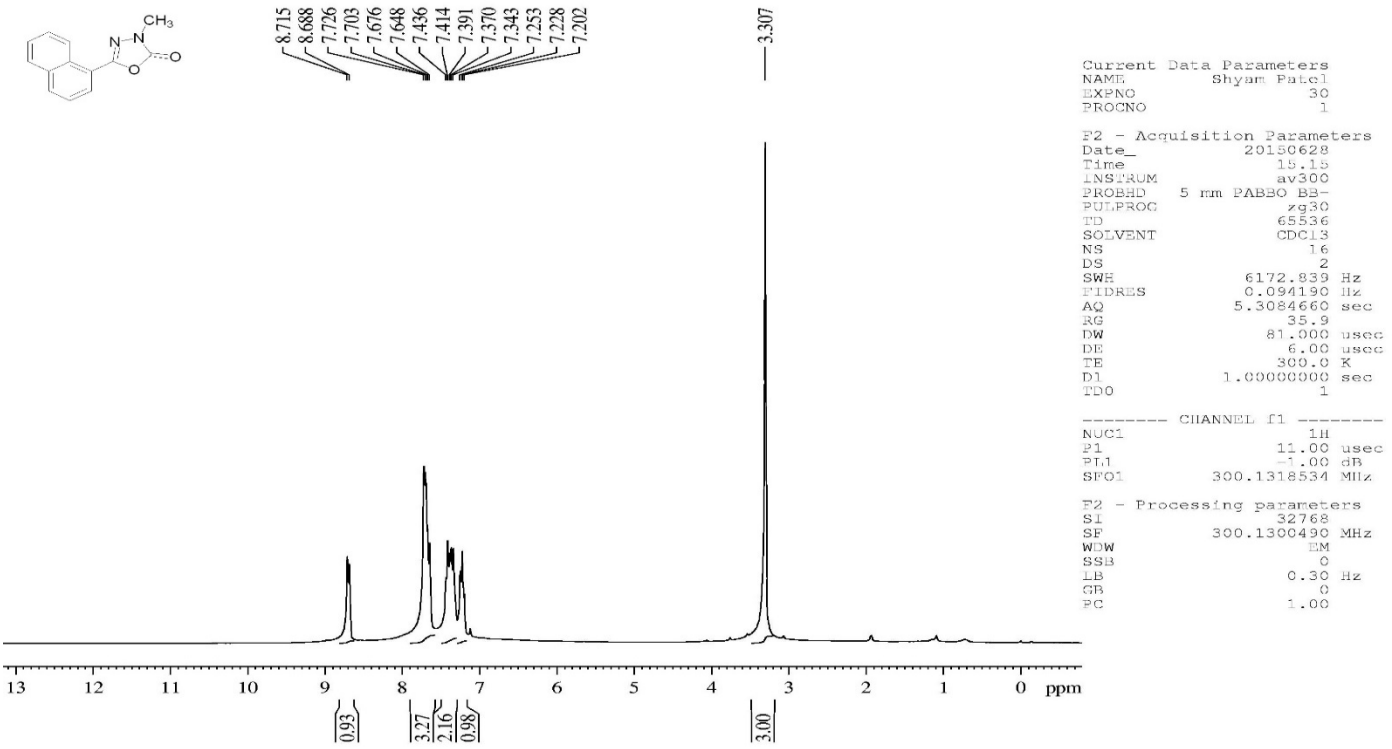
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                32768
DW               27.800 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                8.00 usec
PL1              -3.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           80.00 usec
PL2              -1.00 dB
PL12             16.23 dB
PL13             20.23 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

3-methyl-5-(naphthalen-2-yl)-1,3,4-oxadiazol-2(*3H*)-one (4p):



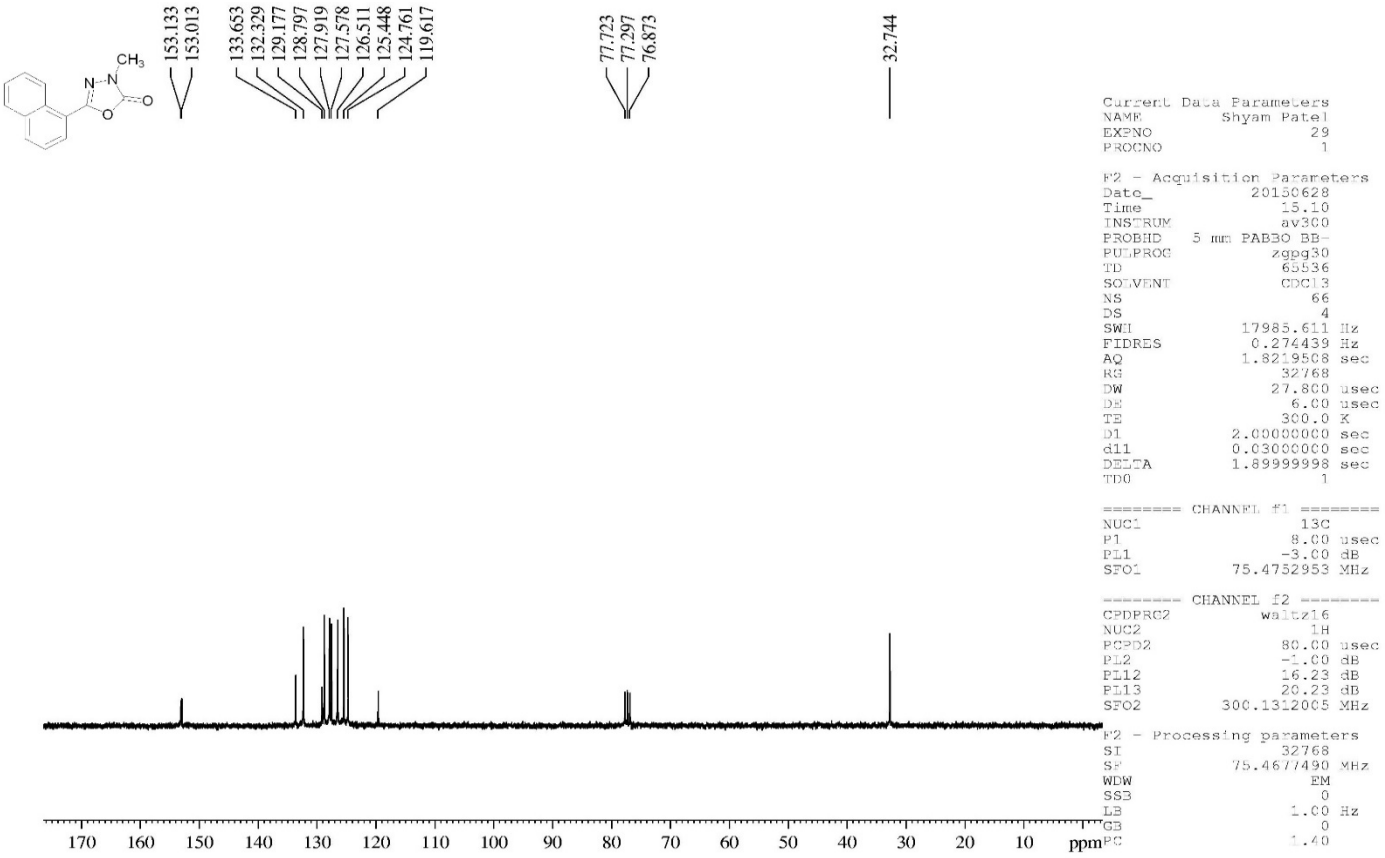

```
Current Data Parameters
NAME          Shyam Patel
EXPNO                  30
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150628
Time               15.15
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                  35.9
DW                 81.000 usec
DE                  6.00 usec
TE                 300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                -1.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300490 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3-methyl-5-(naphthalen-2-yl)-1,3,4-oxadiazol-2(*3H*)-one (4p):




```
Current Data Parameters
NAME          Shyam Patel
EXPNO                  29
PROCNO                  1

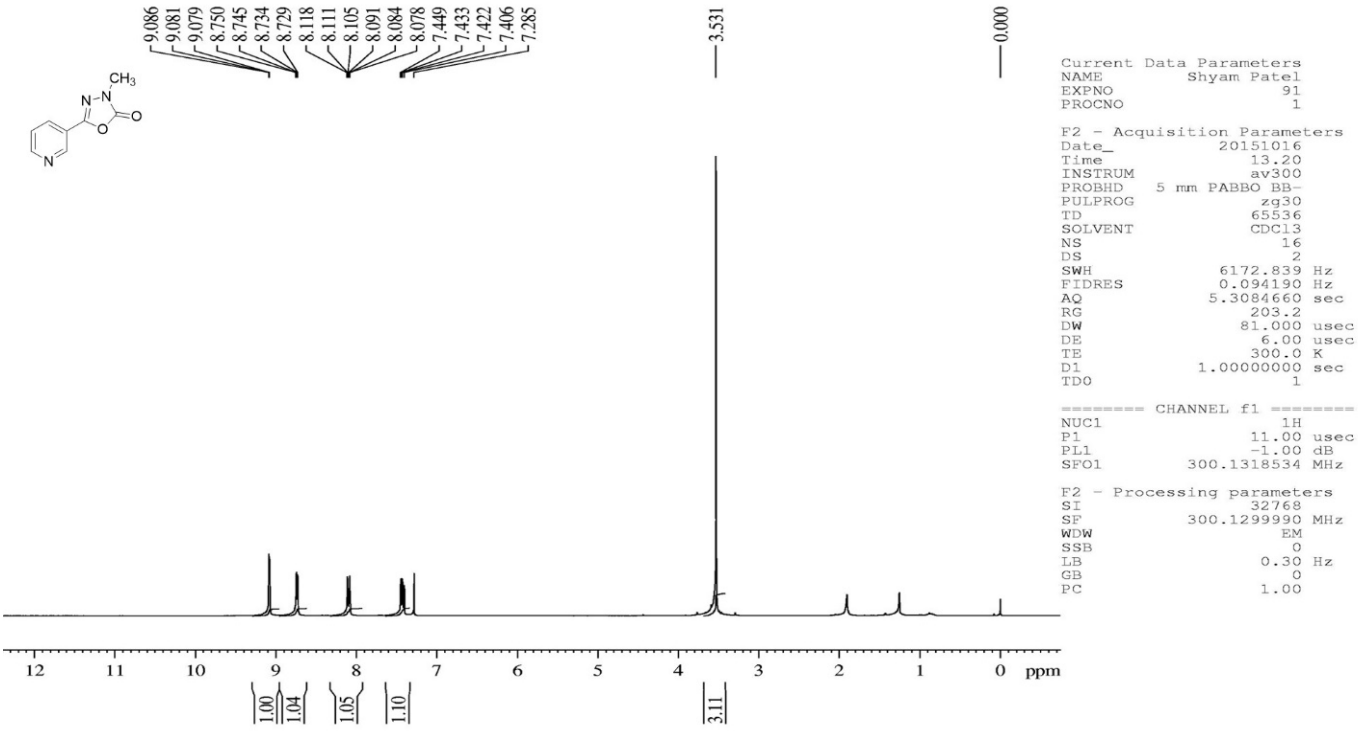
F2 - Acquisition Parameters
Date_           20150628
Time               15.10
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    66
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                  32768
DW                 27.800 usec
DE                  6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.00 usec
PL1                -3.00 dB
SFO1          75.4752953 MHz

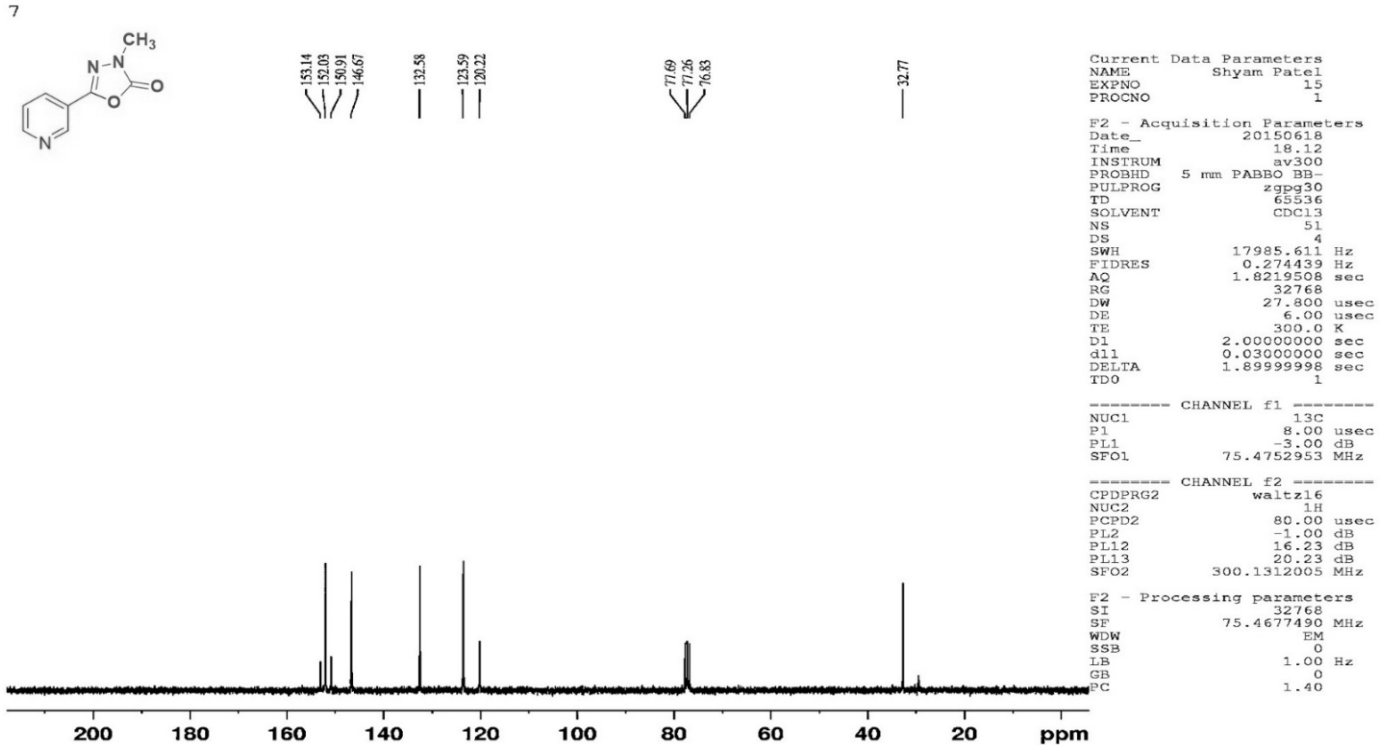
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.23 dB
PL13               20.23 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

