

Supplementary Information

Diversity oriented synthesis of 6-Nitro- and 6-Aminoquinolones and their activity as alkaline phosphatase inhibitors

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peter.langer@uni-rostock.de; iva108@googlemail.com

^b Centre for Advanced Drug Research, COMSATS Institute of Information Technology, Abbottabad, Pakistan

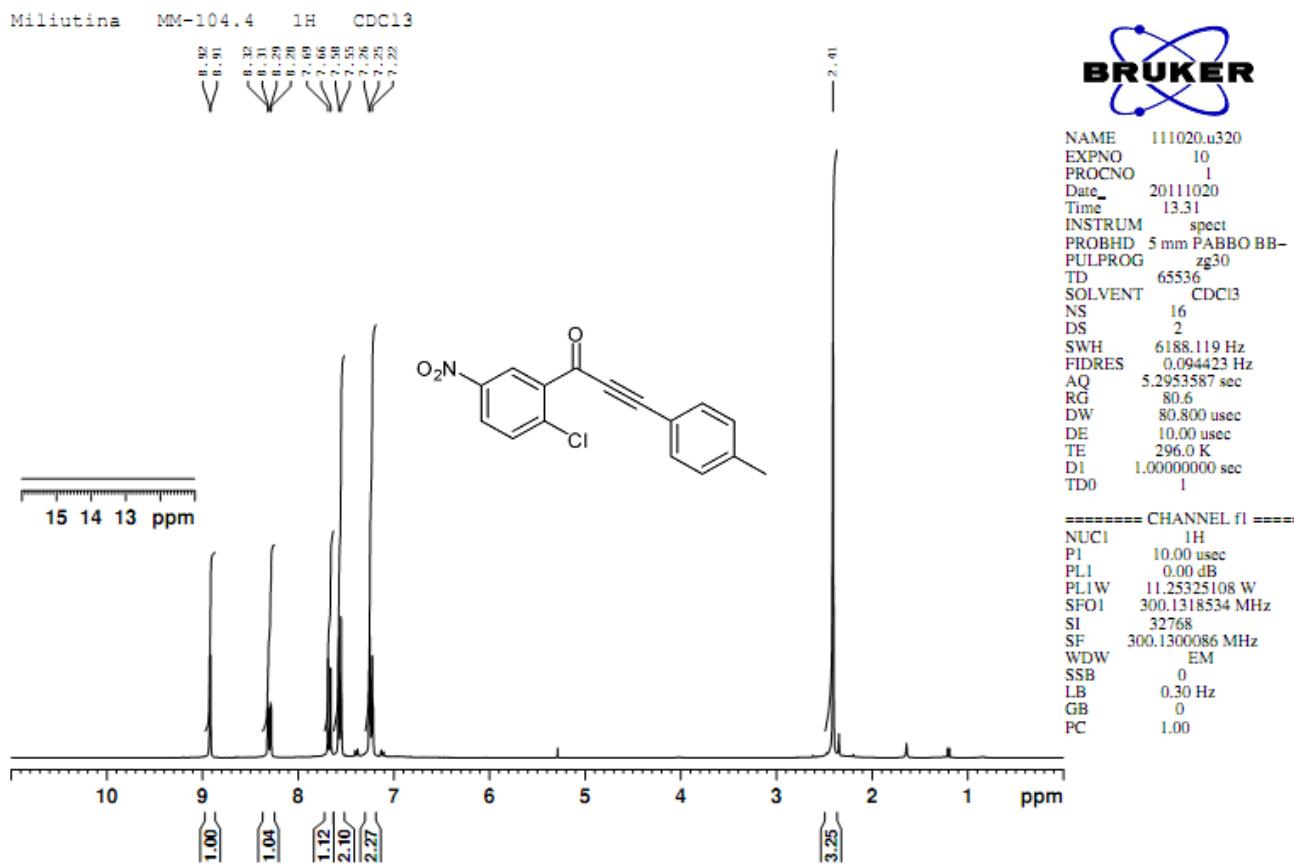
^c National Taras Shevchenko University, 62 Volodymyrska Str., 01033 Kyiv, Ukraine.

^d Leibniz Institut für Katalyse an der Universität Rostock e.V., Albert Einstein Str. 29a, 18059 Rostock, Germany

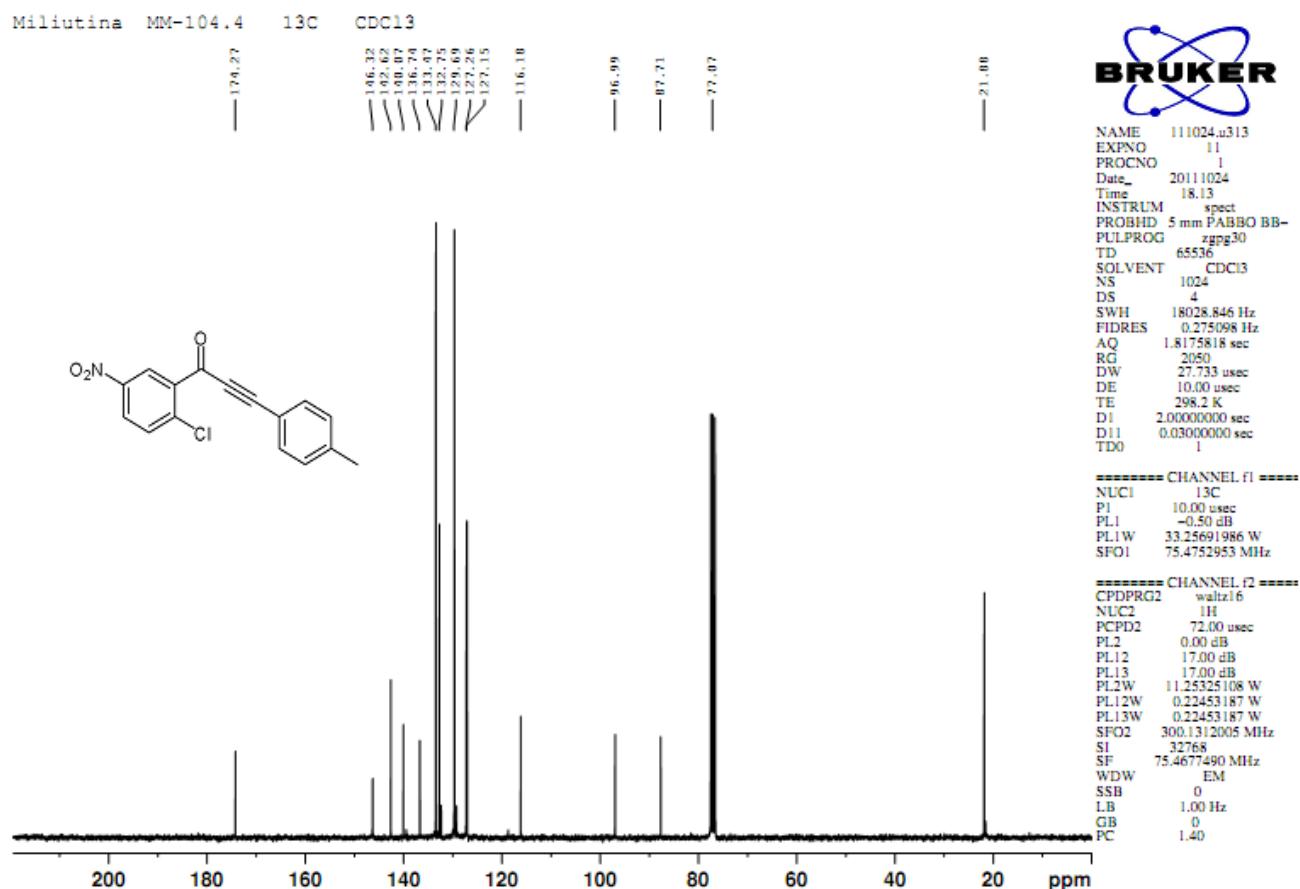
Copies of ¹ H and ¹³ C NMR spectra	1
X-Ray structure of compound 7ab	146
X-Ray structure of compound 7ac.....	147
X-Ray structure of compound 7bd	148
X-Ray structure of compound 15	149
X-Ray structure of compound 16.....	150

Copies of ¹H and ¹³C NMR spectra

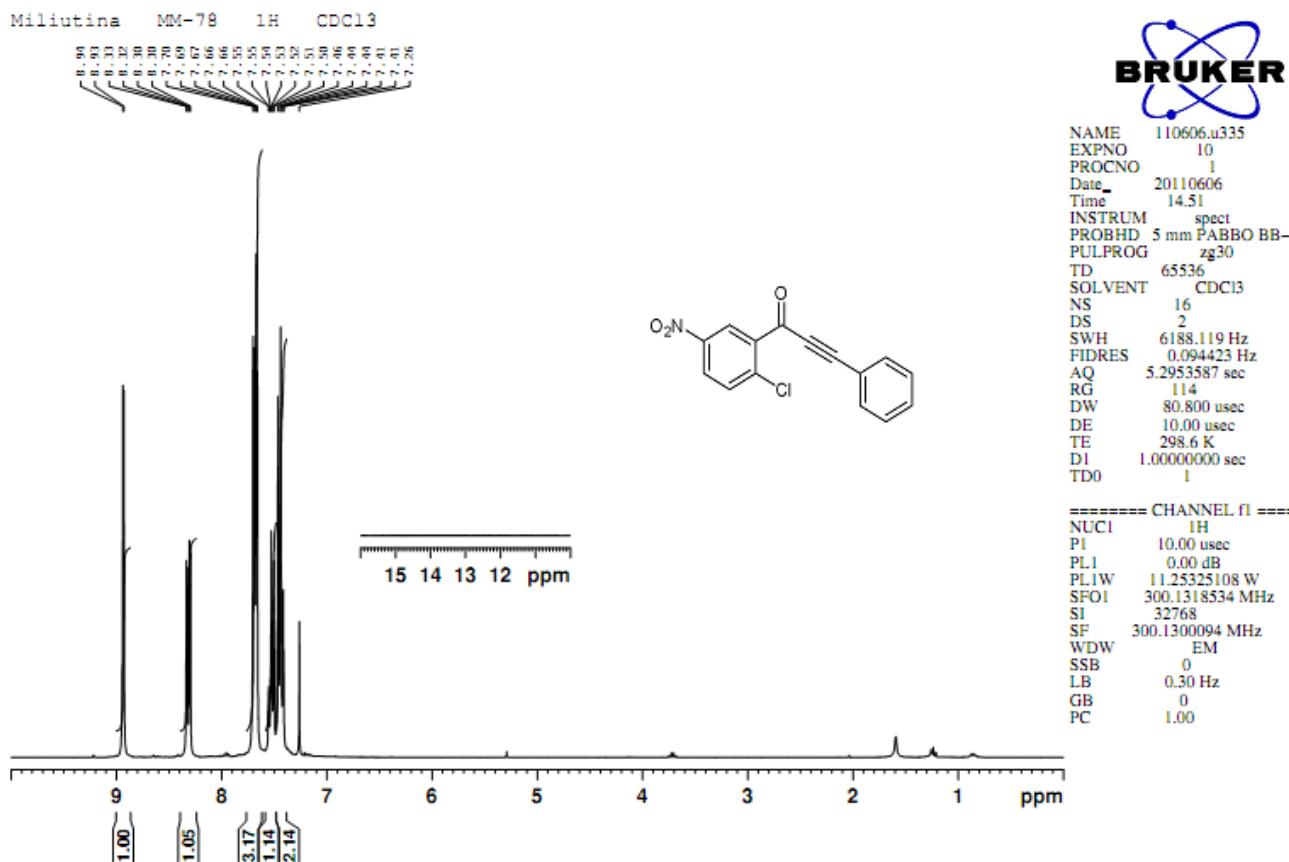
1-(2-Chloro-5-nitrophenyl)-3-p-tolylprop-2-yn-1-one (6a).



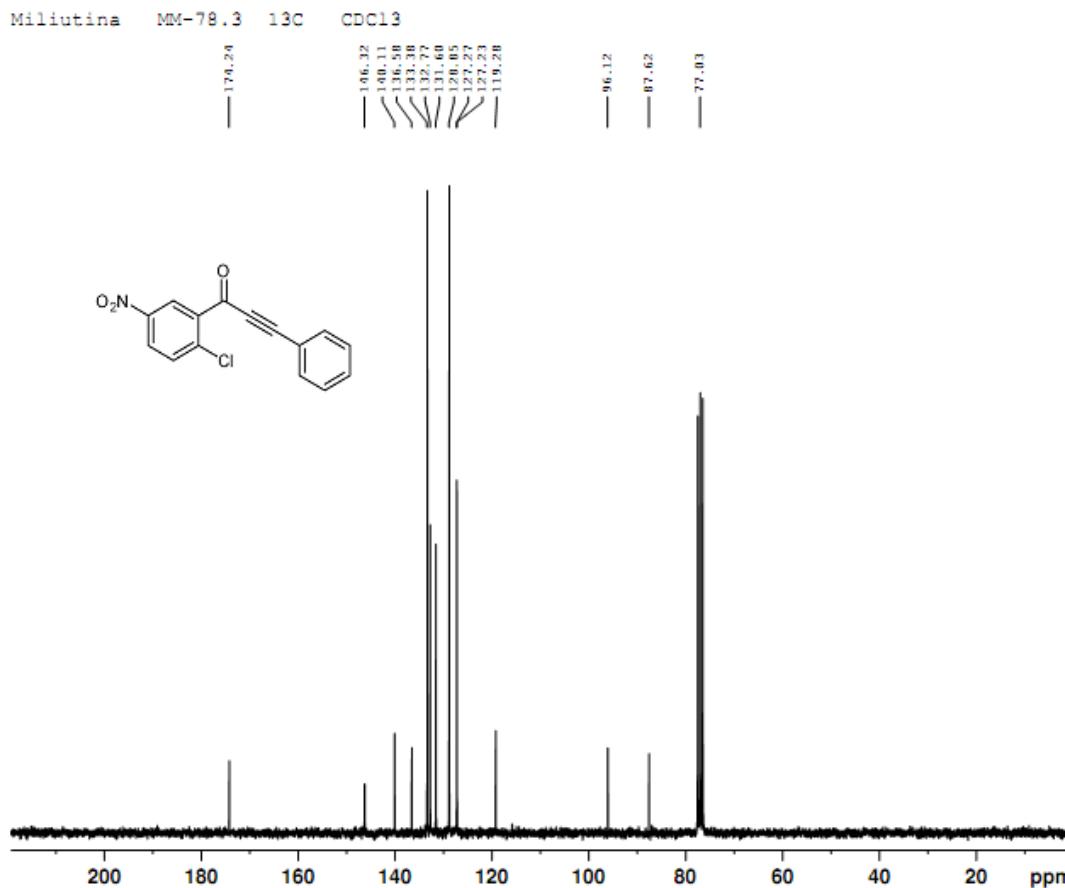
1-(2-Chloro-5-nitrophenyl)-3-p-tolylprop-2-yn-1-one (6a).



1-(2-Chloro-5-nitrophenyl)-3-phenylprop-2-yn-1-one (6b).



1-(2-Chloro-5-nitrophenyl)-3-phenylprop-2-yn-1-one (6b).



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SFO1 62.9015280 MHz

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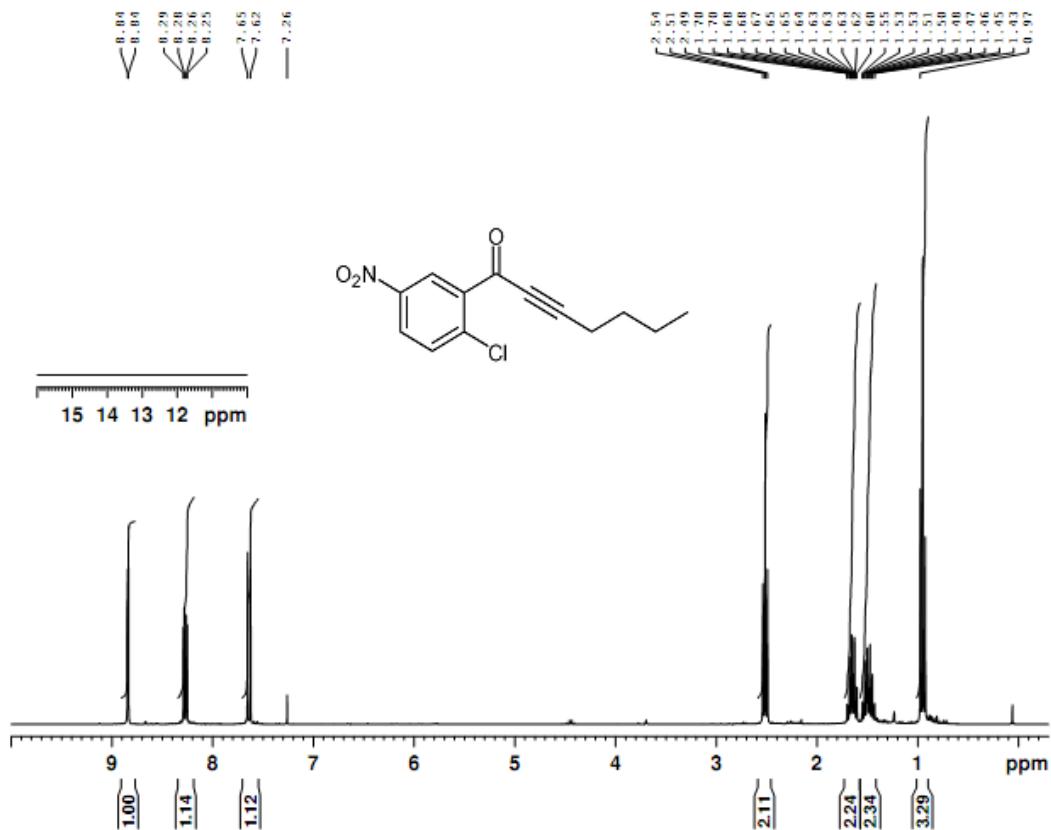
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PC 1.40

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1-(2-chloro-5-nitrophenyl)hept-2-yne-1-one (6c).

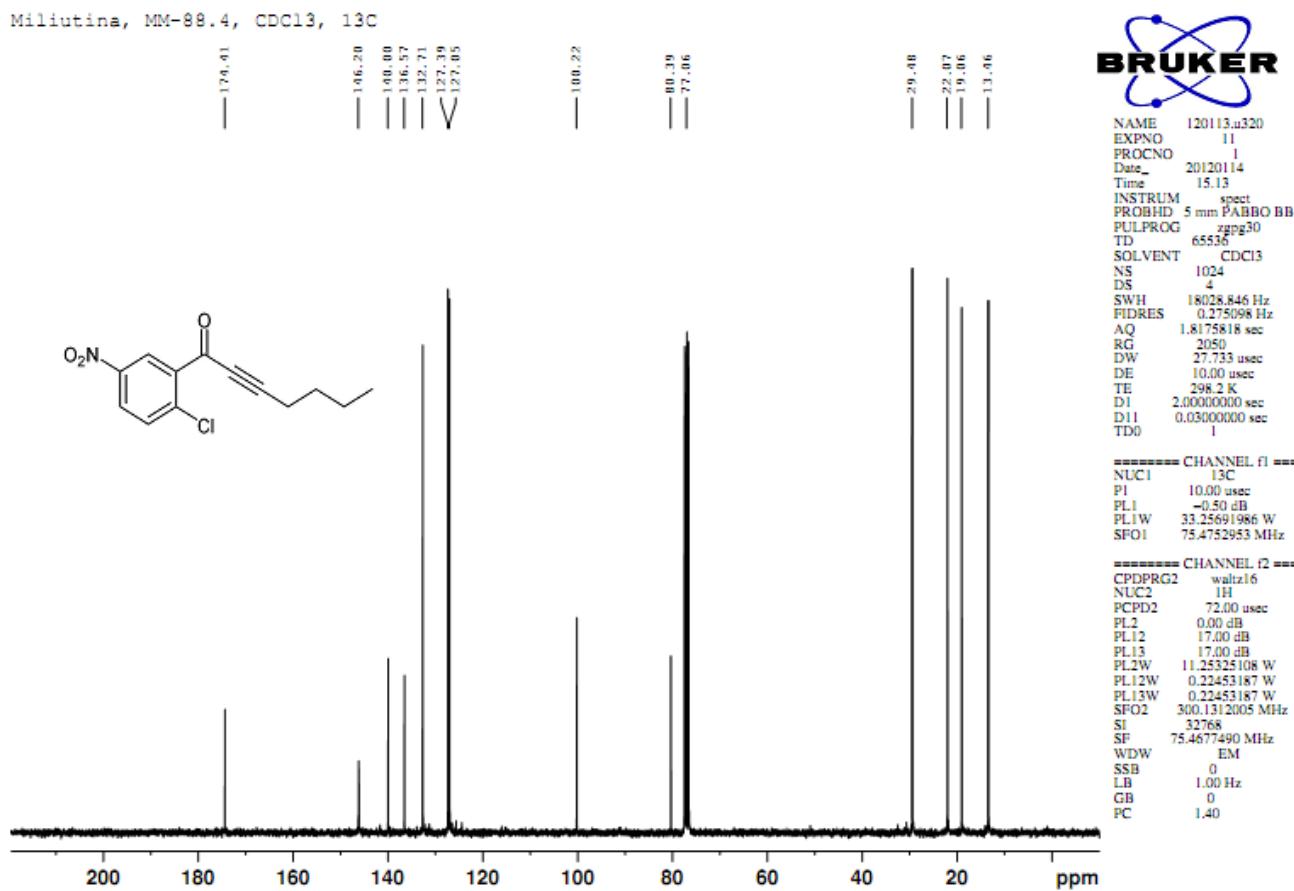
Miliutina, MM-88.4, CDCl₃, 1H



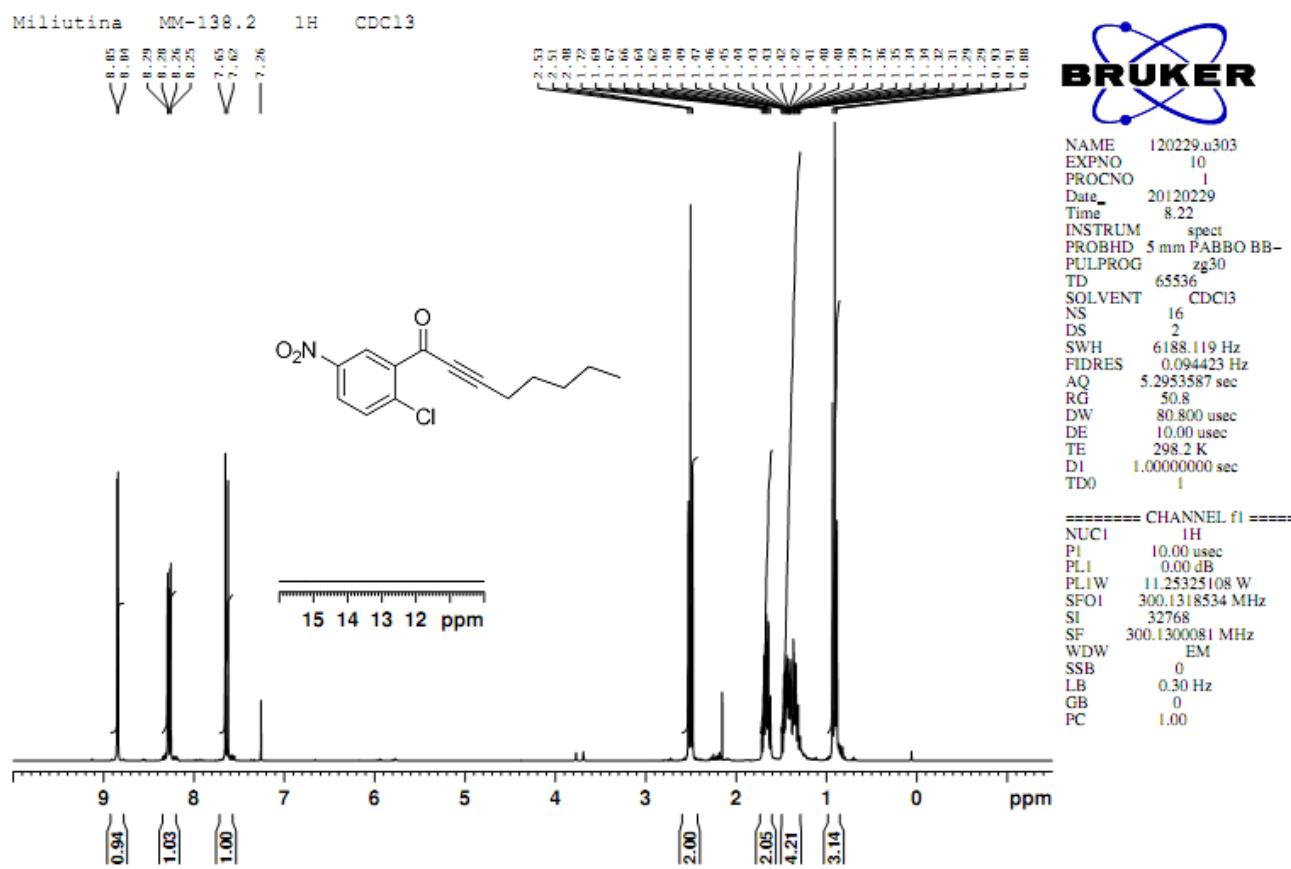
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 RG 50.8
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 DE 10.00 usec
 TE 298.2 K
 DI 1.0000000 sec
 TD0 1

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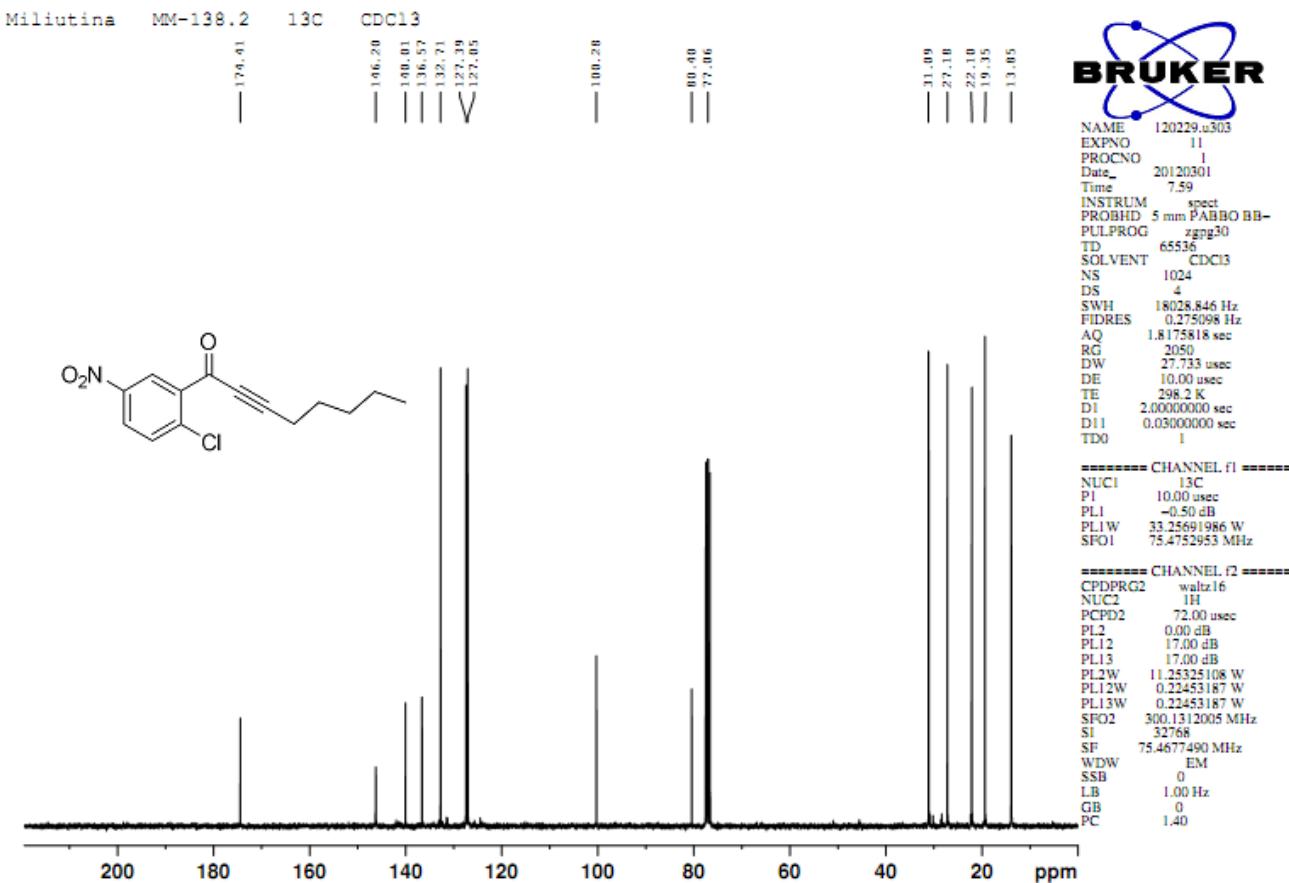
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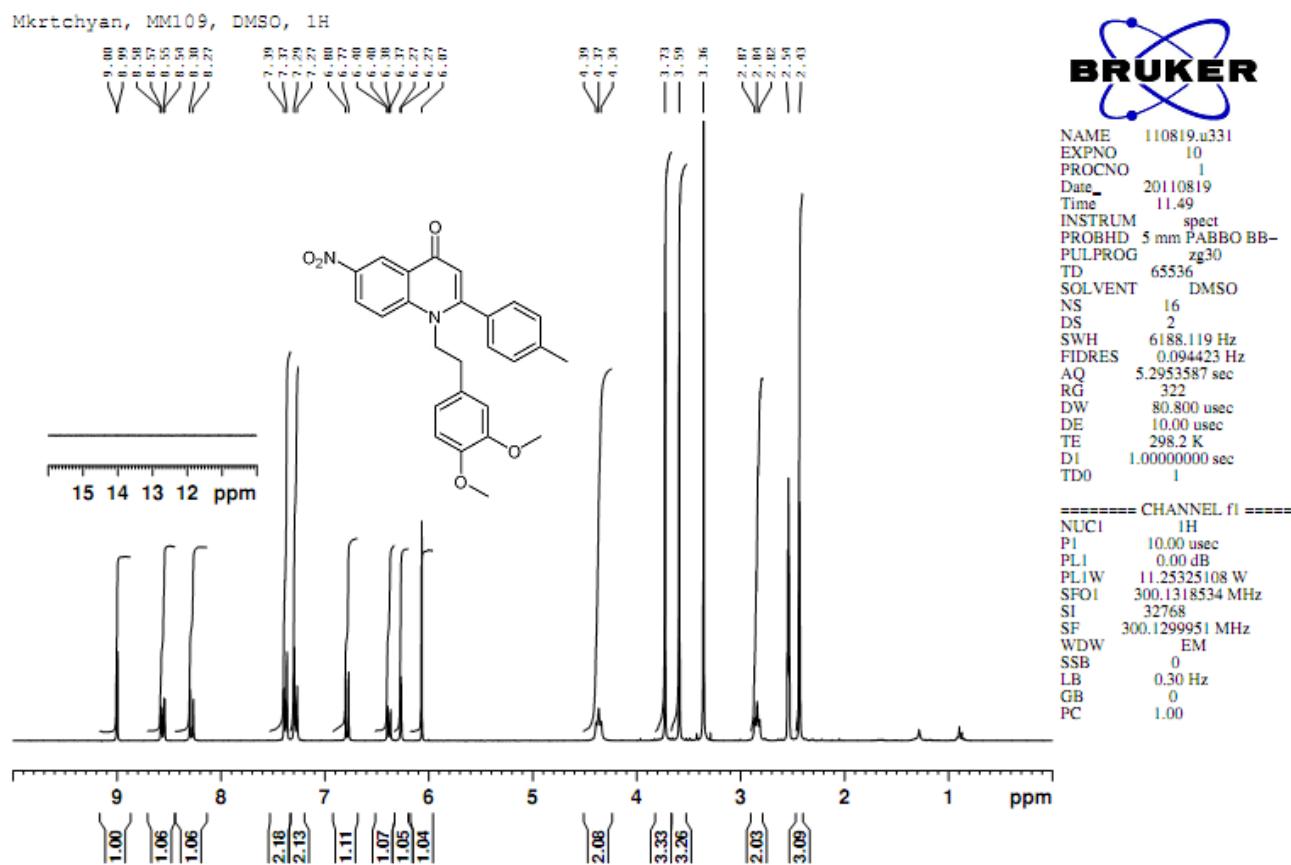
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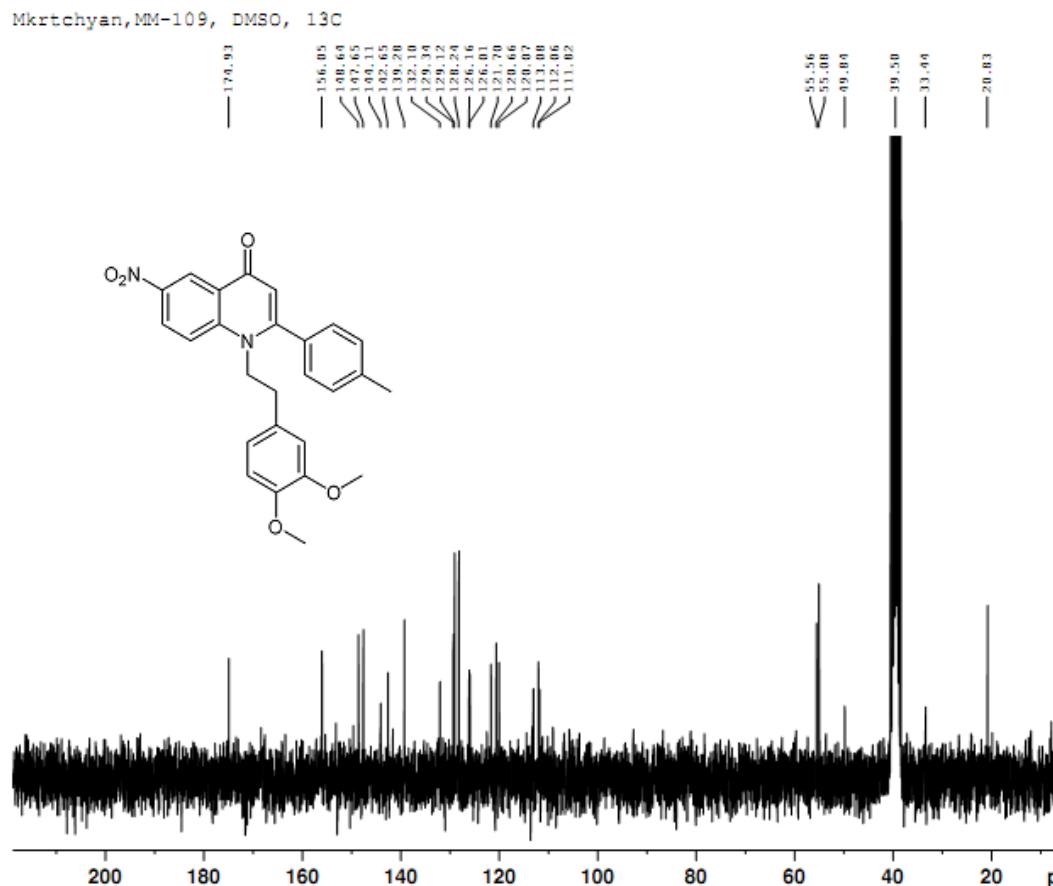
1-(2-chloro-5-nitrophenyl)oct-2-yn-1-one (6d).