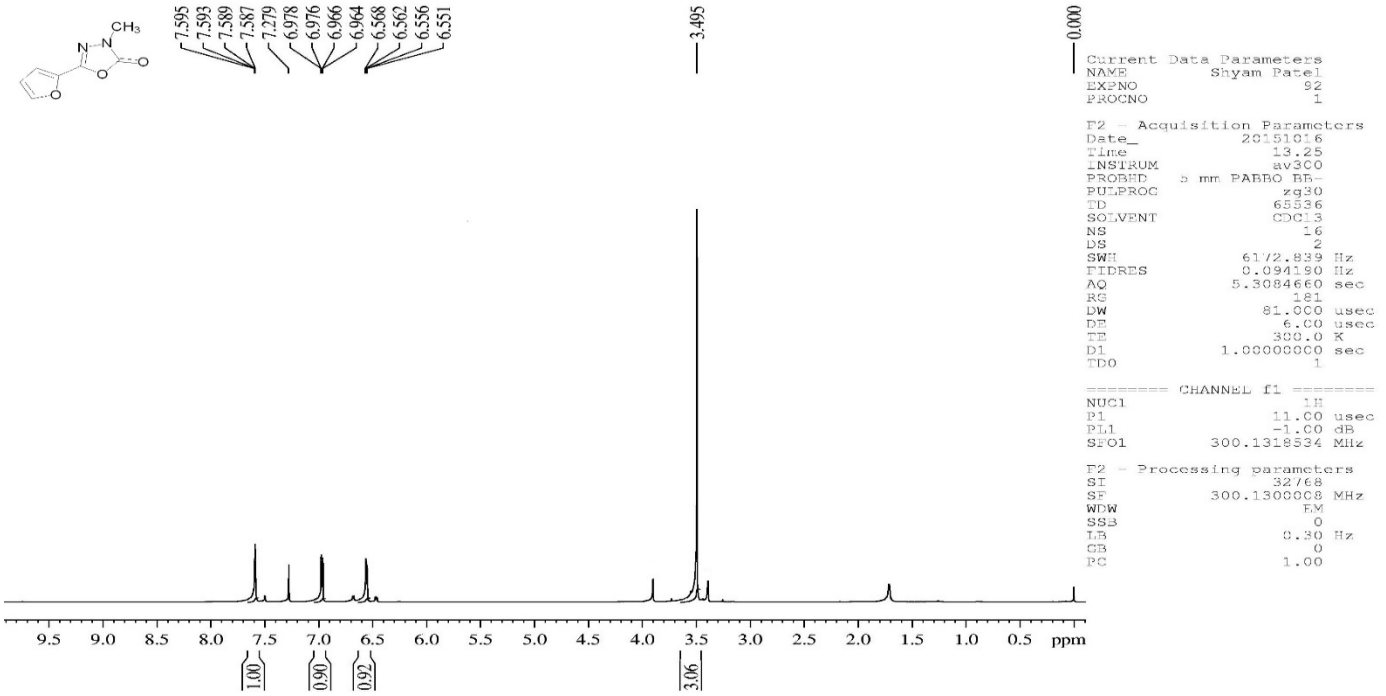
3-methyl-5-(pyridin-3-yl)-1,3,4-oxadiazol-2(*3H*)-one (4q):



3-methyl-5-(pyridin-3-yl)-1,3,4-oxadiazol-2(*3H*)-one (4q):



5-(furan-2-yl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4r):



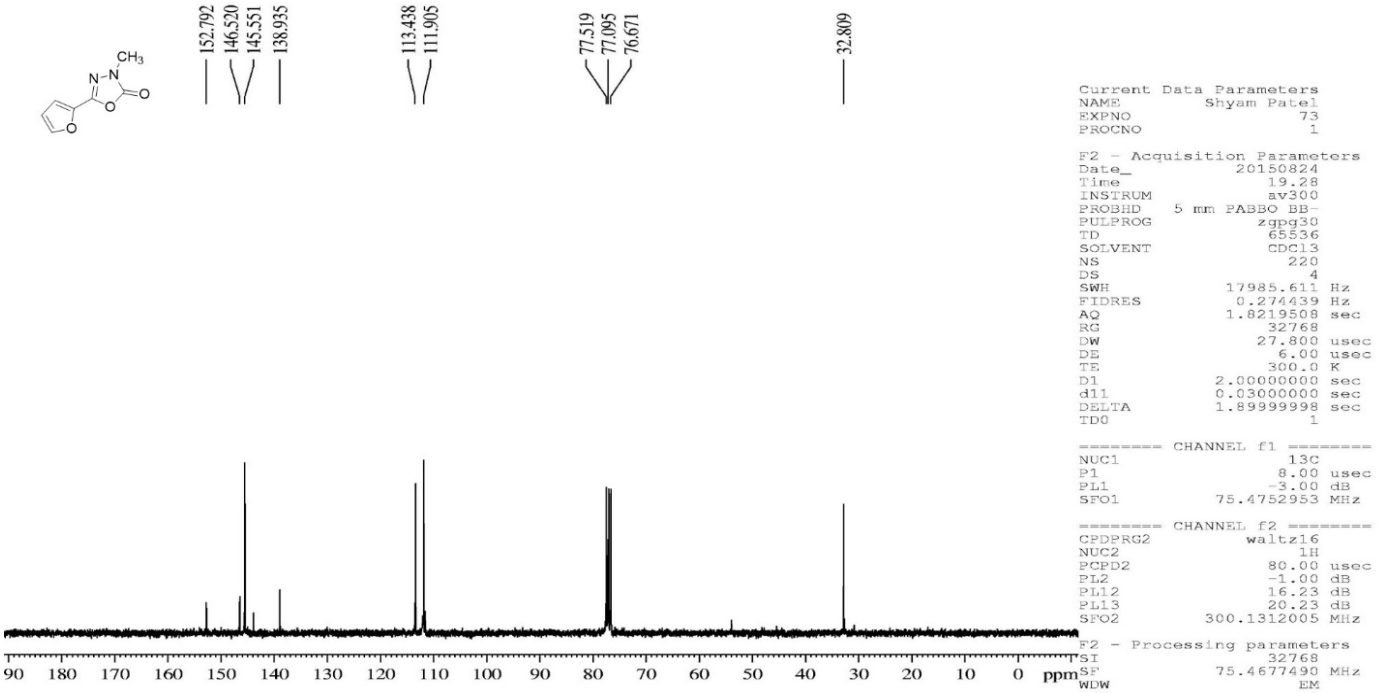

```
Current Data Parameters
NAME                 Shyam Patel
EXPNO                         92
PROCNO                         1

F2 - Acquisition Parameters
Date_               20151016
Time                     13.25
INSTRUM                  av3C0
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  6172.839 Hz
FIDRES               0.094190 Hz
AQ                   5.3084660 sec
RG                         181
DW                      81.000 usec
DE                       6.00 usec
TE                      300.0 K
D1                   1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         1H
P1                       11.00 usec
PL1                      -1.00 dB
SFO1                300.1318534 MHz

F2 - Processing parameters
SI                         32768
SF                  300.1300008 MHz
WDW                           EM
SSB                            0
LB                        0.30 Hz
GB                             0
PC                          1.00
```

5-(furan-2-yl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4r):




```
Current Data Parameters
NAME                 Shyam Patel
EXPNO                         73
PROCNO                         1

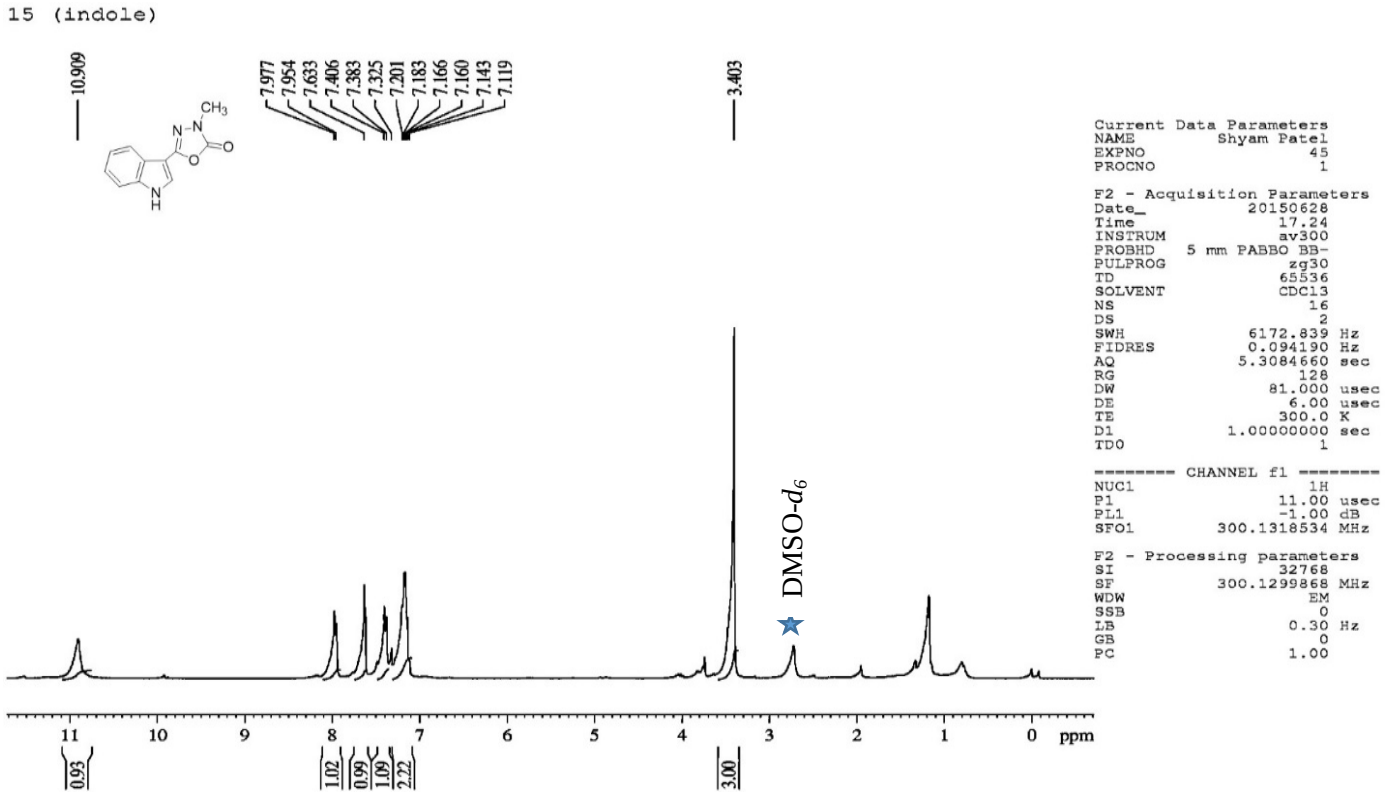
F2 - Acquisition Parameters
Date_               20150824
Time                     19.28
INSTRUM                  av300
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  CDCl3
NS                         220
DS                           4
SWH                 17985.611 Hz
FIDRES               0.274439 Hz
AQ                   1.8219508 sec
RG                         32768
DW                      27.800 usec
DE                       6.00 usec
TE                      300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                        13C
P1                       8.00 usec
PL1                      -3.00 dB
SFO1                75.4752953 MHz

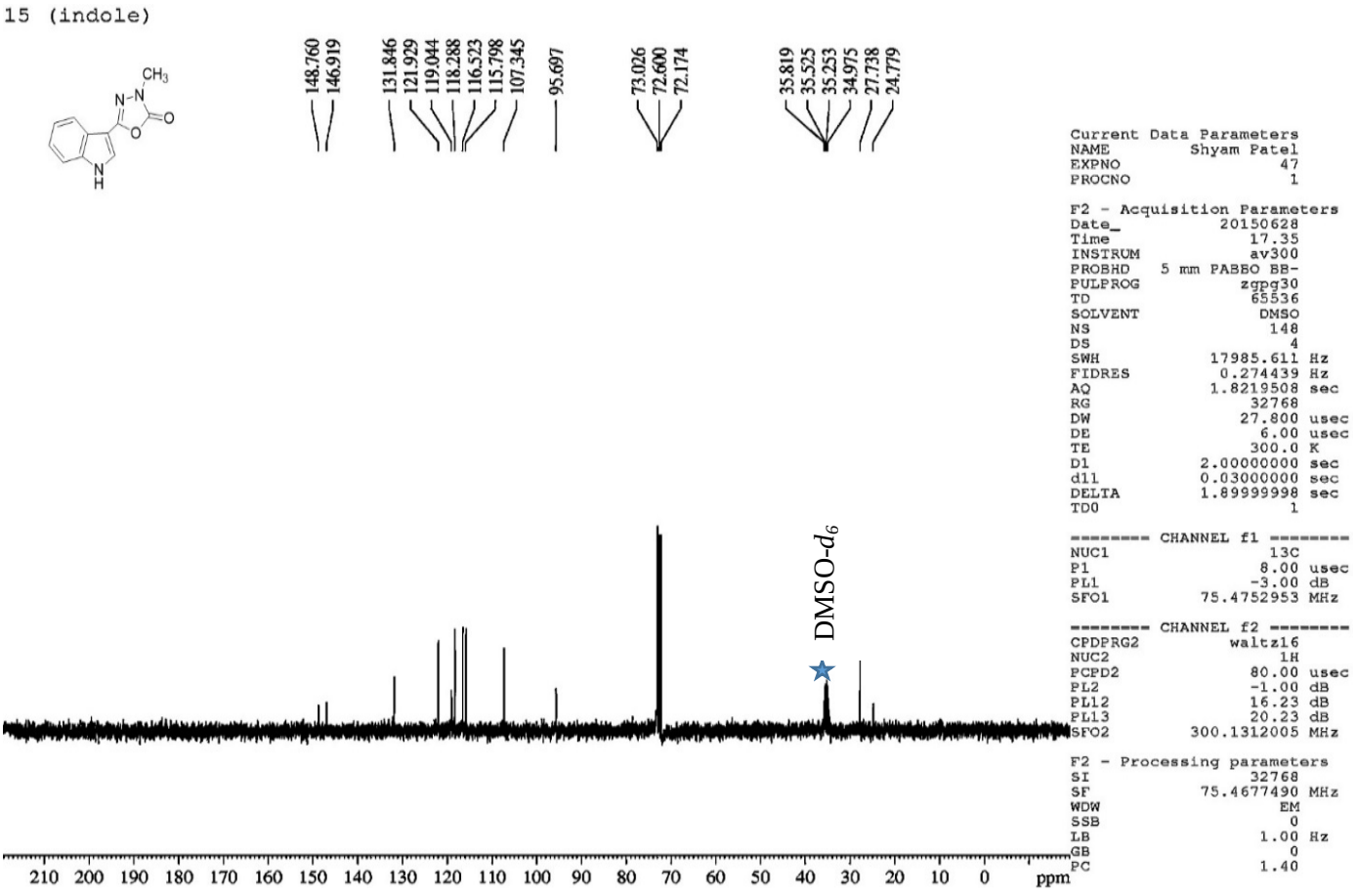
======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     16.23 dB
PL13                     20.23 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                  75.4677490 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                          1.40
```