1-(3,4-Dimethoxyphenethyl)-6-nitro-2-*p*-tolylquinolin-4(1*H*)-one (7aa).



1-(3,4-Dimethoxyphenethyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7aa).



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RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.4 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

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P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

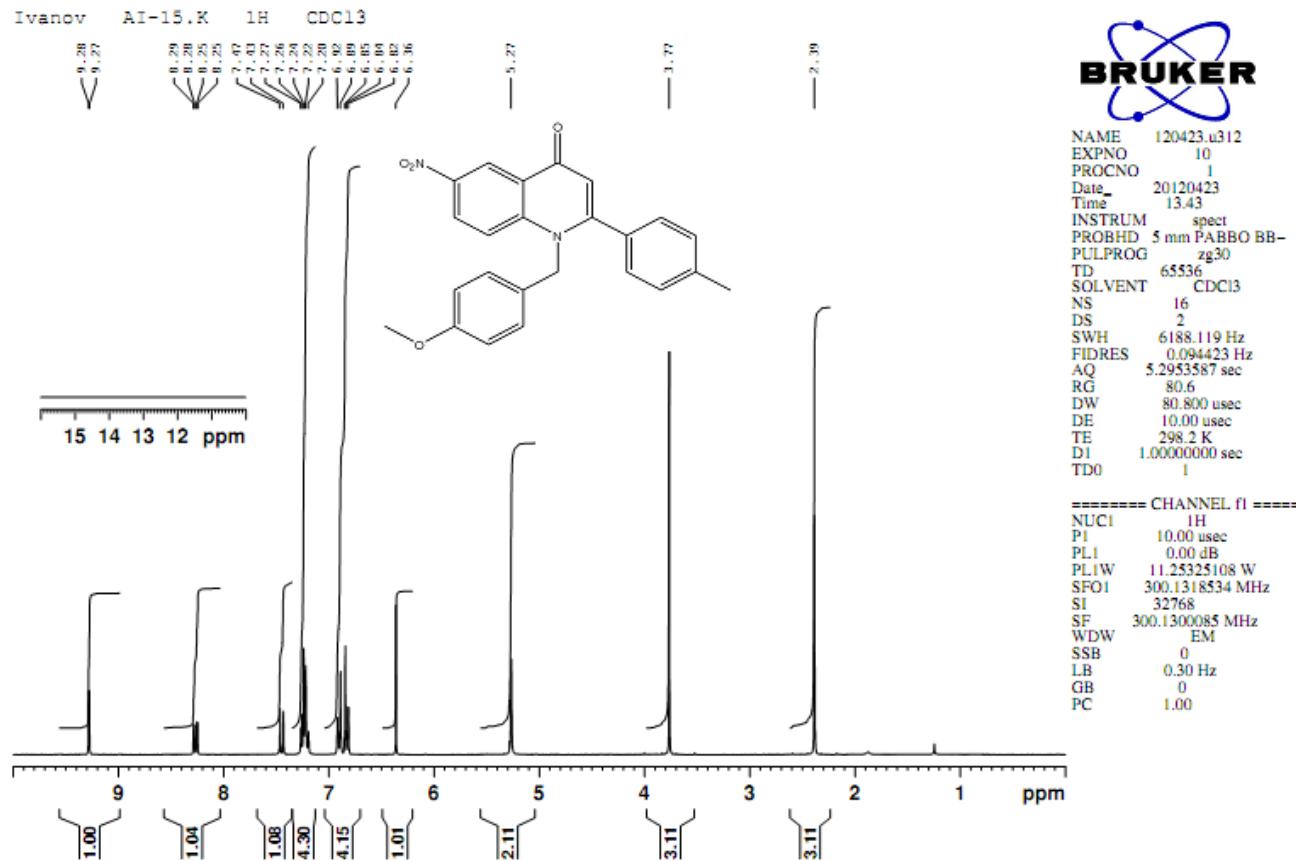
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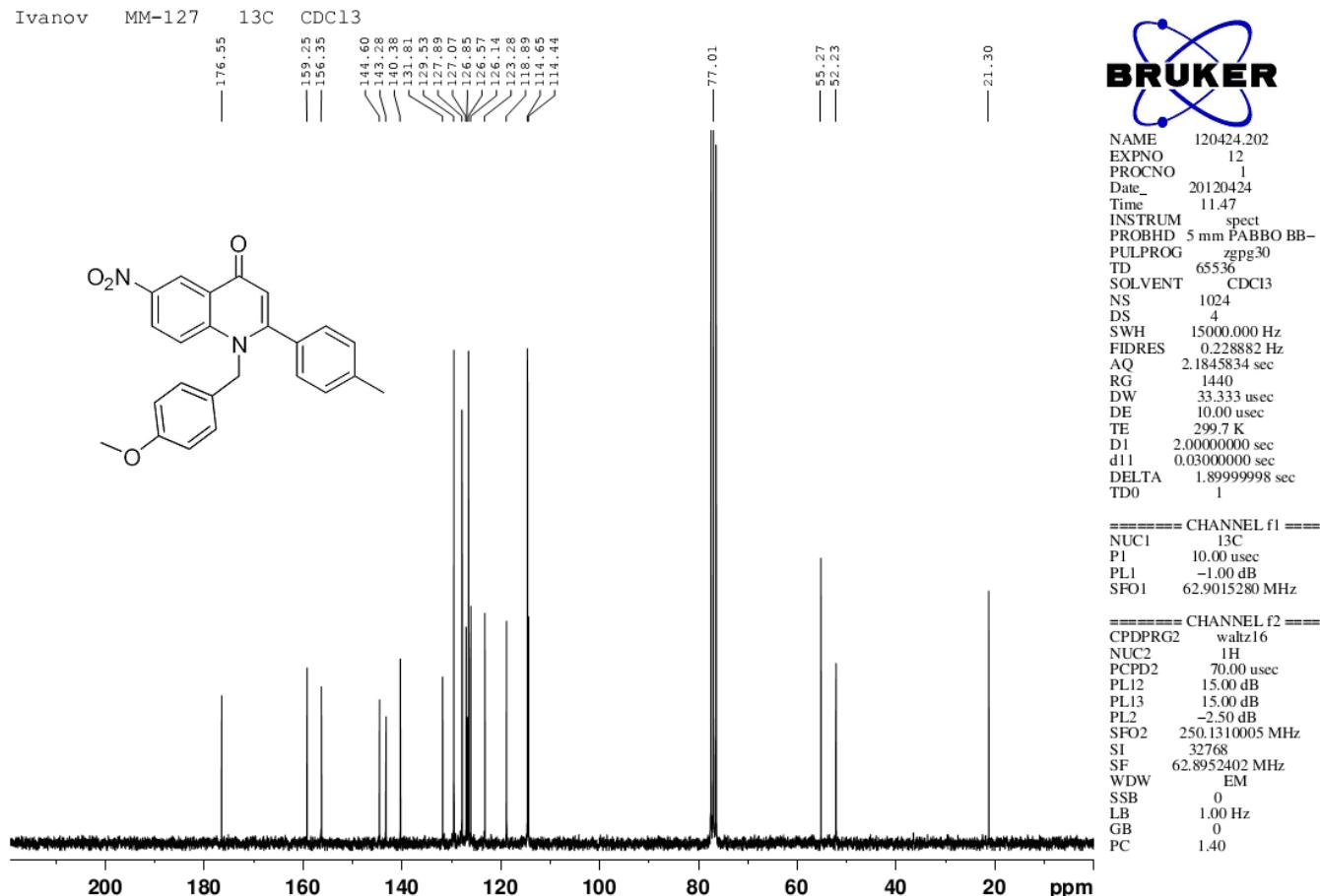
===== CHANNEL f2 ====
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NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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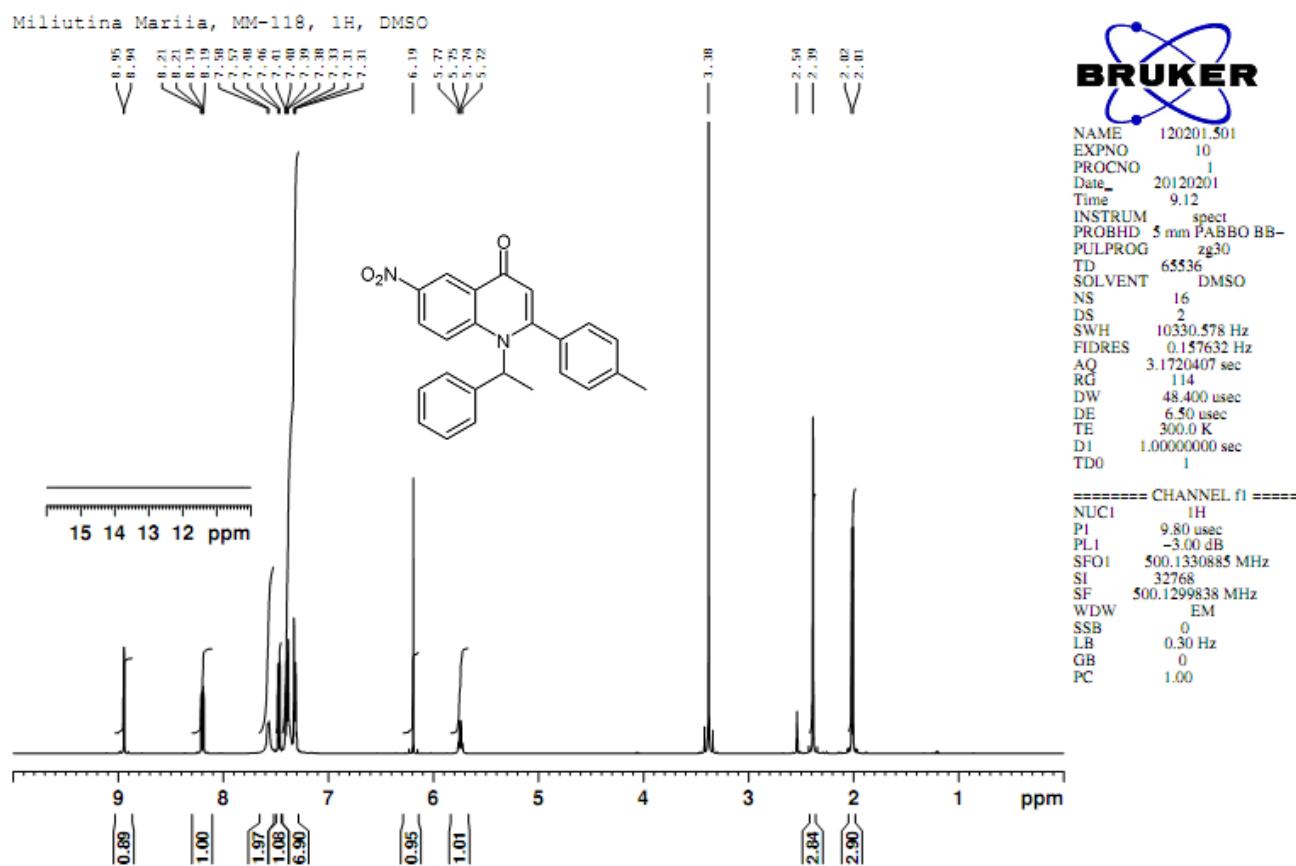
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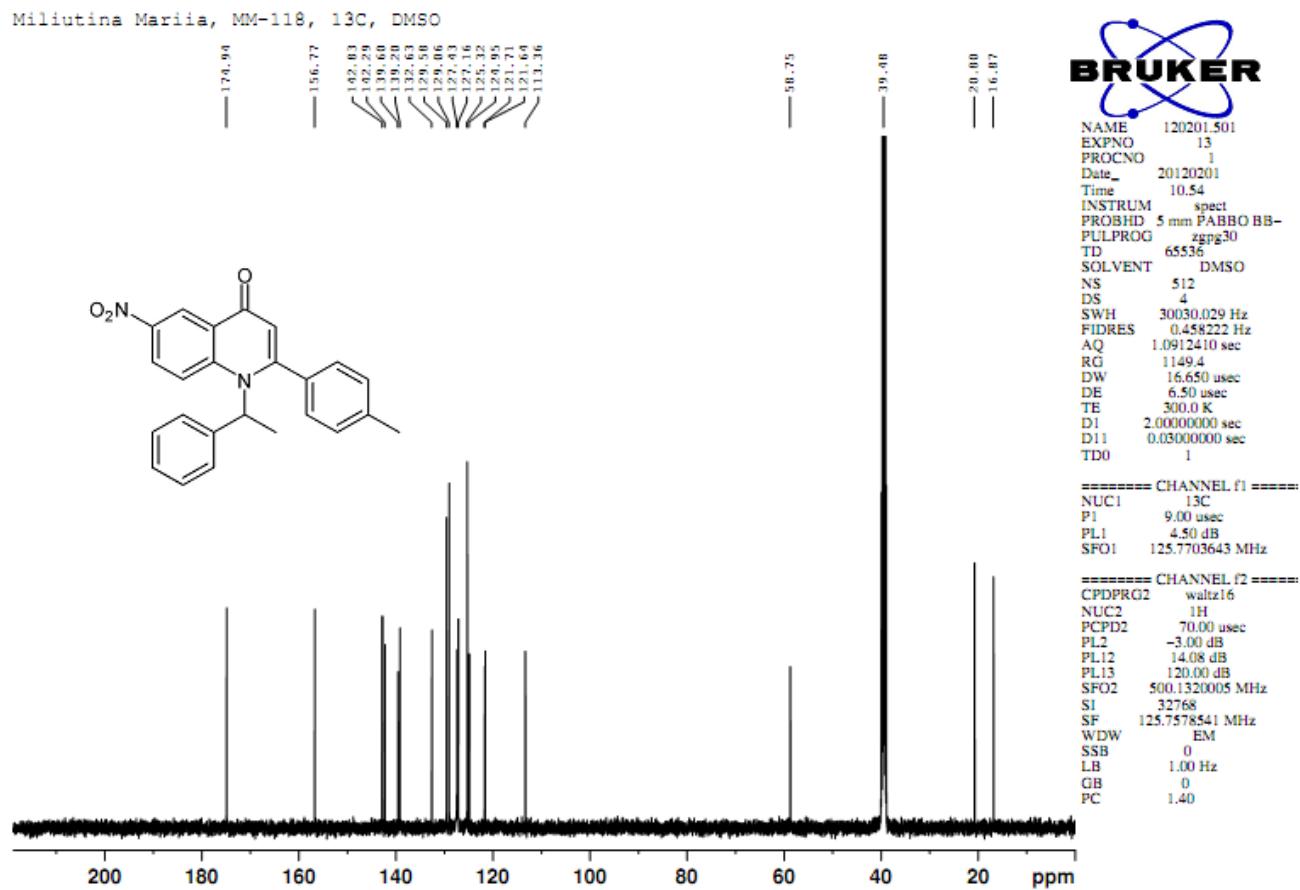
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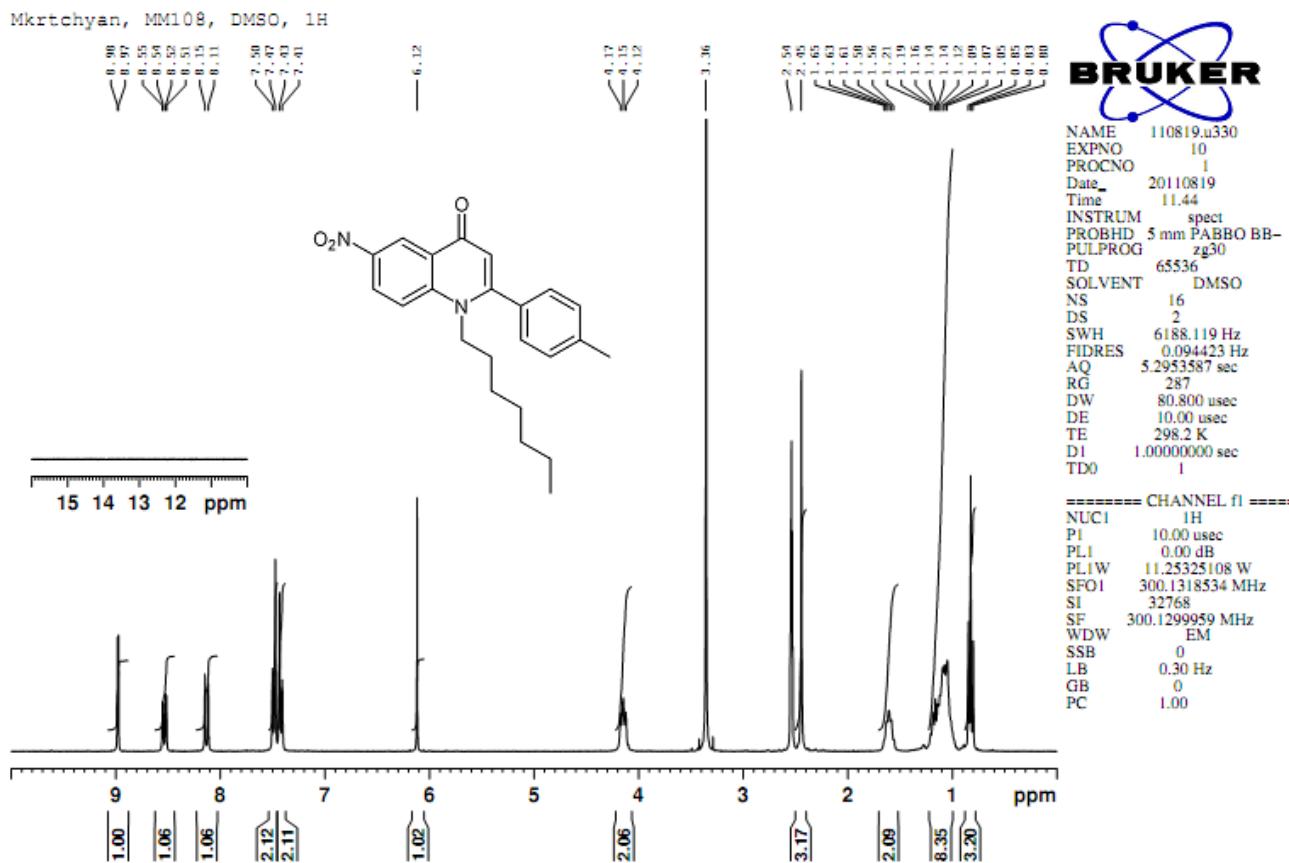
(R)-6-Nitro-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (7ac).



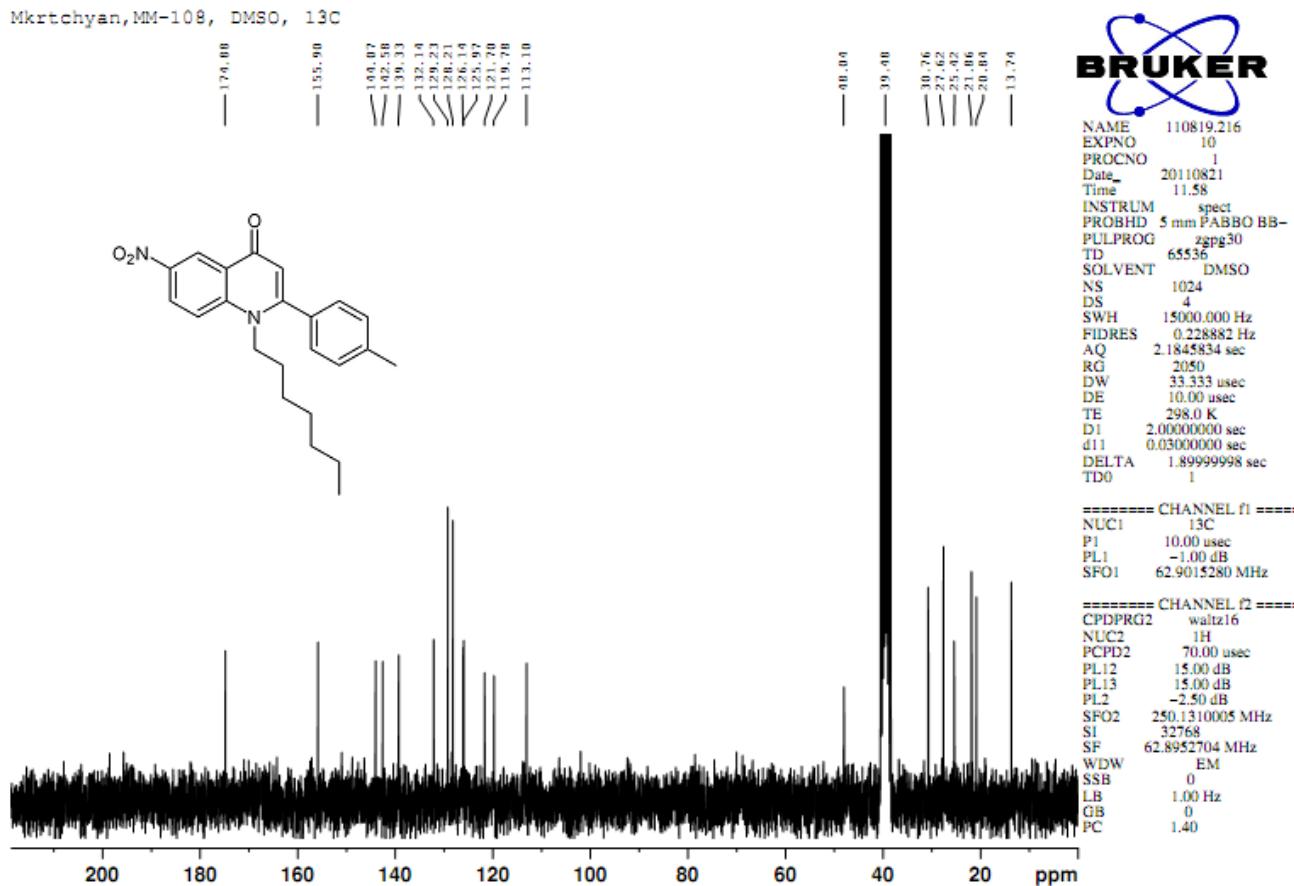
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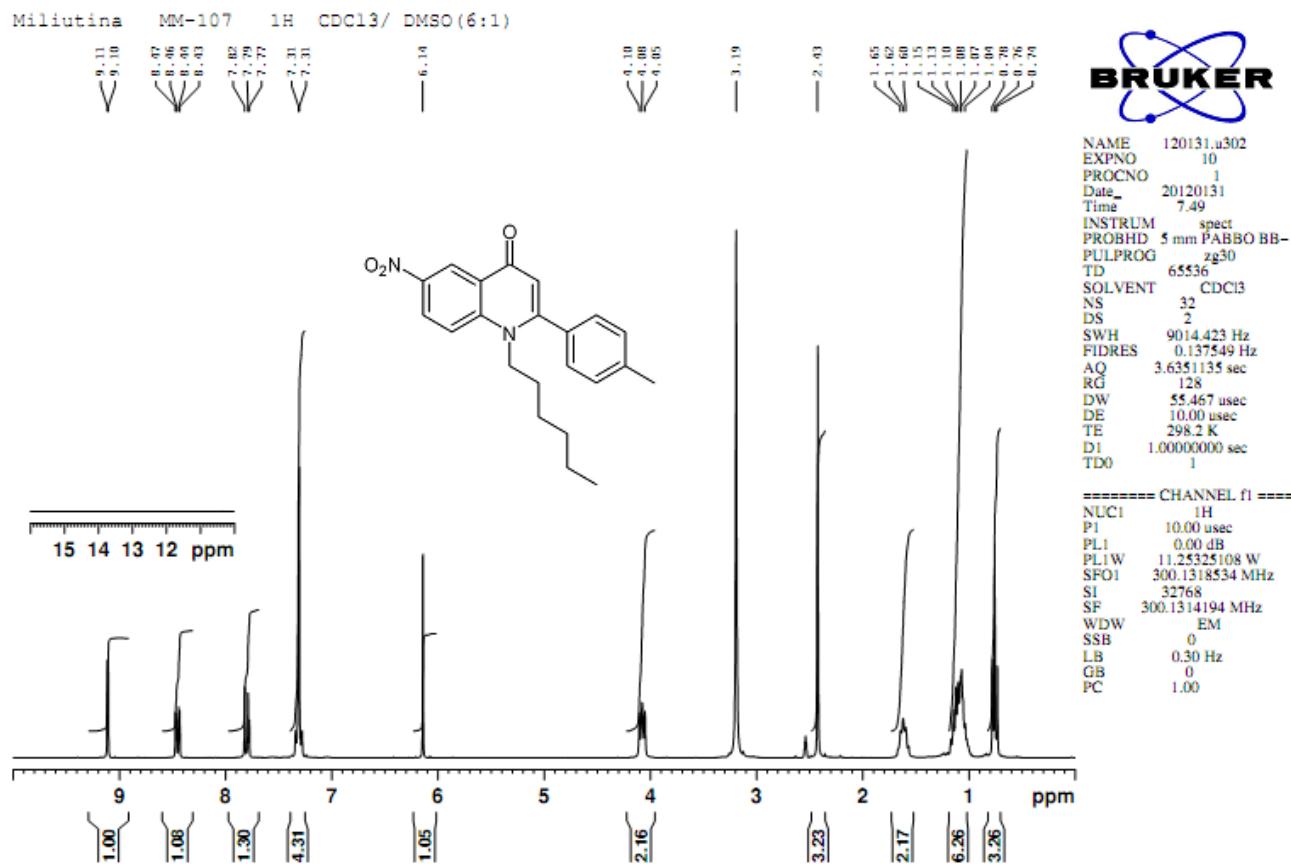
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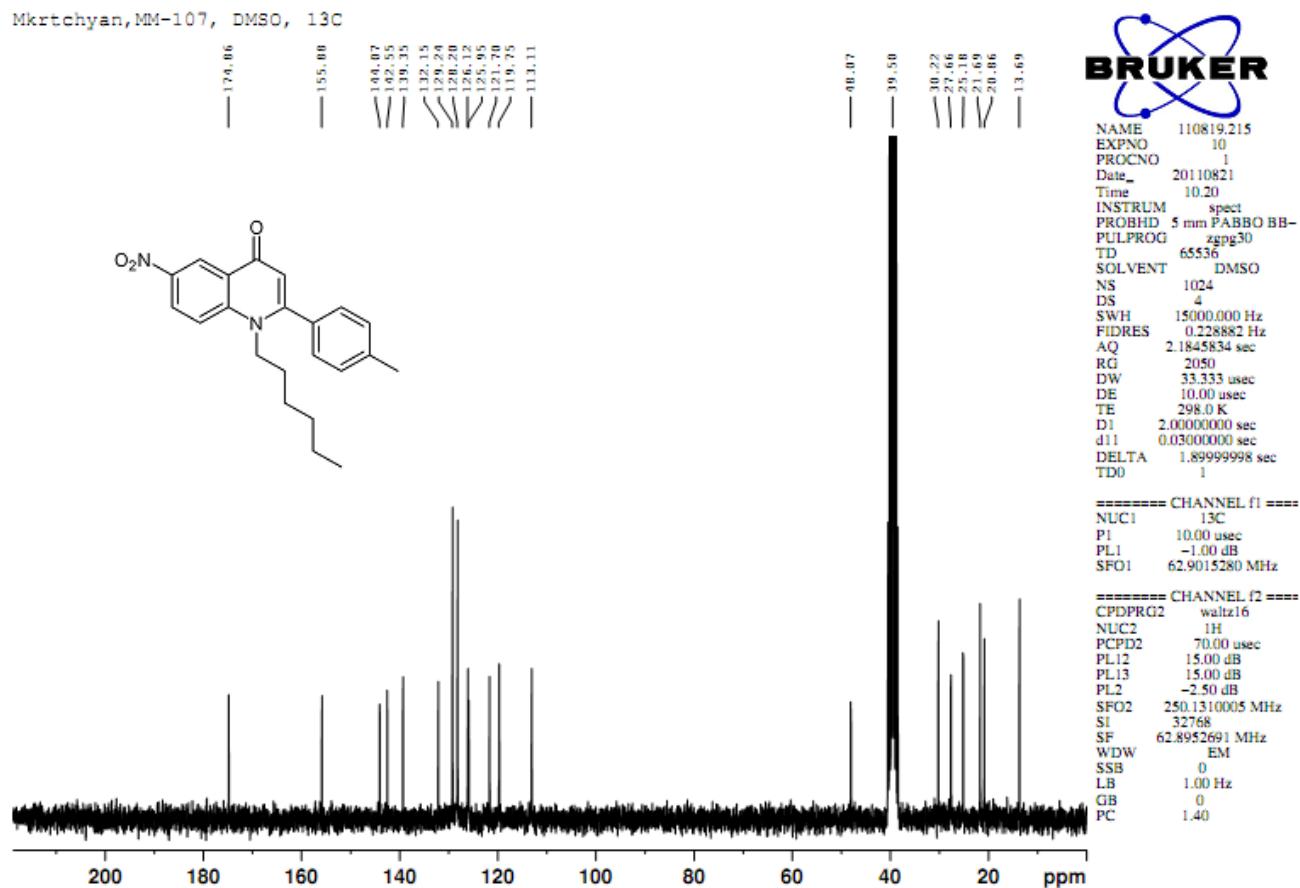
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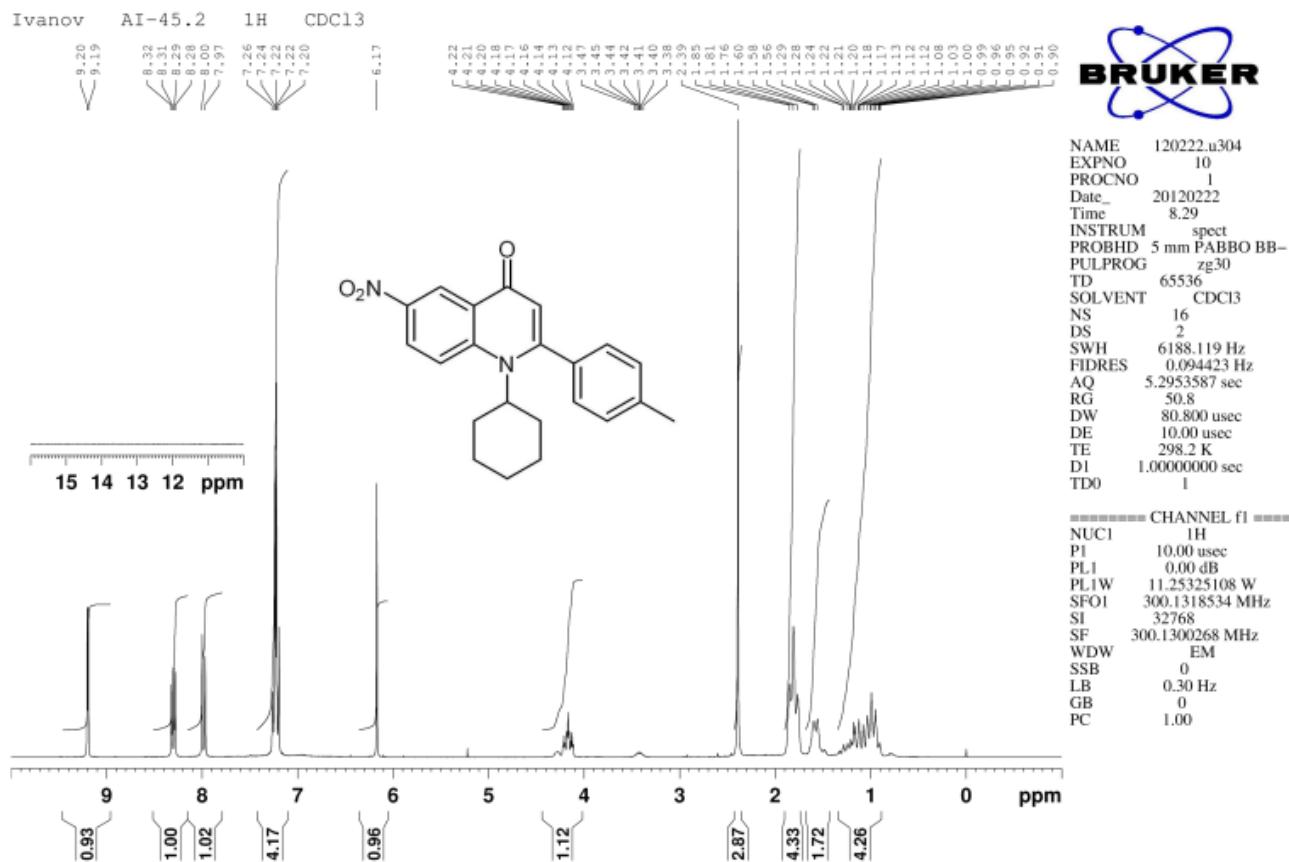