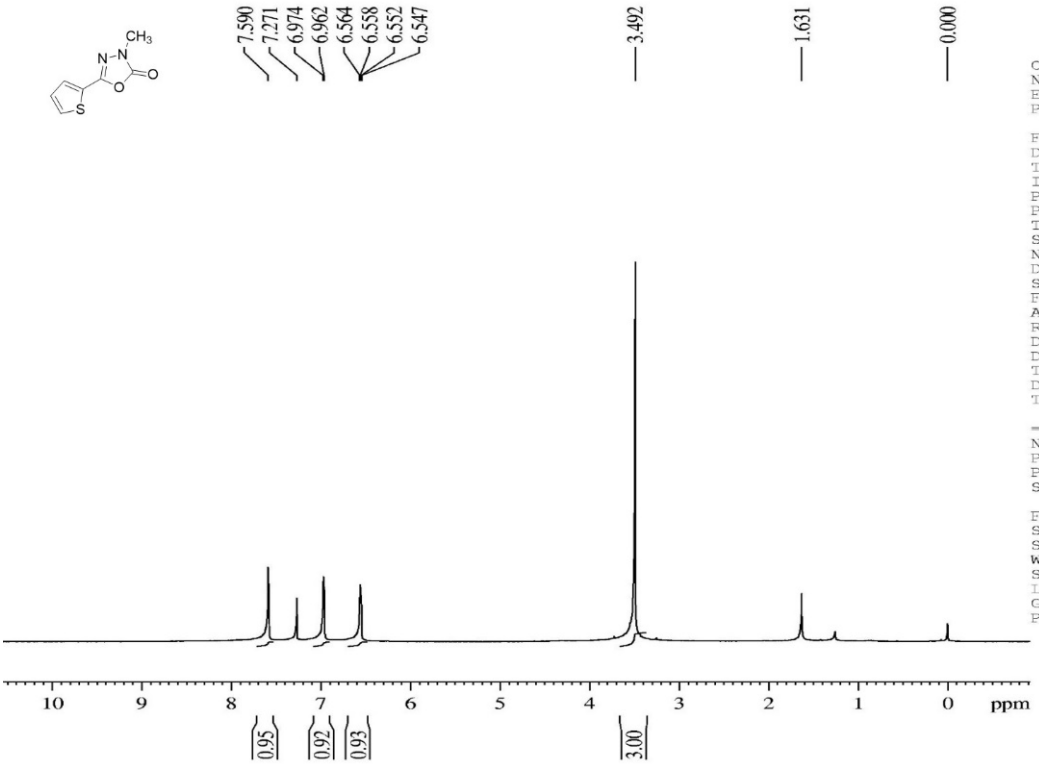
5-(1H-indol-2-yl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4s):



5-(1H-indol-2-yl)-3-methyl-1,3,4-oxadiazol-2(*3H*)-one (4s):



3-methyl-5-(thiophen-2-yl)-1,3,4-oxadiazol-2(*3H*)-one (4t):



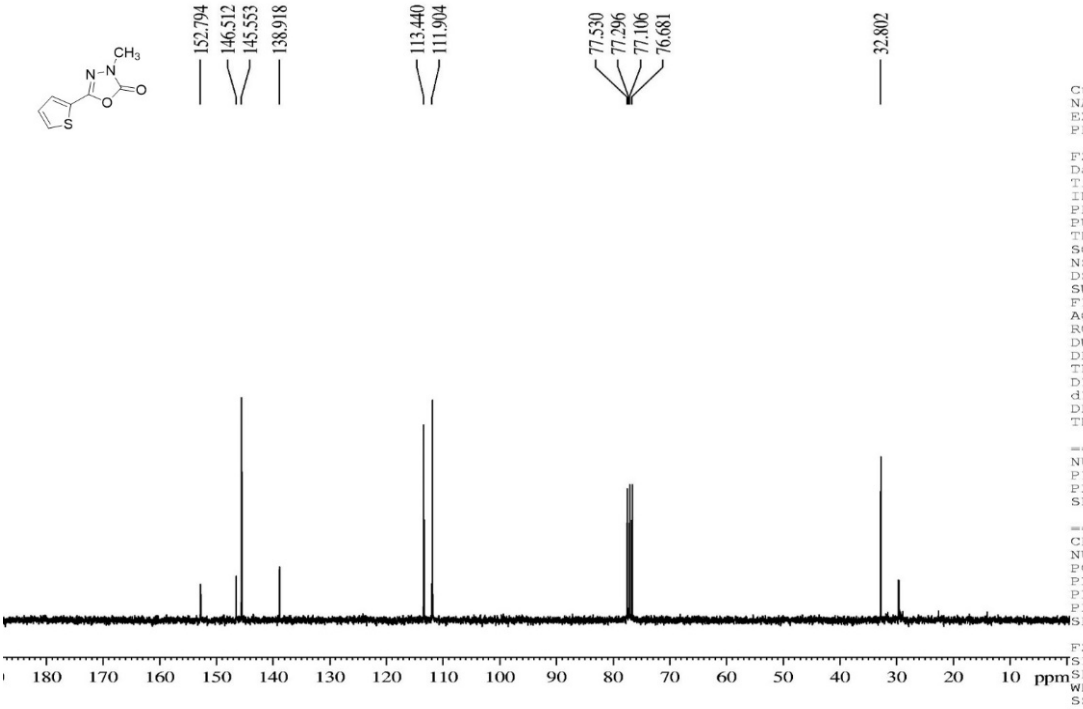

```
Current Data Parameters
NAME                 Shyam Patel
EXPNO                         96
PROCNO                         1

F2 - Acquisition Parameters
Date_               20151017
Time                    9.30
INSTRUM                av300
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 6172.839 Hz
FIDRES              0.094190 Hz
AQ                  5.3084660 sec
RG                      322.5
DW                     81.000 usec
DE                      6.00 usec
TE                     300.0 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.00 usec
PL1                    -1.00 dB
SFO1               300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF                 300.1300022 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

3-methyl-5-(thiophen-2-yl)-1,3,4-oxadiazol-2(*3H*)-one (4t):




```
Current Data Parameters
NAME                 Shyam Patel
EXPNO                         66
PROCNO                         1

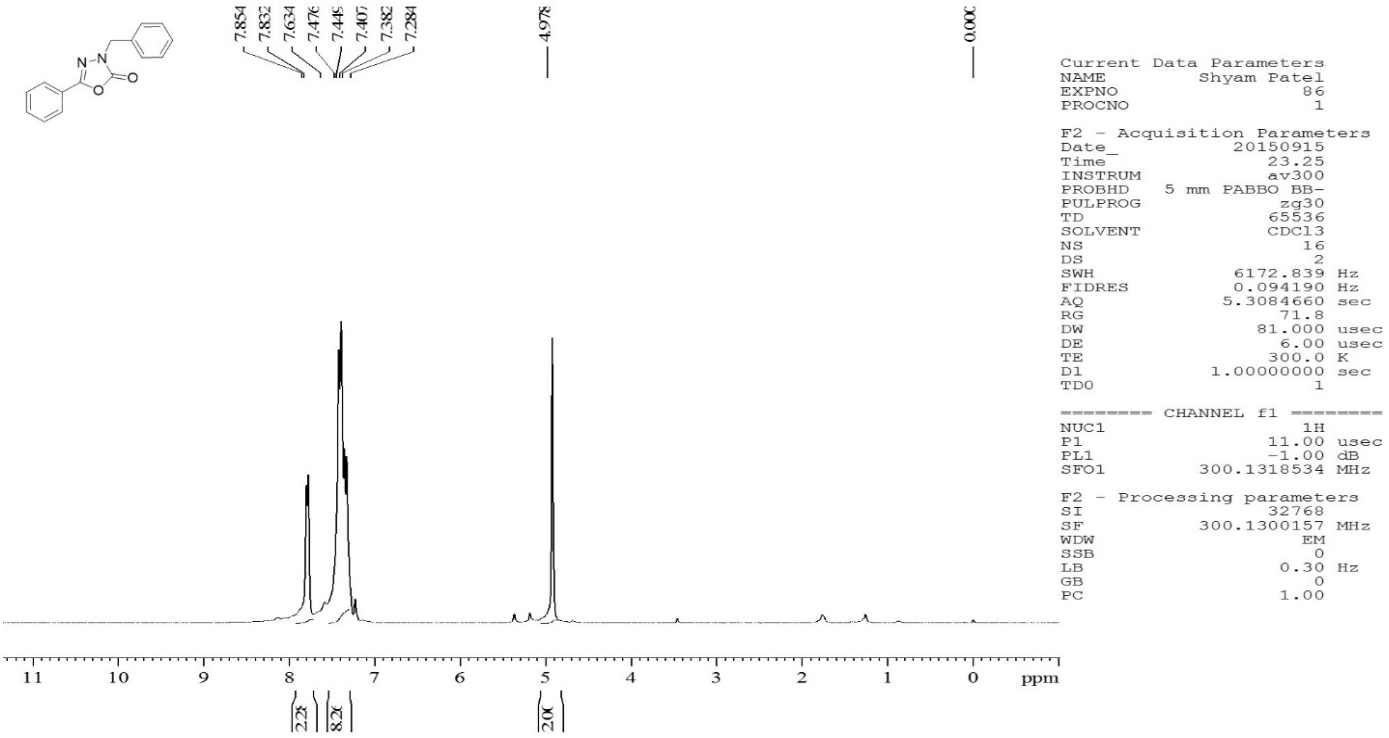
F2 - Acquisition Parameters
Date_               20150813
Time                   19.06
INSTRUM                av300
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        94
DS                         4
SWH                17985.611 Hz
FIDRES              0.274439 Hz
AQ                  1.8219508 sec
RG                      32768
DW                     27.800 usec
DE                      6.00 usec
TE                     300.0 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.00 usec
PL1                    -3.00 dB
SFO1               75.4752953 MHz