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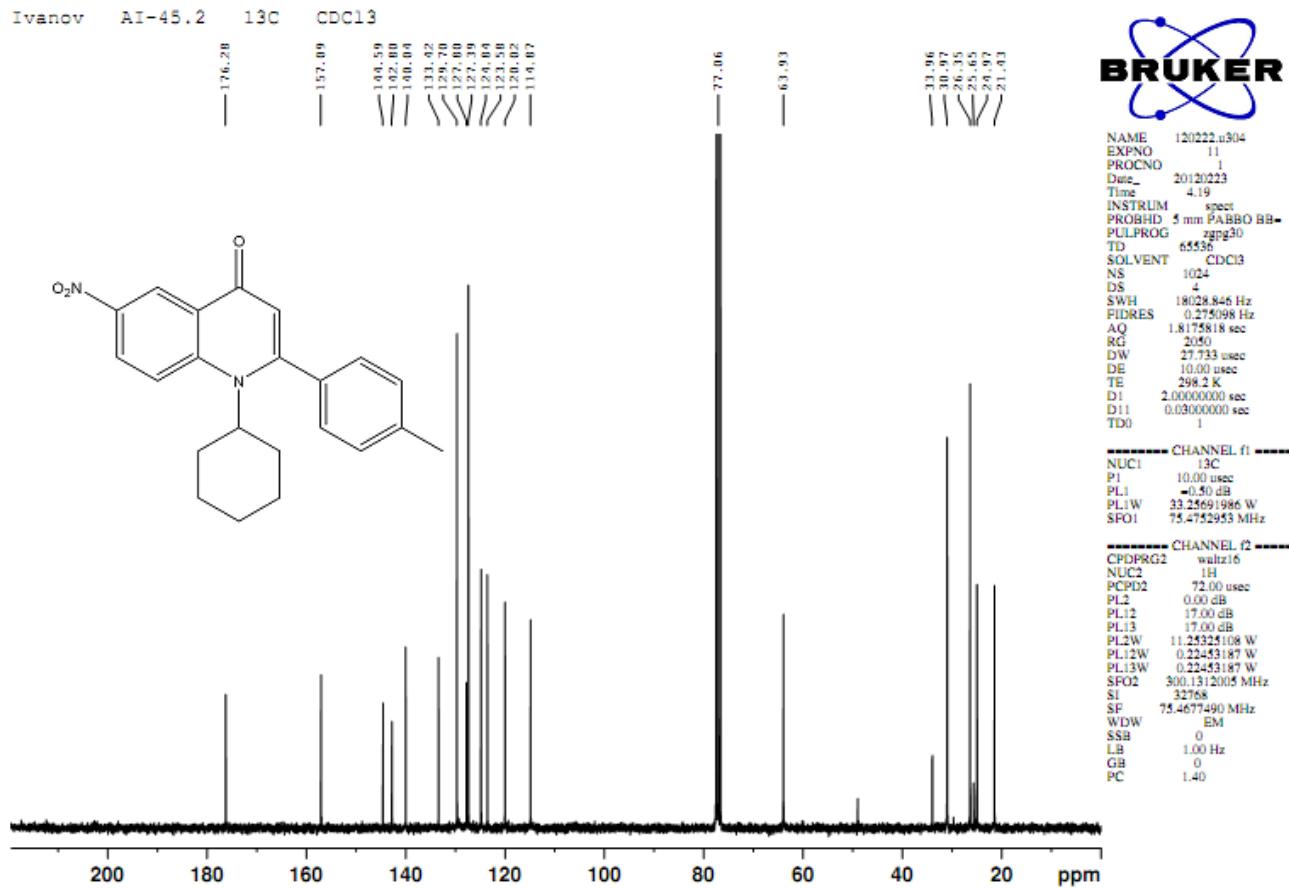
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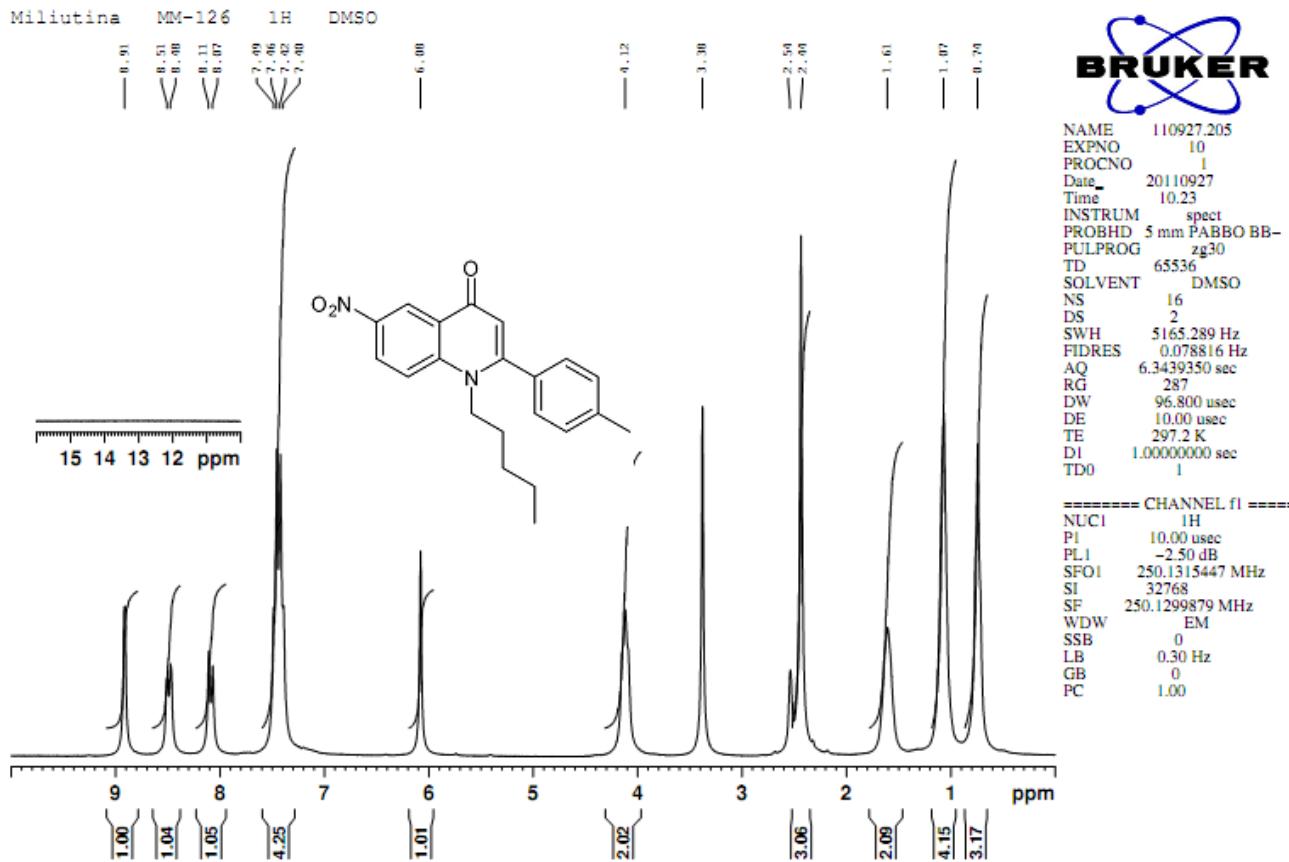
6-Nitro-1-cyclohexyl-2-p-tolyl-4-quinolone (7af).



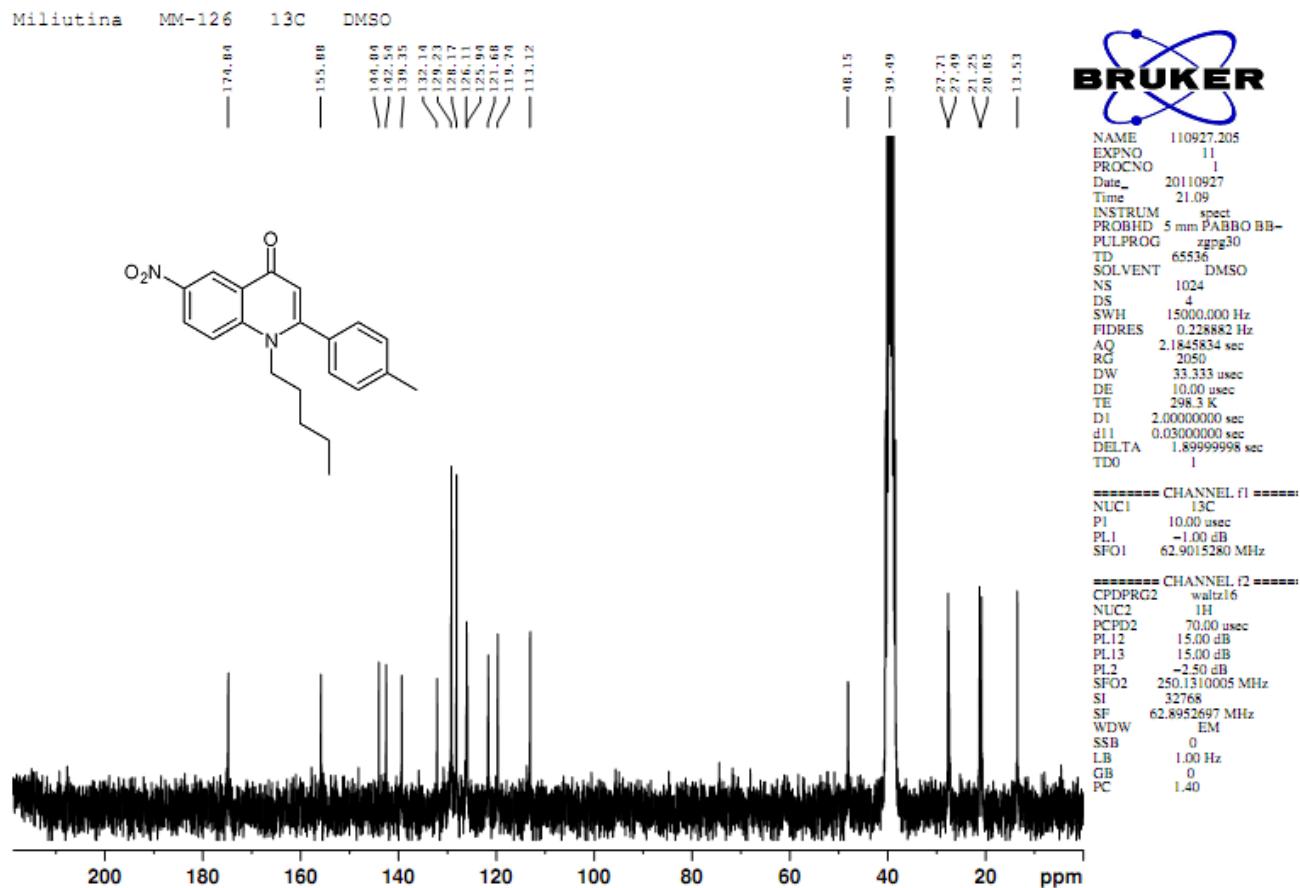
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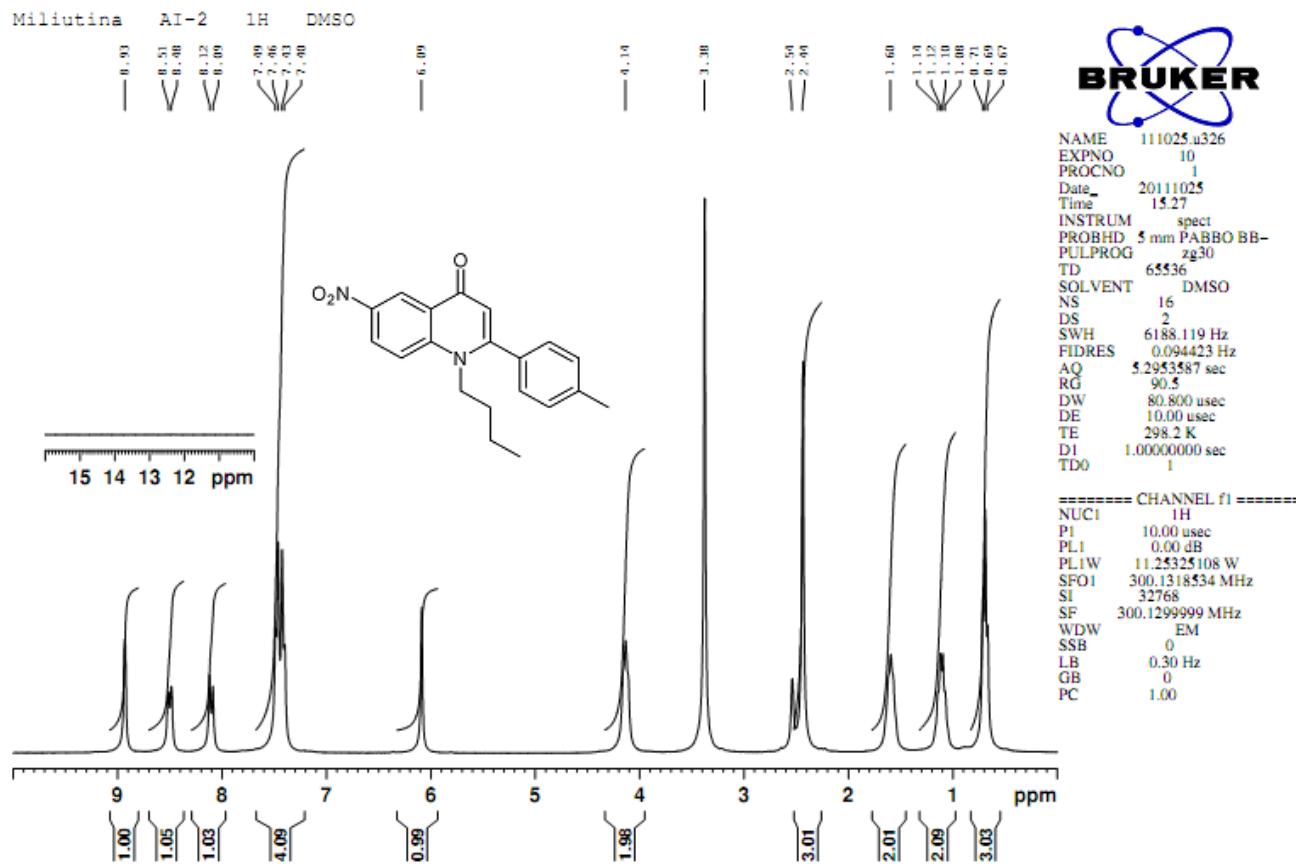
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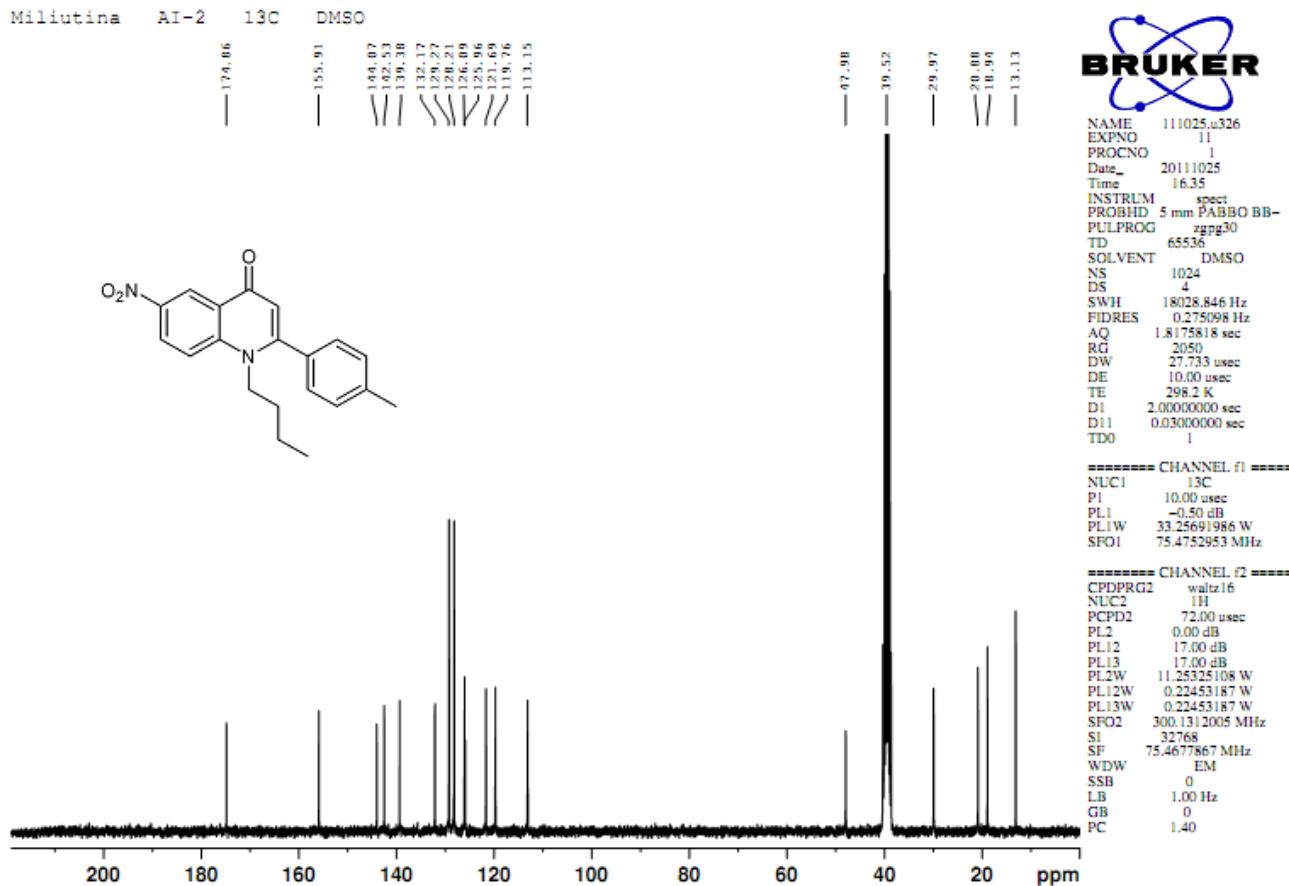
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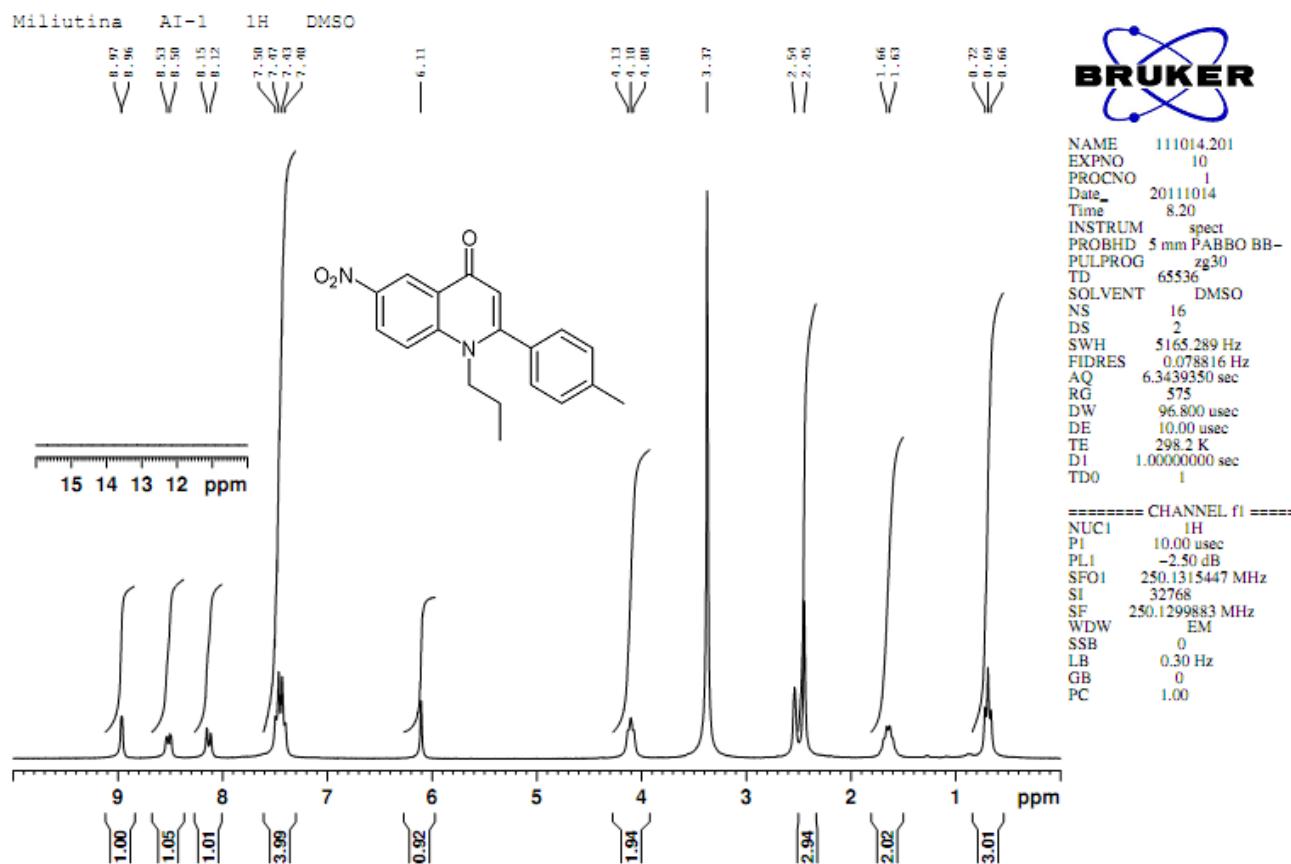
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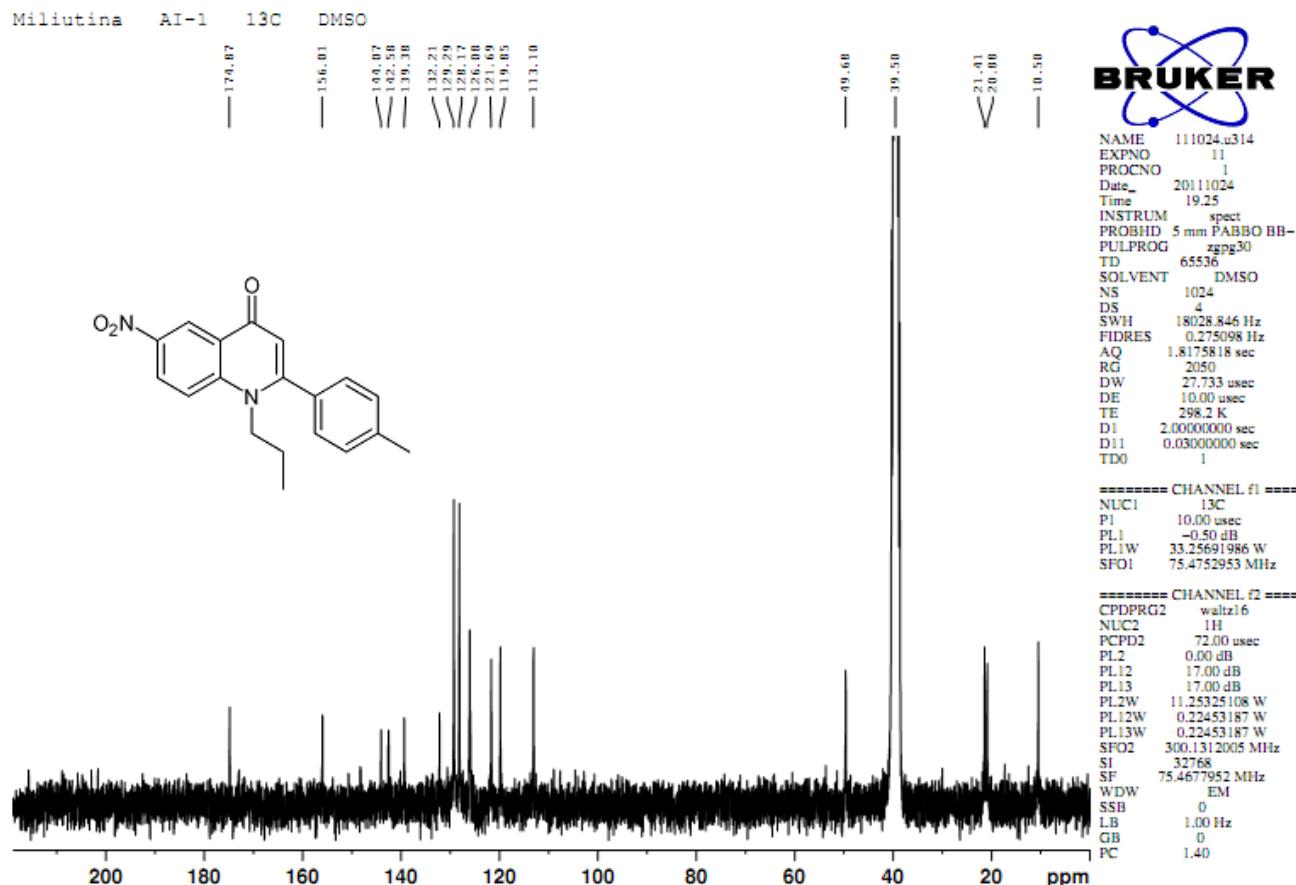