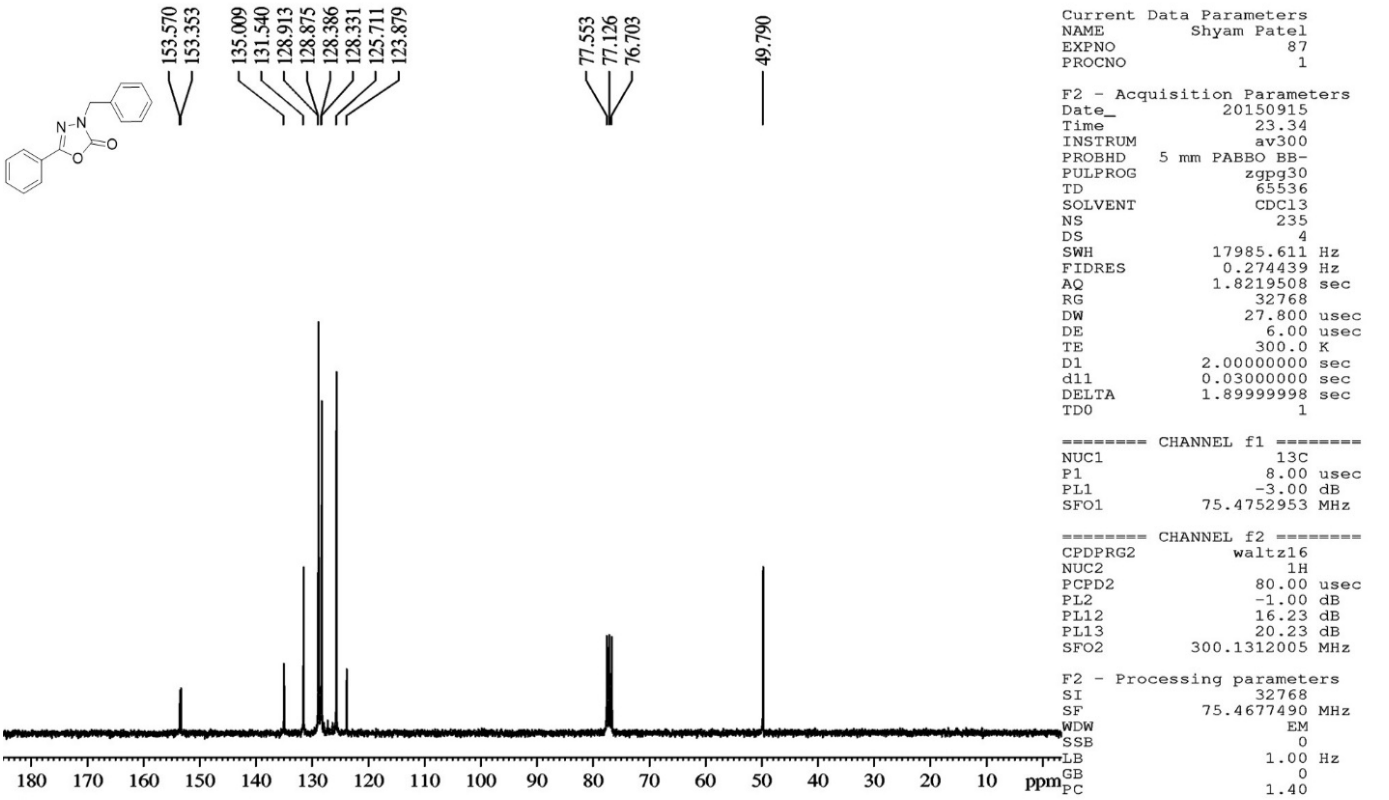
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.23 dB
PL13                   20.23 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF                 75.4677490 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

3-benzyl-5-phenyl-1,3,4-oxadiazol-2(*3H*)-one (5a):

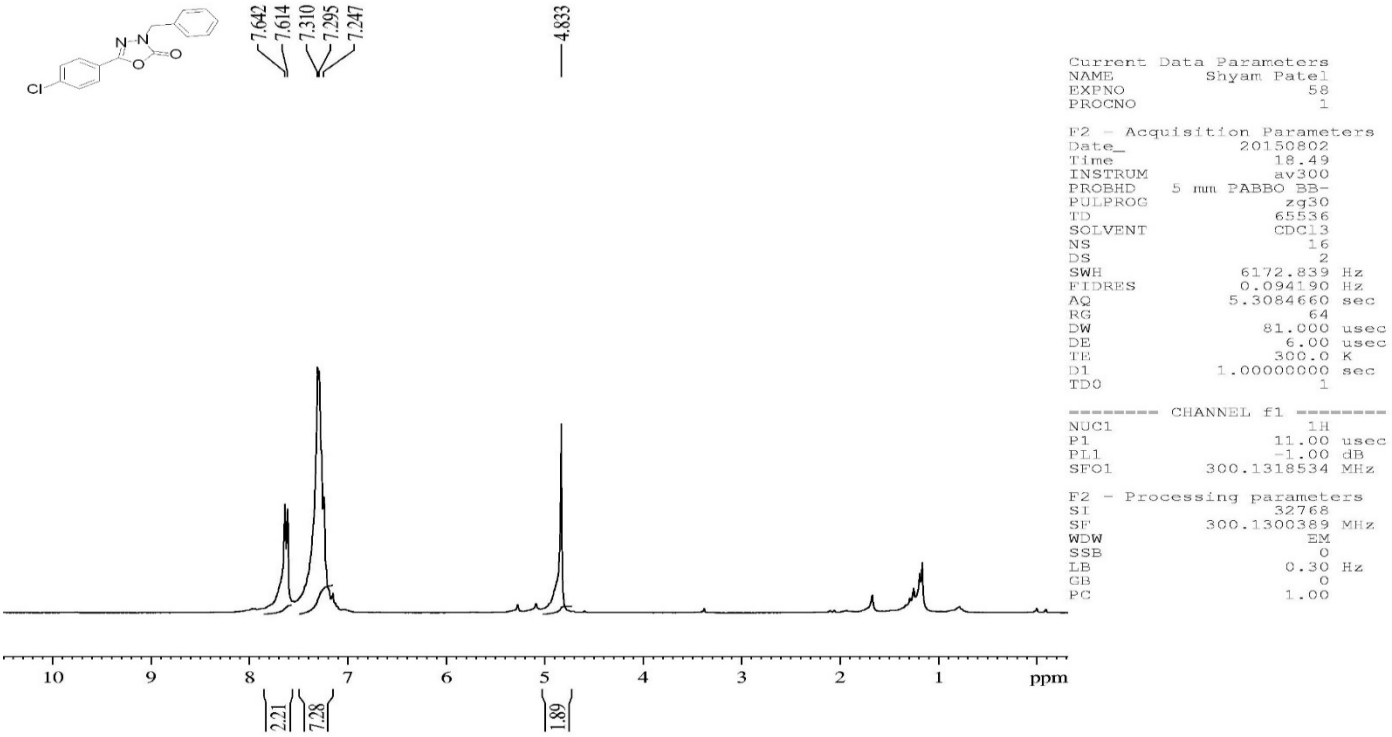


3-benzyl-5-phenyl-1,3,4-oxadiazol-2(*3H*)-one (5a):



\

3-benzyl-5-(4-chlorophenyl)-1,3,4-oxadiazol-2(*3H*)-one (**5b**):



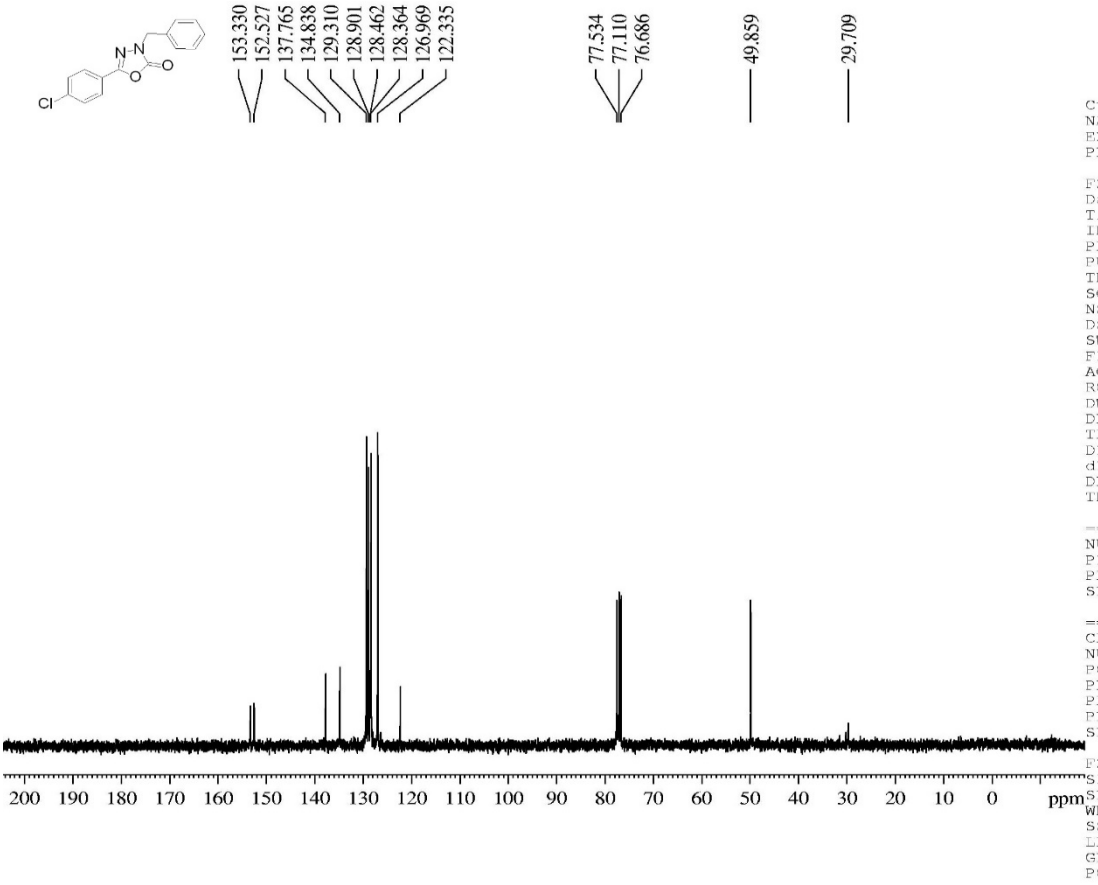

```
Current Data Parameters
NAME                 Shyam Patel
EXPNO                         58
PROCNO                         1

F2 - Acquisition Parameters
Date_               20150802
Time                    18.49
INSTRUM                 av300
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 6172.839 Hz
FIDRES              0.094190 Hz
AQ                  5.3084660 sec
RG                        64
DW                    81.000 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.00 usec
PL1                    -1.00 dB
SFO1              300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF                300.1300389 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

3-benzyl-5-(4-chlorophenyl)-1,3,4-oxadiazol-2(*3H*)-one (**5b**):




```
Current Data Parameters
NAME                 Shyam Patel
EXPNO                         59
PROCNO                         1

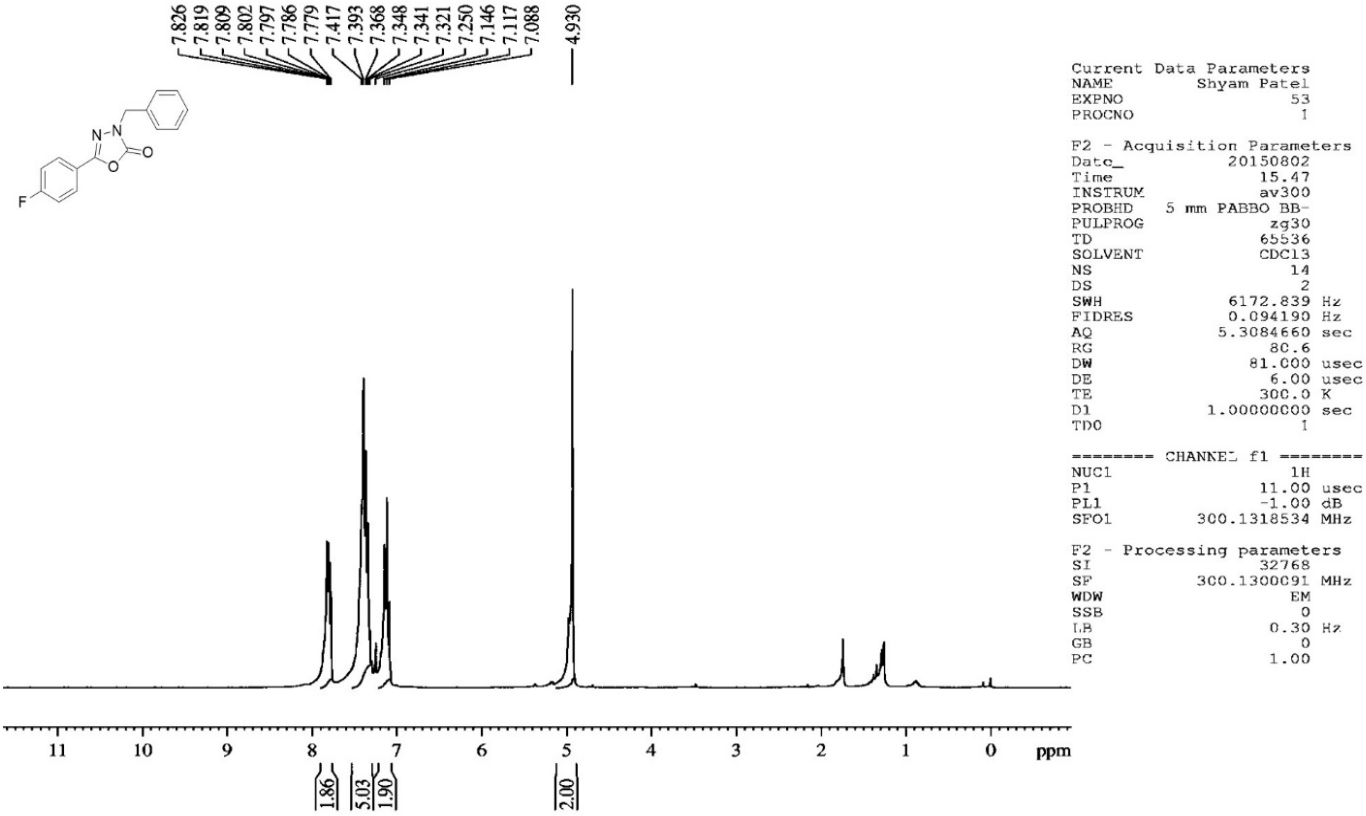
F2 - Acquisition Parameters
Date_               20150802
Time                    18.53
INSTRUM                 av300
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       159
DS                         4
SWH                17985.611 Hz
FIDRES              0.274439 Hz
AQ                  1.8219508 sec
RG                        32768
DW                    27.800 usec
DE                     6.00 usec
TE                    300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      8.00 usec
PL1                    -3.00 dB
SFO1              75.4752953 MHz

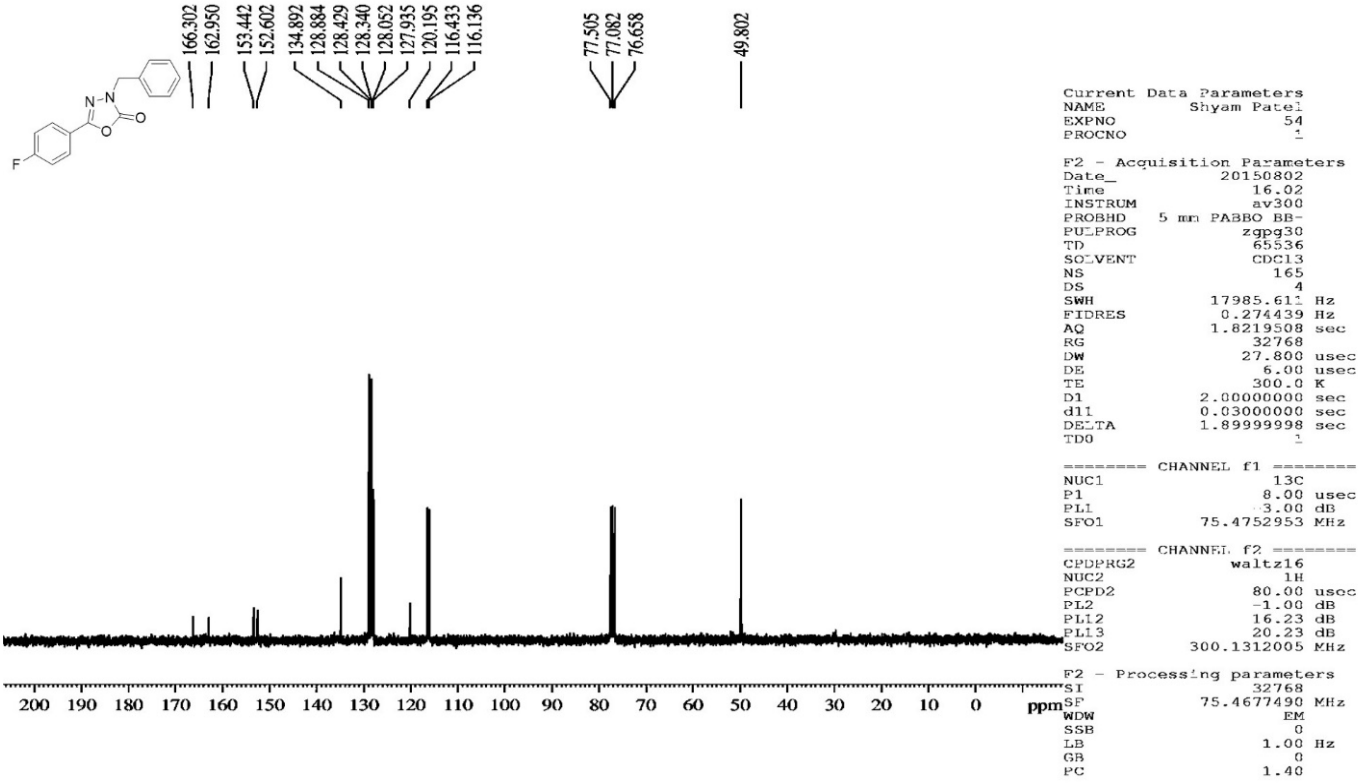
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.23 dB
PL13                   20.23 dB
SFO2              300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF                75.4677490 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

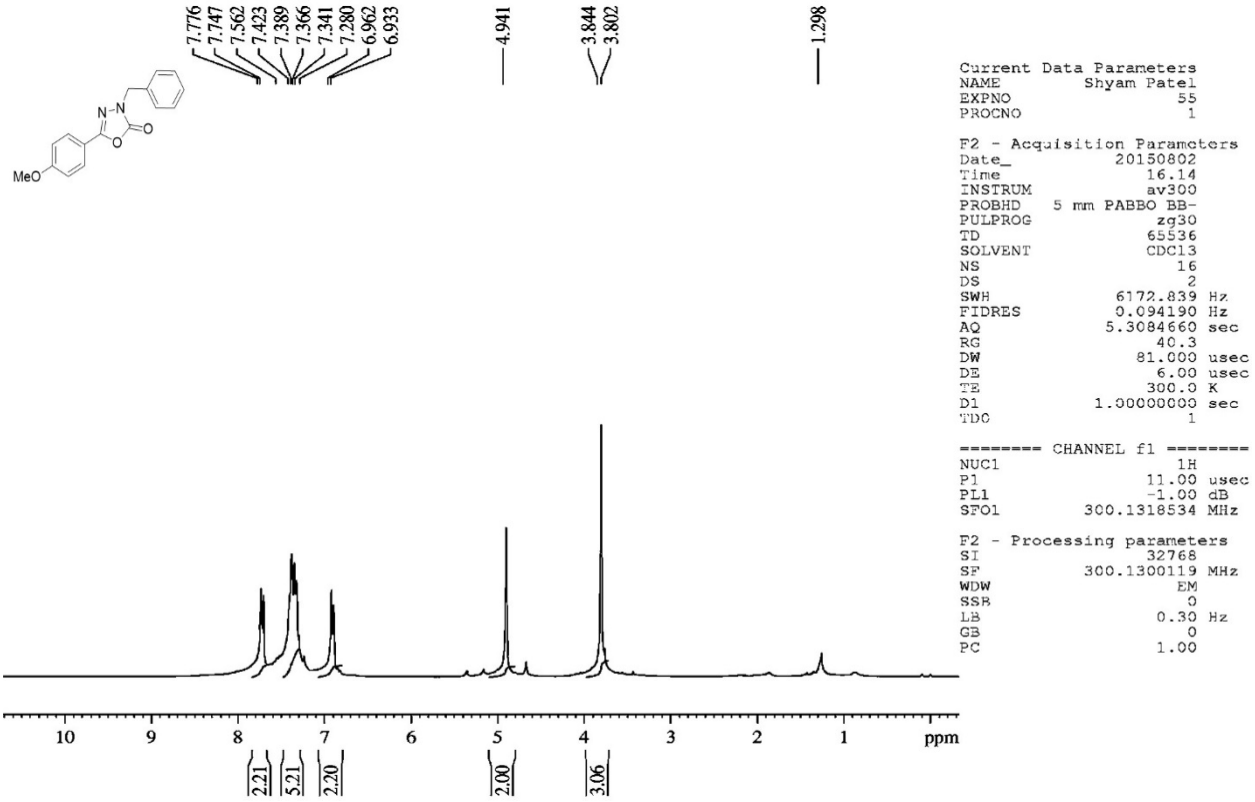
3-benzyl-5-(4-fluorophenyl)-1,3,4-oxadiazol-2(*3H*)-one (**5c**):



3-benzyl-5-(4-fluorophenyl)-1,3,4-oxadiazol-2(*3H*)-one (**5c**):



3-benzyl-5-(4-methoxyphenyl)-1,3,4-oxadiazol-2(*3H*)-one (**5d**):



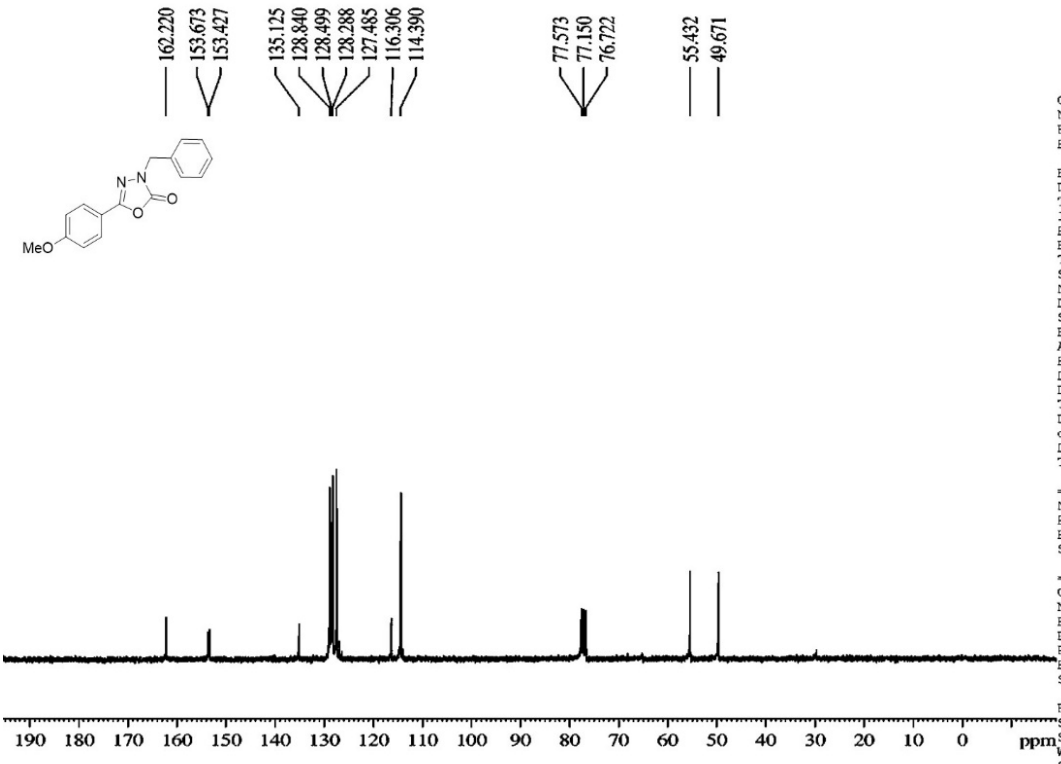

```
Current Data Parameters
NAME         Shyam Patel
EXPNO                 55
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150802
Time               16.14
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                  40.3
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                -1.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300119 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3-benzyl-5-(4-methoxyphenyl)-1,3,4-oxadiazol-2(*3H*)-one (**5d**):




```
Current Data Parameters
NAME         Shyam Patel
EXPNO                 56
PROCNO                 1