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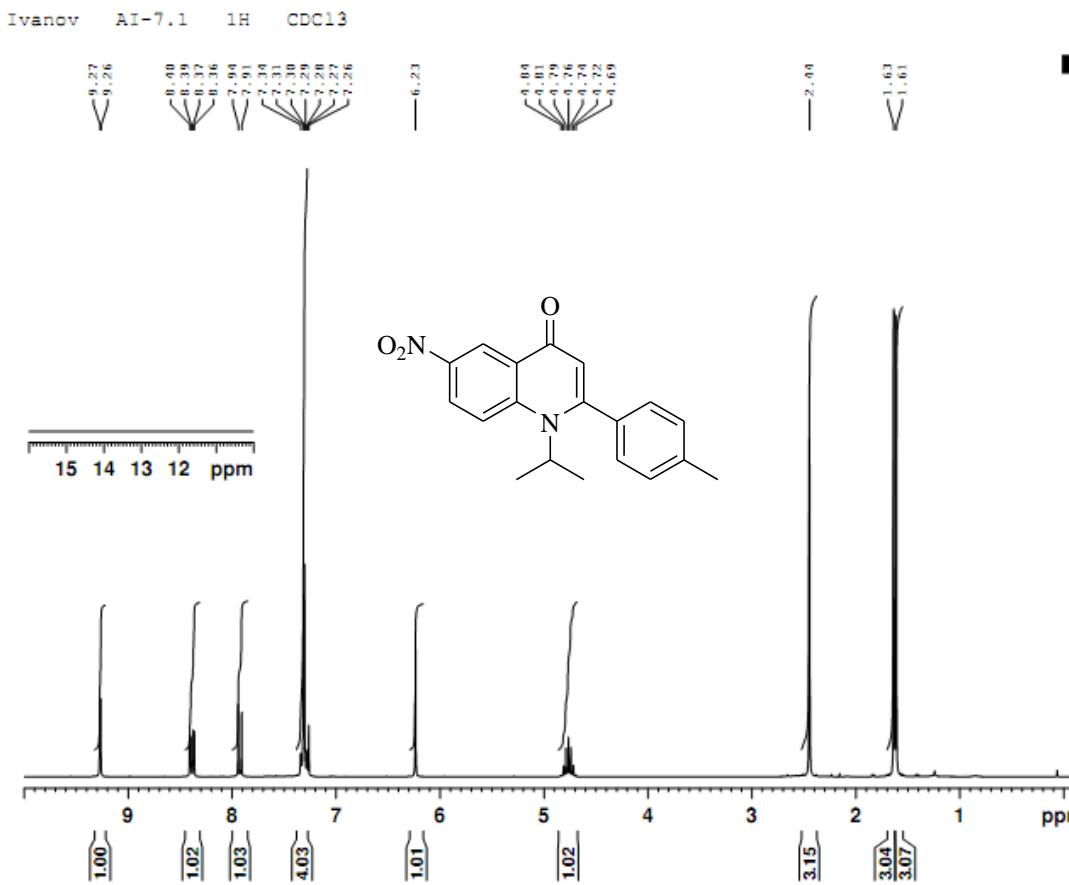
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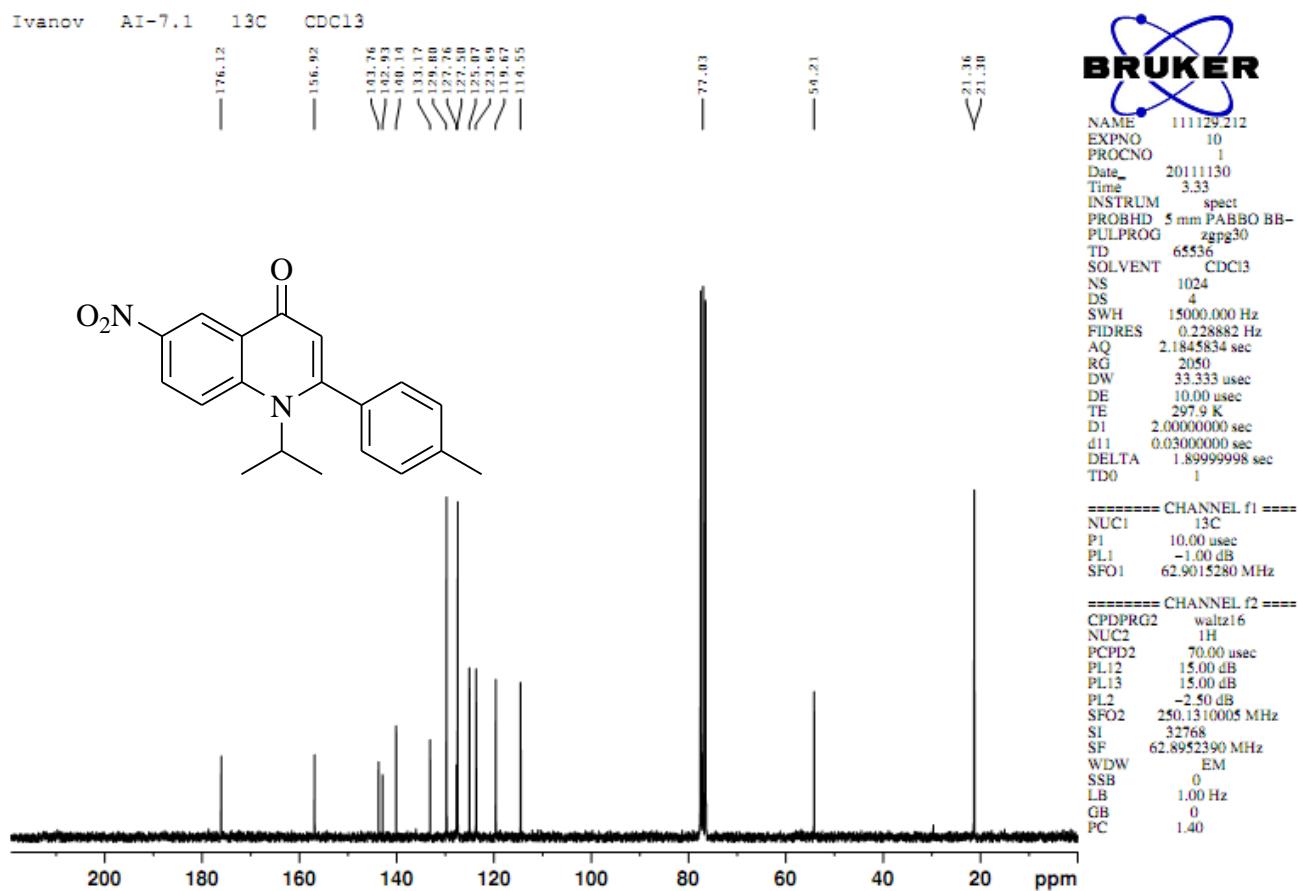
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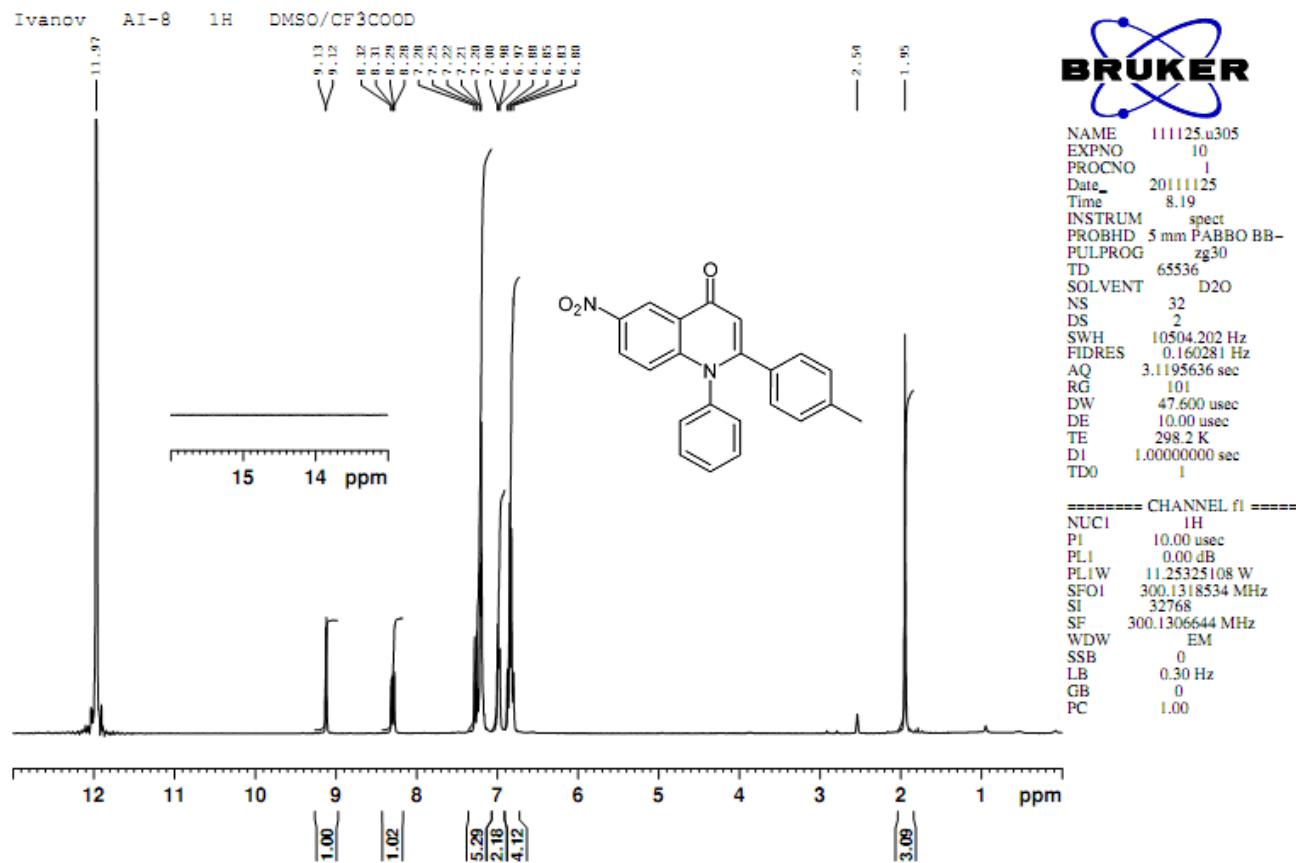
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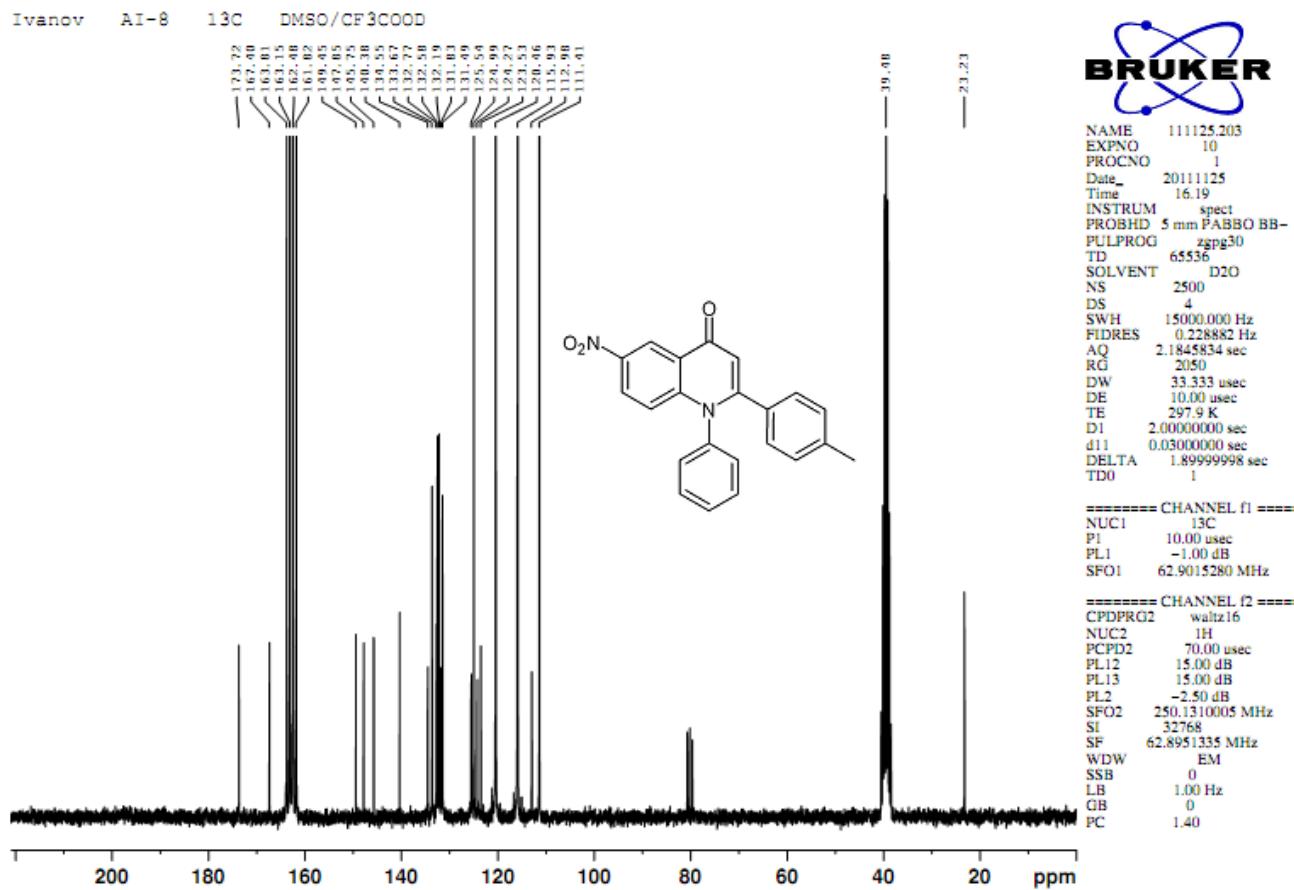
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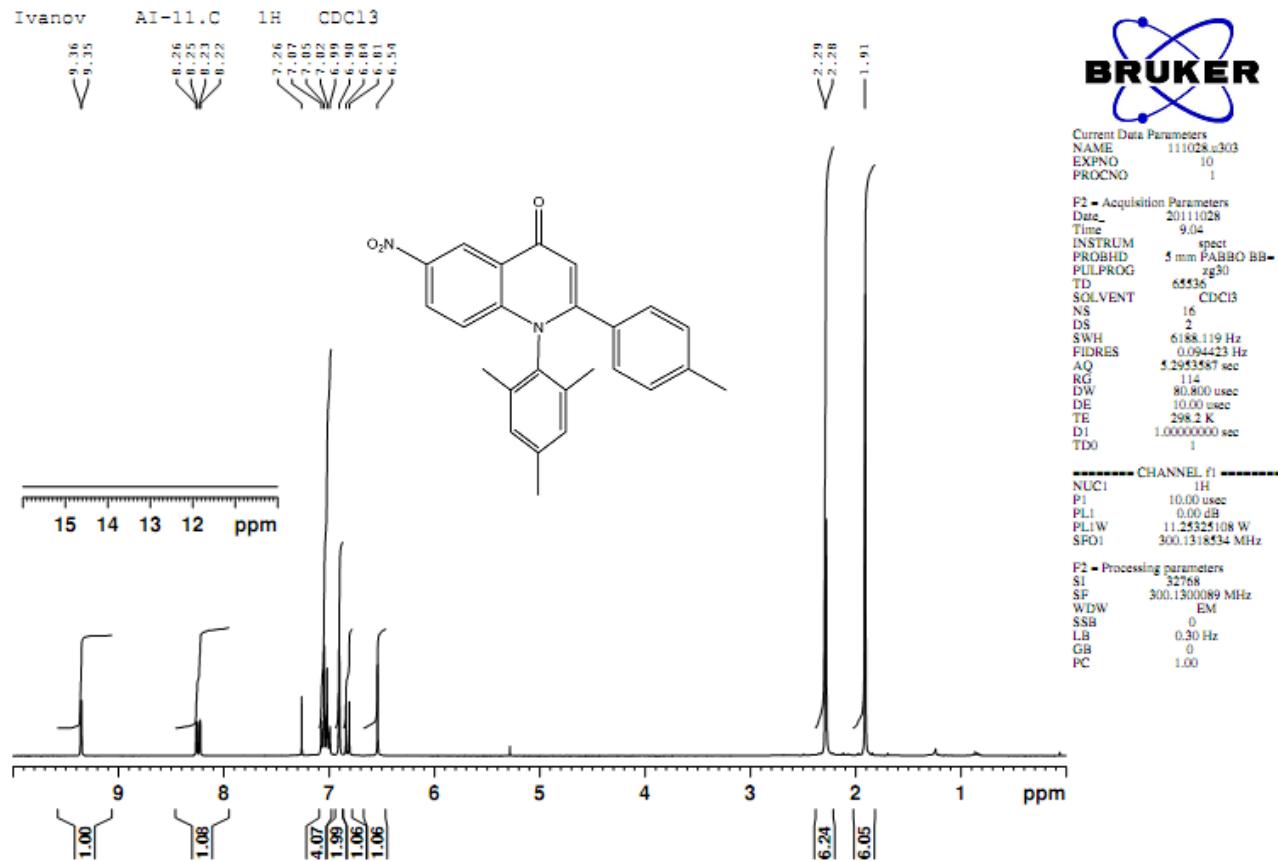