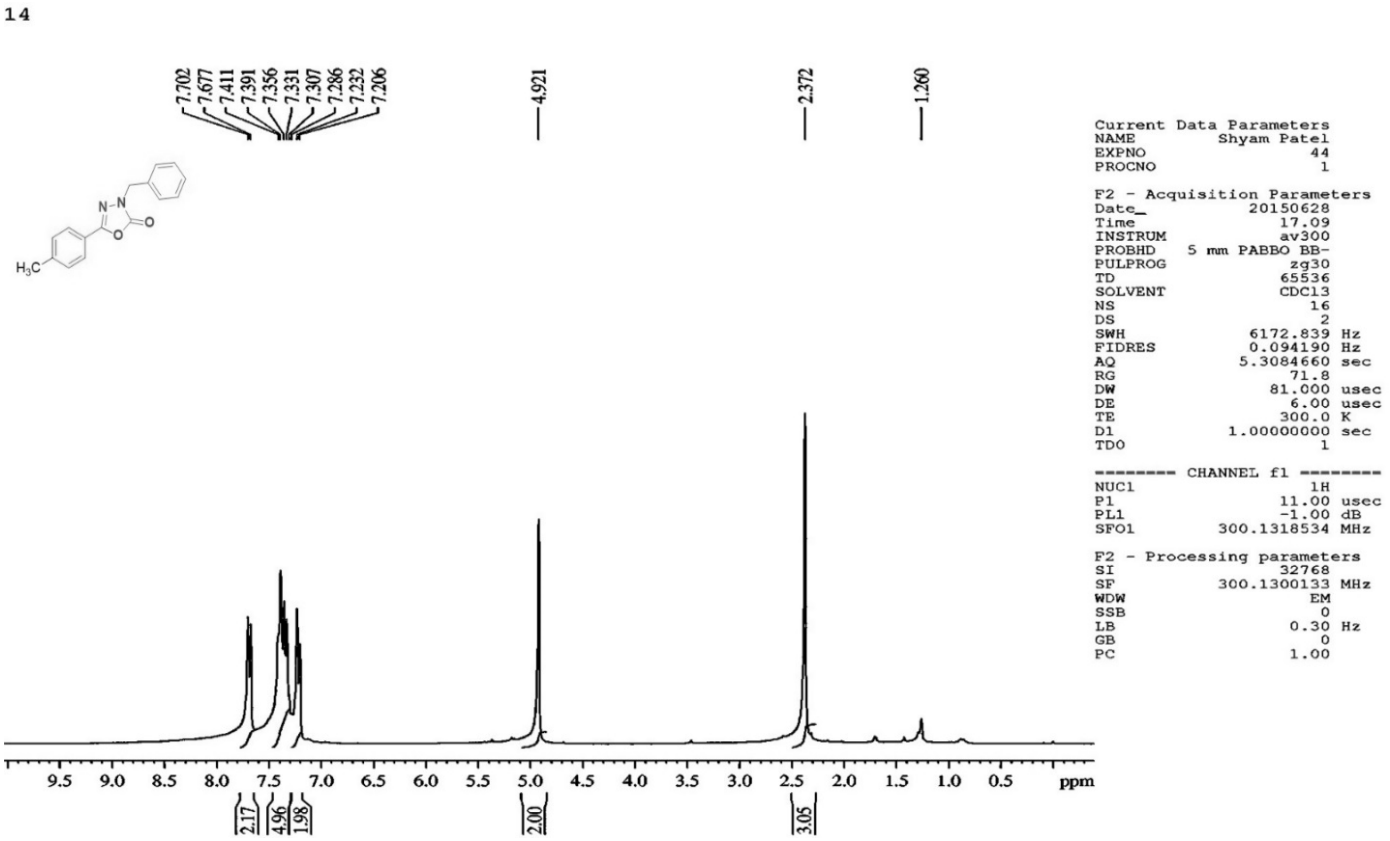
F2 - Acquisition Parameters
Date_           20150802
Time               16.32
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   175
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                 32768
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.00 usec
PL1                -3.00 dB
SFO1          75.4752953 MHz

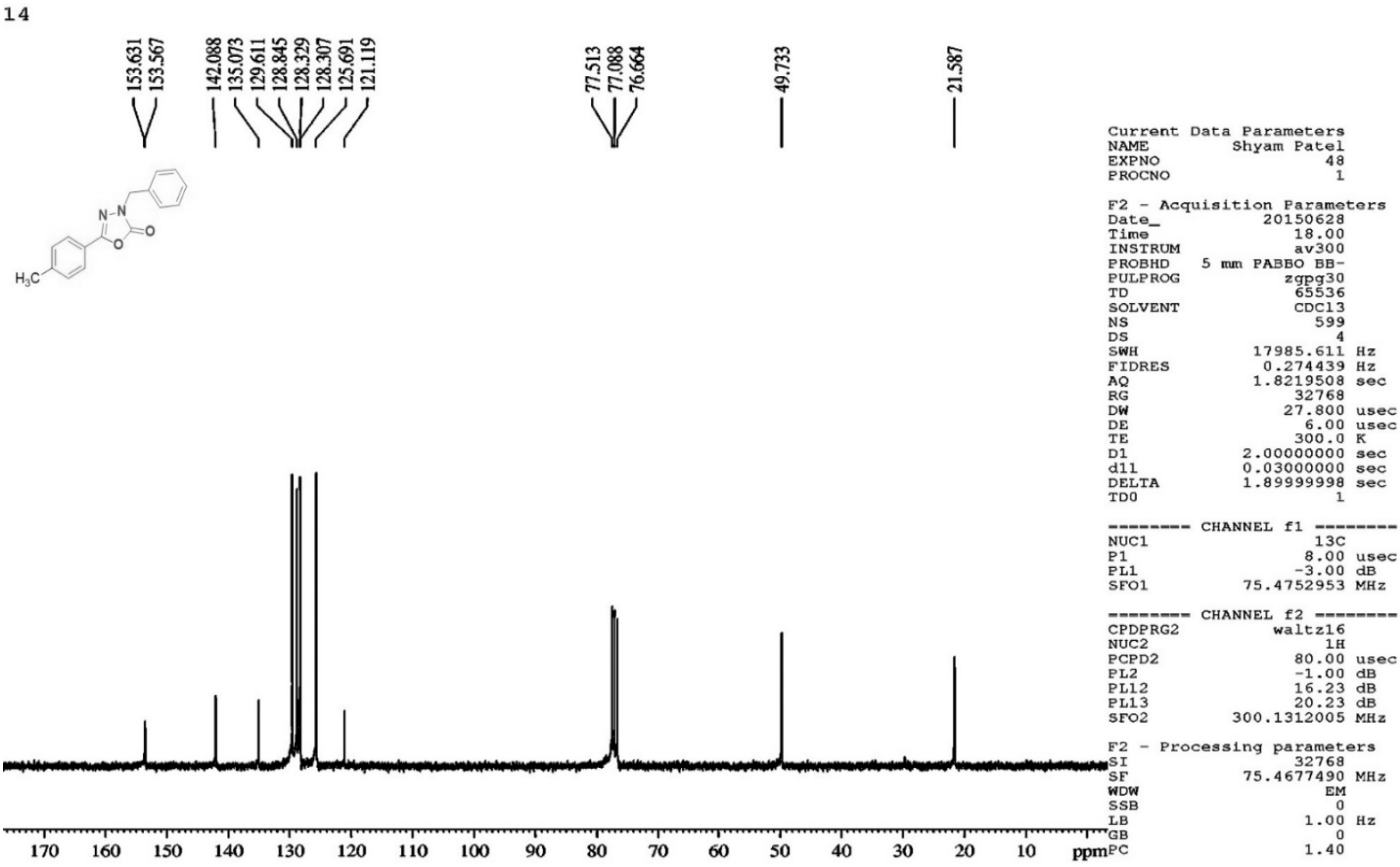
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.23 dB
PL13               20.23 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

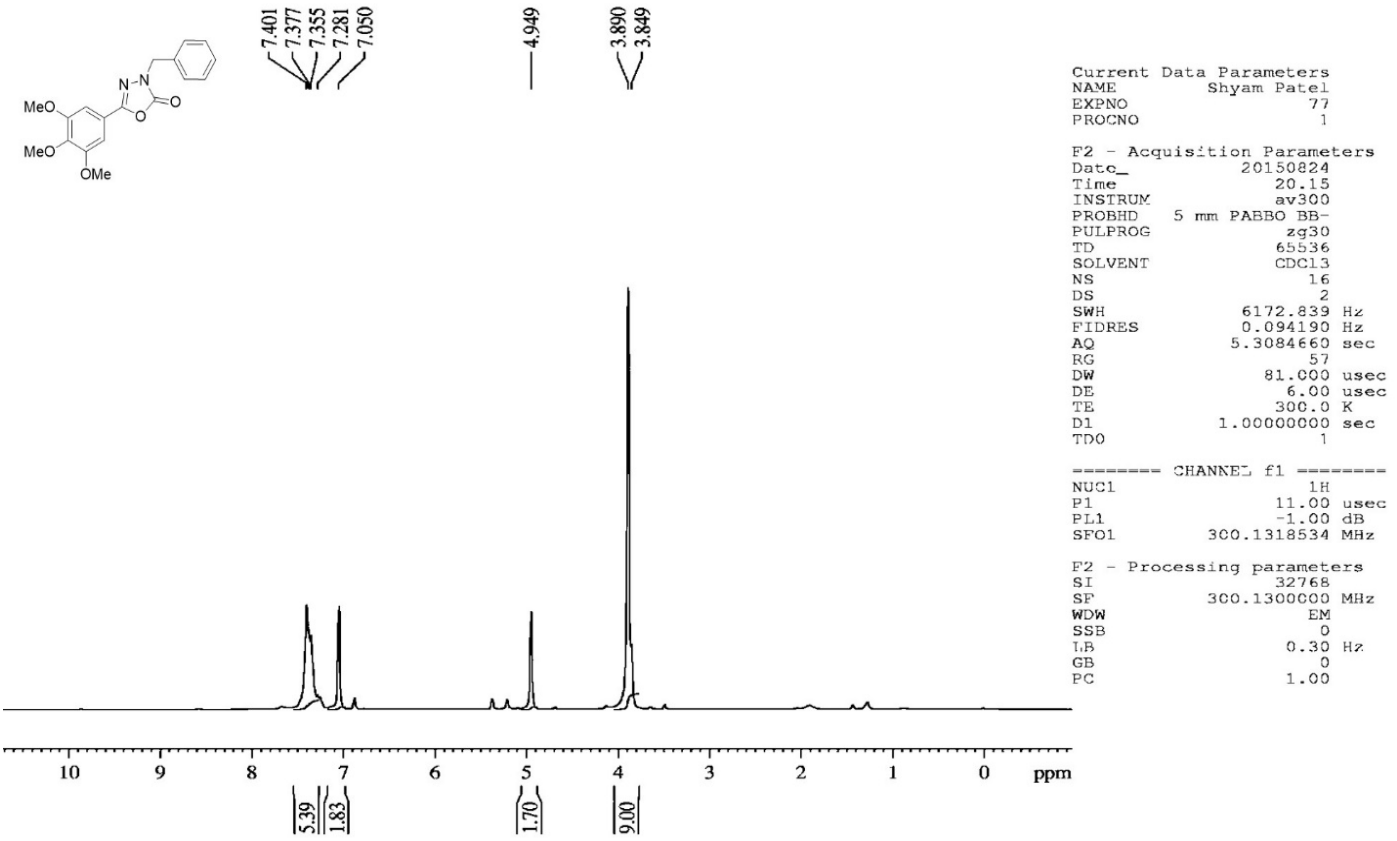
3-benzyl-5-(p-tolyl)-1,3,4-oxadiazol-2(*3H*)-one (5e):



3-benzyl-5-(p-tolyl)-1,3,4-oxadiazol-2(*3H*)-one (5e):



3-benzyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(*3H*)-one (5f):



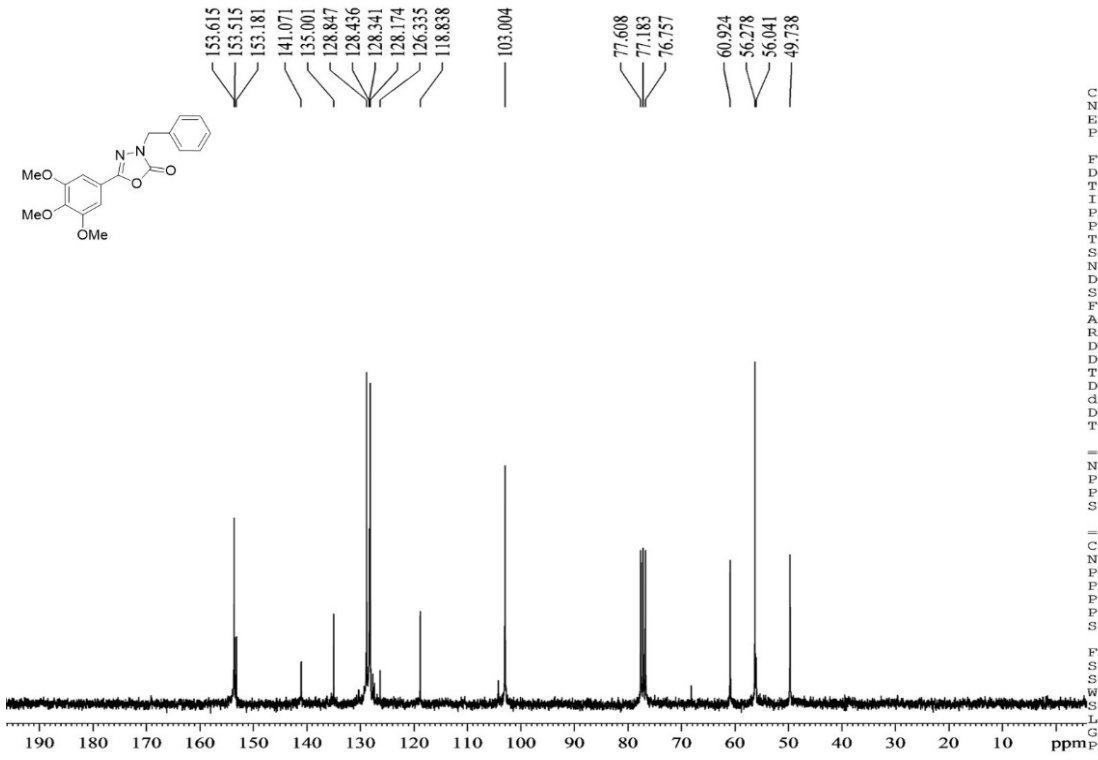

```
Current Data Parameters
NAME          Shyam Patel
EXPNO                  77
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150824
Time               20.15
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                    57
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                -1.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

3-benzyl-5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2(*3H*)-one (5f):




```
Current Data Parameters
NAME          Shyam Patel
EXPNO                  84
PROCNO                  1

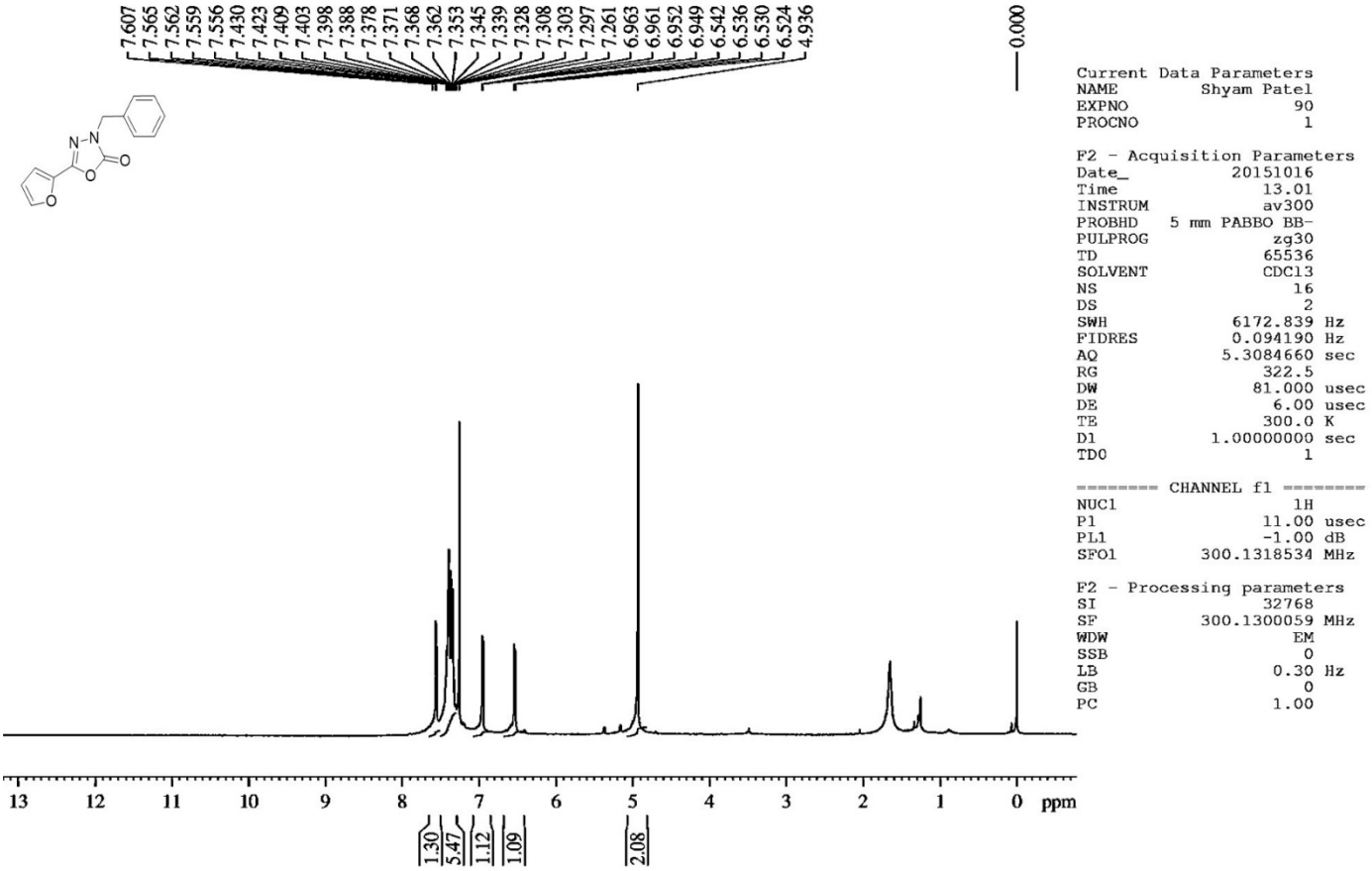
F2 - Acquisition Parameters
Date_           20150915
Time               22.07
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   403
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                 32768
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.00 usec
PL1               -3.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.23 dB
PL13               20.23 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

3-benzyl-5-(furan-2-yl)-1,3,4-oxadiazol-2(*3H*)-one (5g):



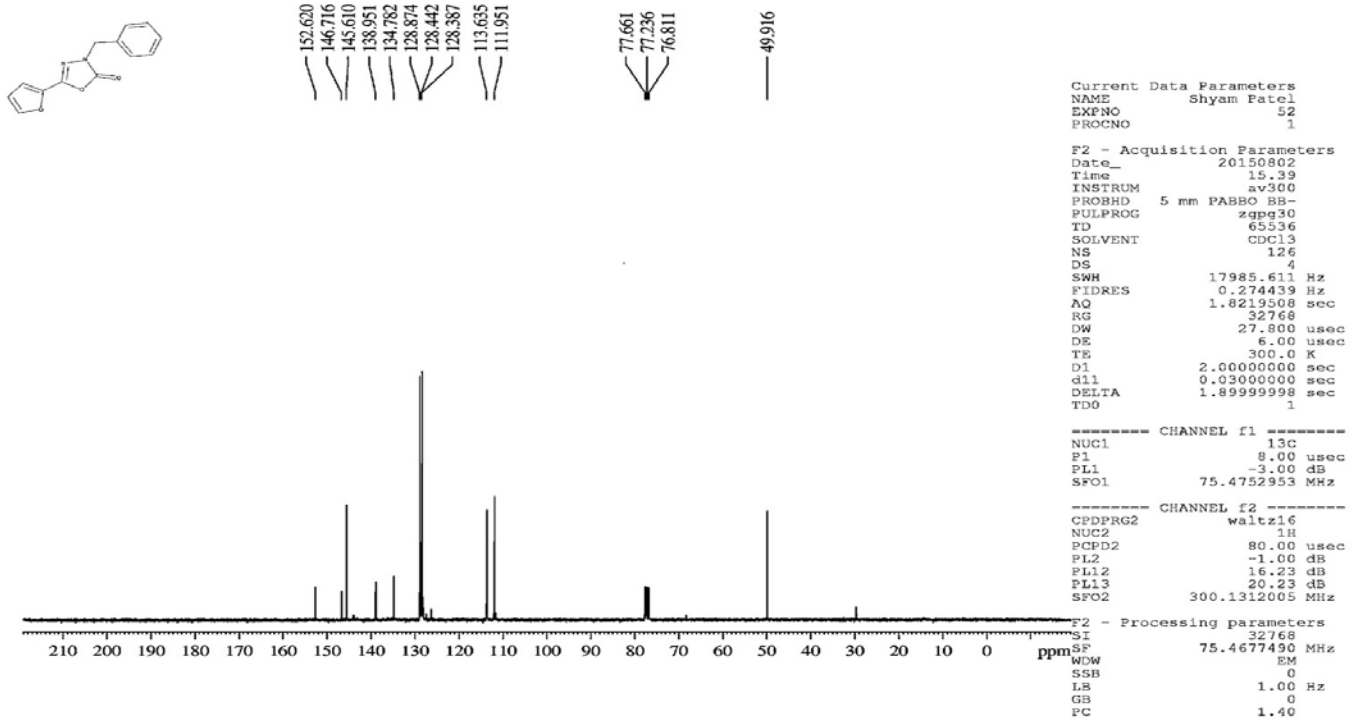

```
Current Data Parameters
NAME          Shyam Patel
EXPNO                  90
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151016
Time               13.01
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ            5.3084660 sec
RG                322.5
DW               81.000 usec
DE                6.00 usec
TE               300.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PL1               -1.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                32768
SF           300.1300059 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                 1.00
```

3-benzyl-5-(furan-2-yl)-1,3,4-oxadiazol-2(*3H*)-one (5g):




```
Current Data Parameters
NAME          Shyam Patel
EXPNO                  52
PROCNO                  1

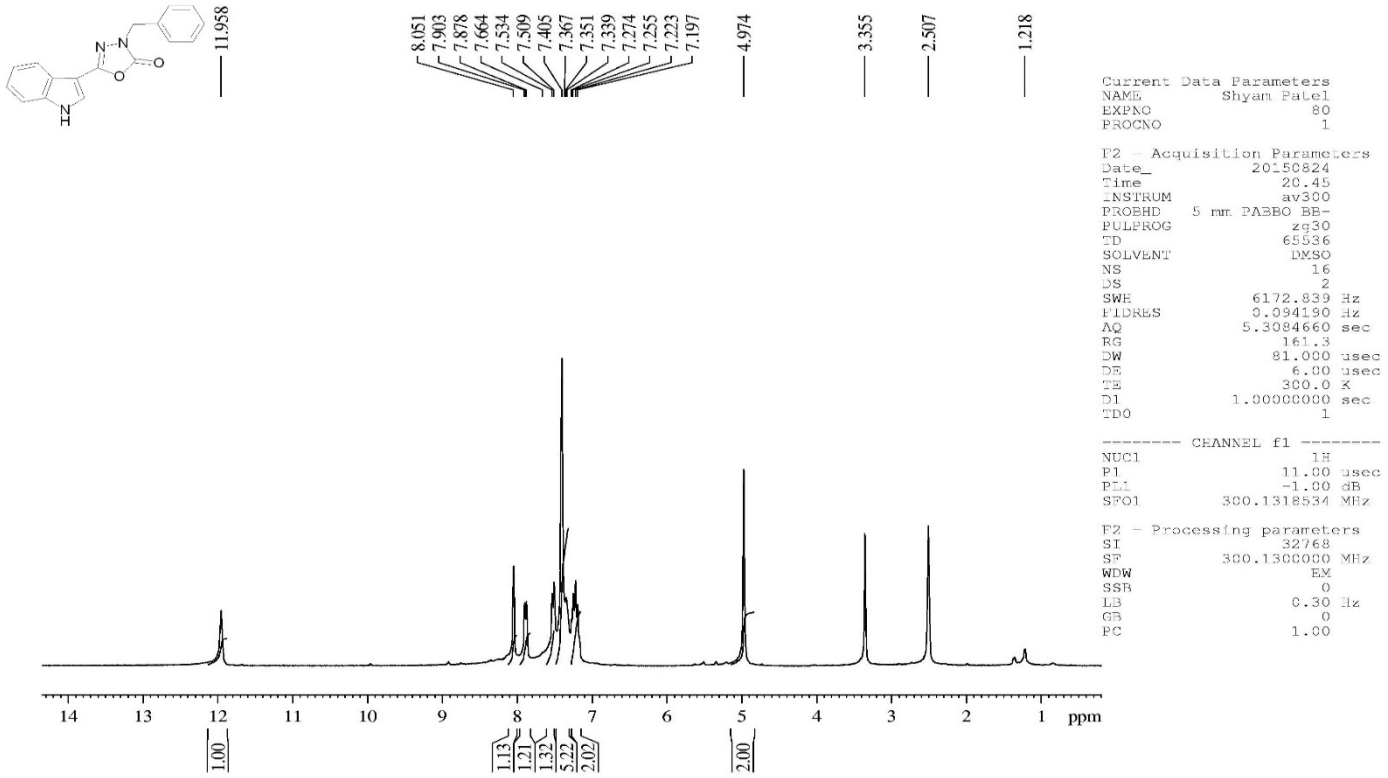
F2 - Acquisition Parameters
Date_           20150802
Time               15.39
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  126
DS                    4
SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                32768
DW               27.800 usec
DE                6.00 usec
TE               300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                8.00 usec
PL1               -3.00 dB
SFO1         75.4752953 MHz

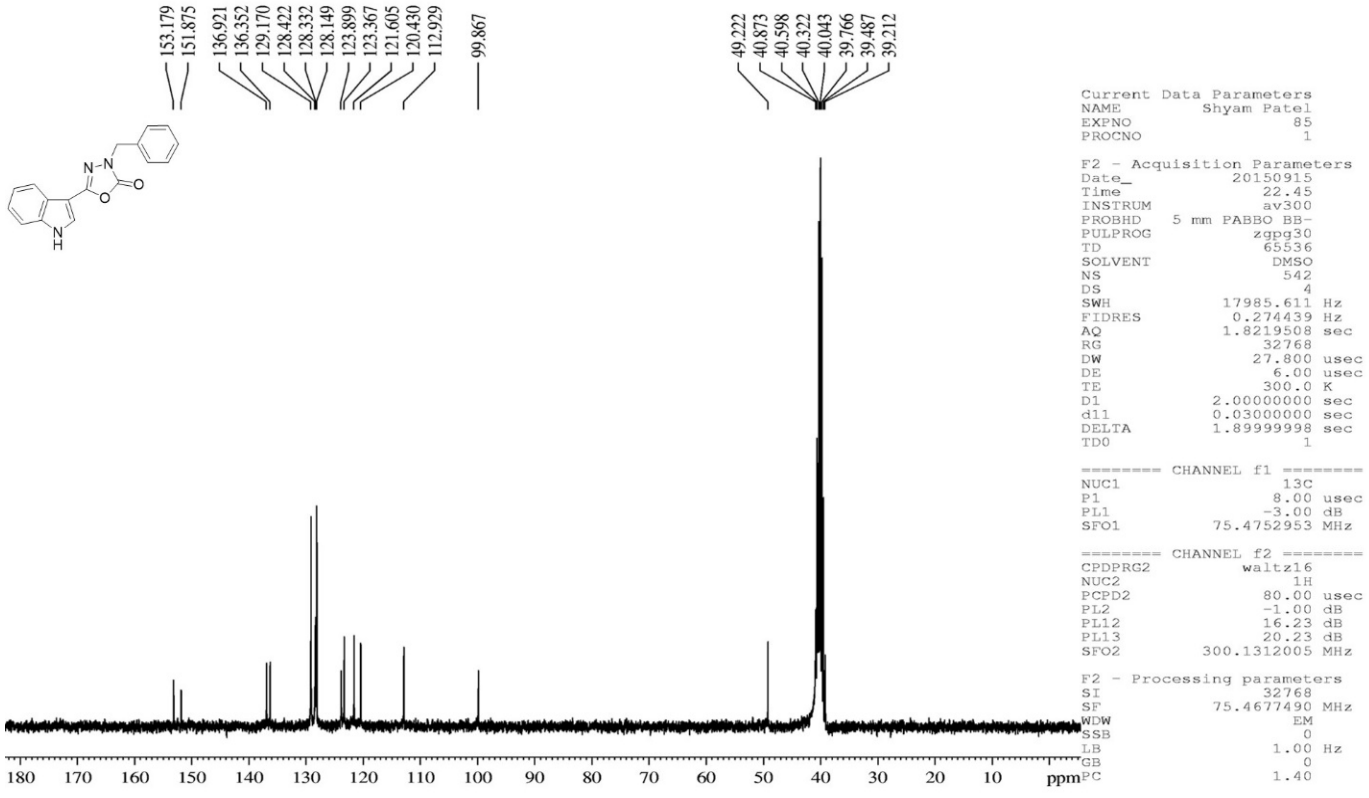
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            80.00 usec
PL2               -1.00 dB
PL12              16.23 dB
PL13              20.23 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677490 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                 1.40
```

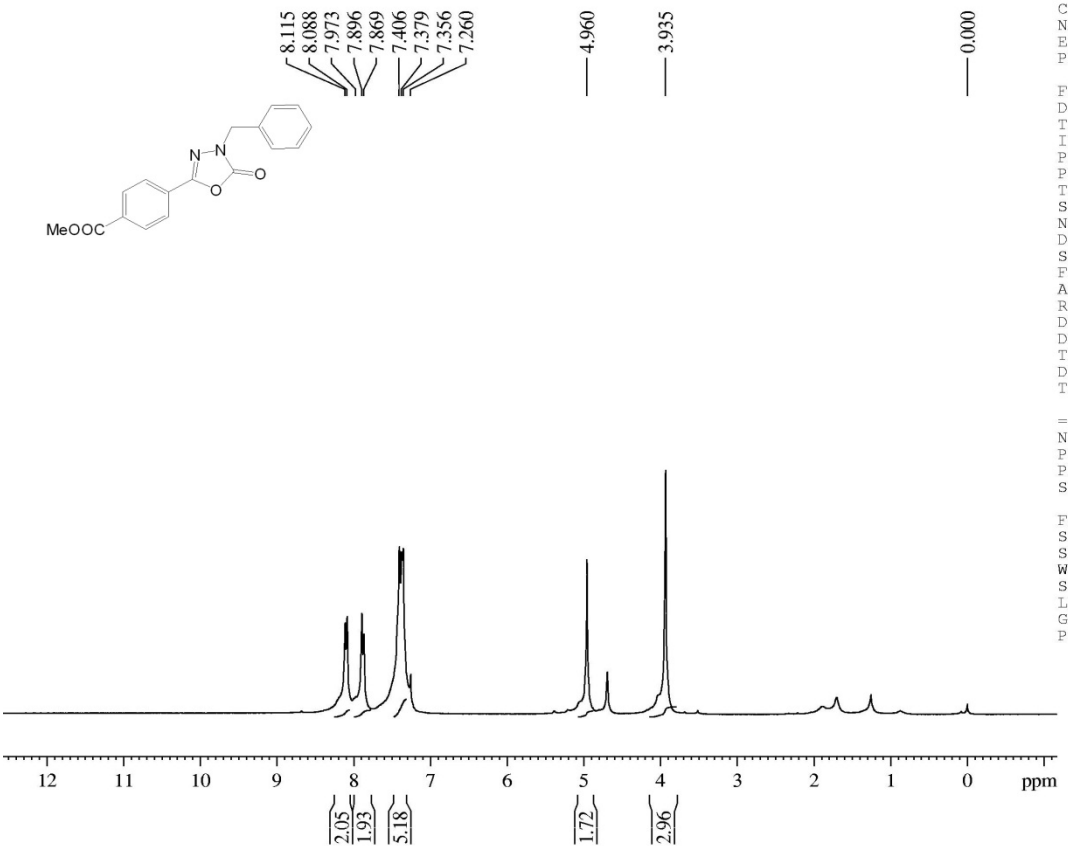
3-benzyl-5-(1H-indol-3-yl)-1,3,4-oxadiazol-2(*3H*)-one (5h):



3-benzyl-5-(1H-indol-3-yl)-1,3,4-oxadiazol-2(*3H*)-one (5h):



Methyl 4-(4-benzyl-5-oxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)benzoate (5i):



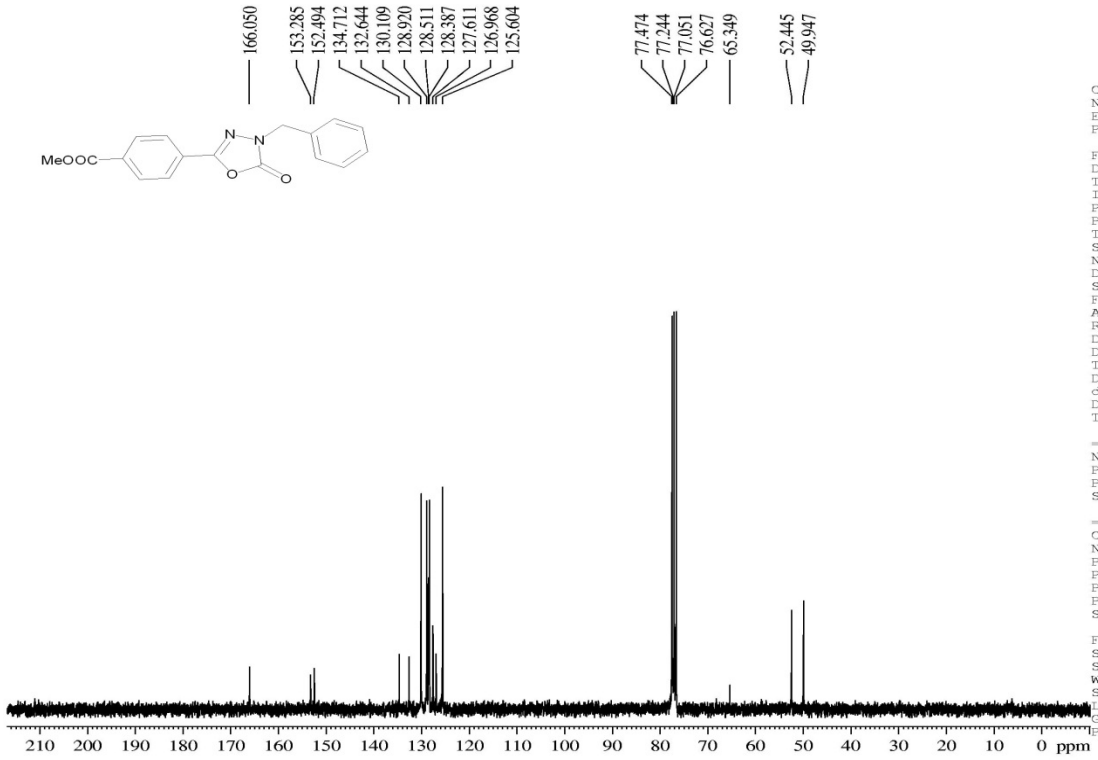

```
Current Data Parameters
NAME         Shyam Patel
EXPNO                153
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170130
Time               20.53
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                   181
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                -1.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300064 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Methyl 4-(4-benzyl-5-oxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)benzoate (5i):




```
Current Data Parameters
NAME         Shyam Patel
EXPNO                154
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170130
Time               21.06
INSTRUM            av300
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   453
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                 32768
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

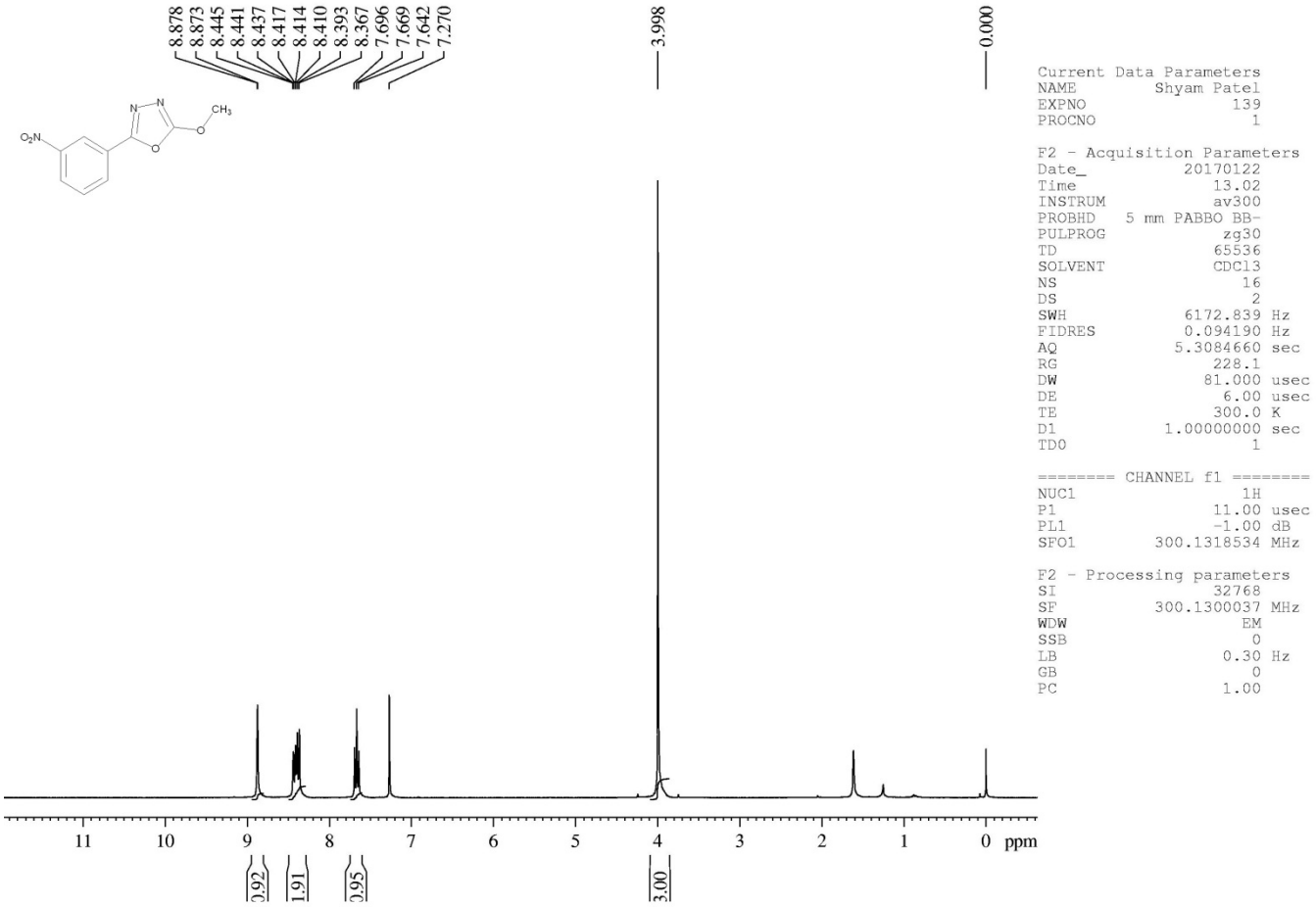
======== CHANNEL f1 ========
NUC1                 13C
P1                 8.00 usec
PL1               -3.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.23 dB
PL13               20.23 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

2-methoxy-5-(3-nitrophenyl)-1,3,4-oxadiazole :

Yield 17 mg, 16%; solid, m.p. 143-145 °C (lit.[3] m.p. 147 °C); ^{1}H NMR (300 MHz, $CDCl_3$): 8.87 (d, 1H, *J* = 1.5 Hz), 8.45-8.37 (m, 2H), 7.67 (t, 1H), 4.0 (s, 3H)



References:

1. SADABS V2.10 (Sheldrick, G. M. 2003).

2. (a) Sheldrick, G. M. Acta Crystallogr., Sect. A: Found. Crystallogr., 1990, **46**, 467; (b) Sheldrick, G. M. SHELXL-NT Version 6.12, University of Gottingen, Germany, 2000

3. Shang, Z., Chu, Q., & Tan, S. *Synthesis.*, 2015, **47**, 1032-1040.