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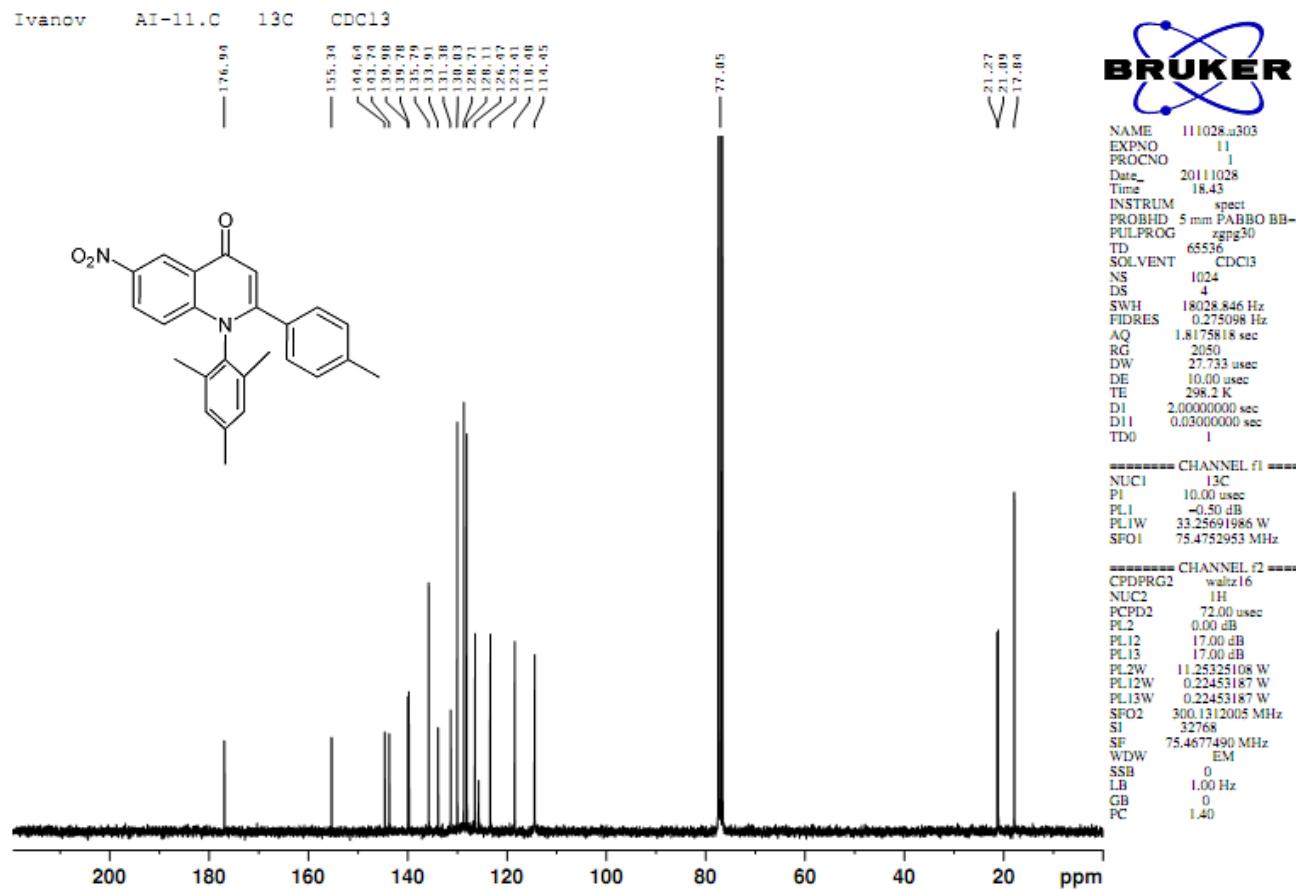
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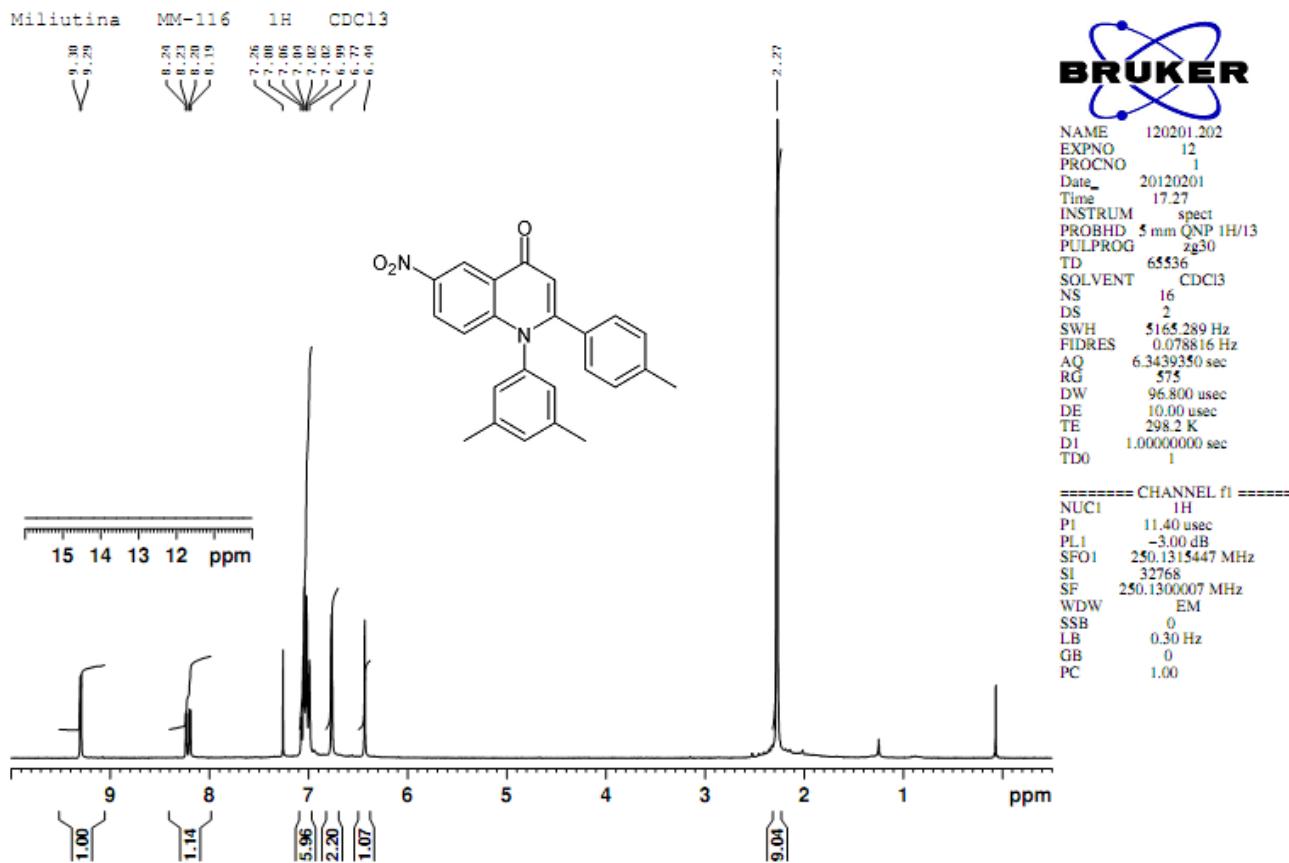
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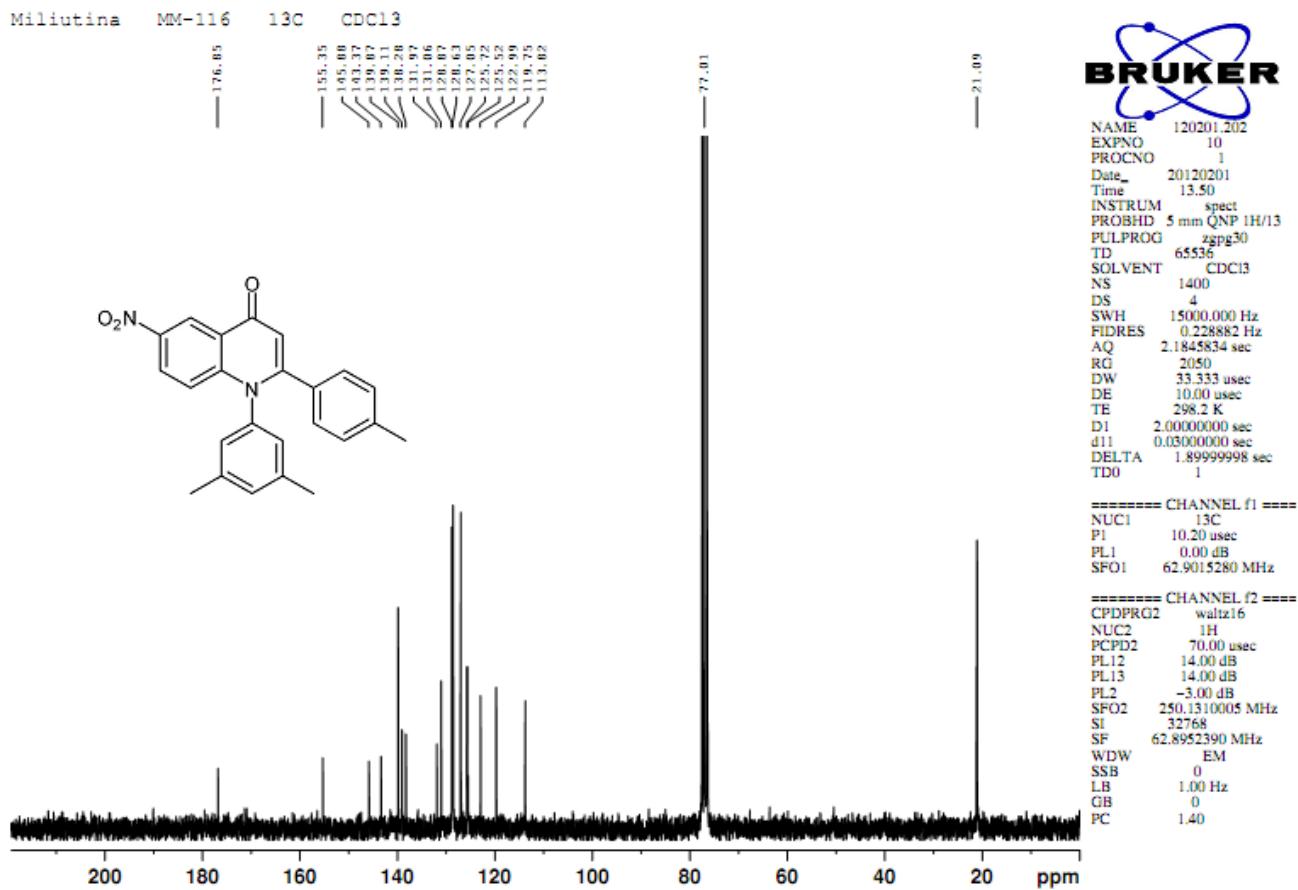
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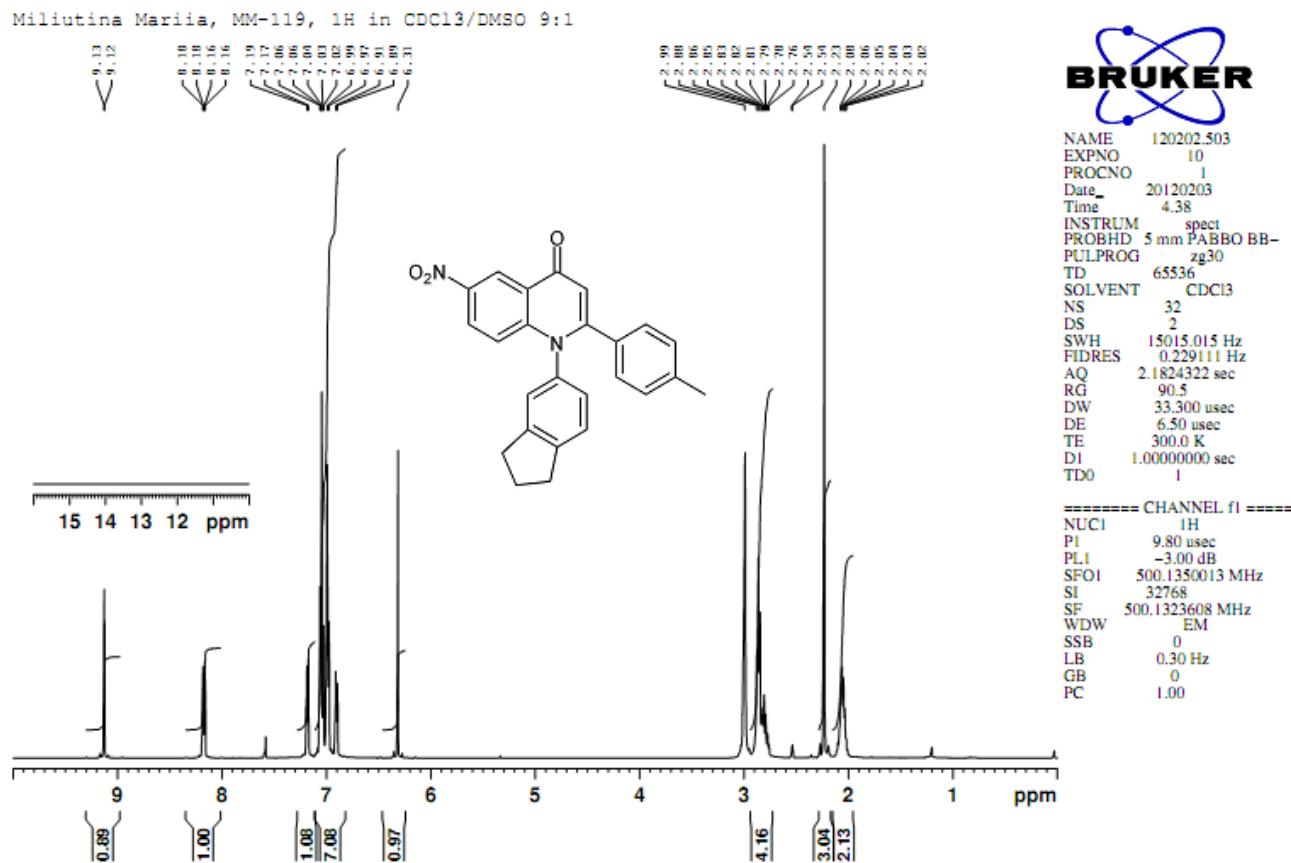
1-(3,5-Dimethylphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7am).



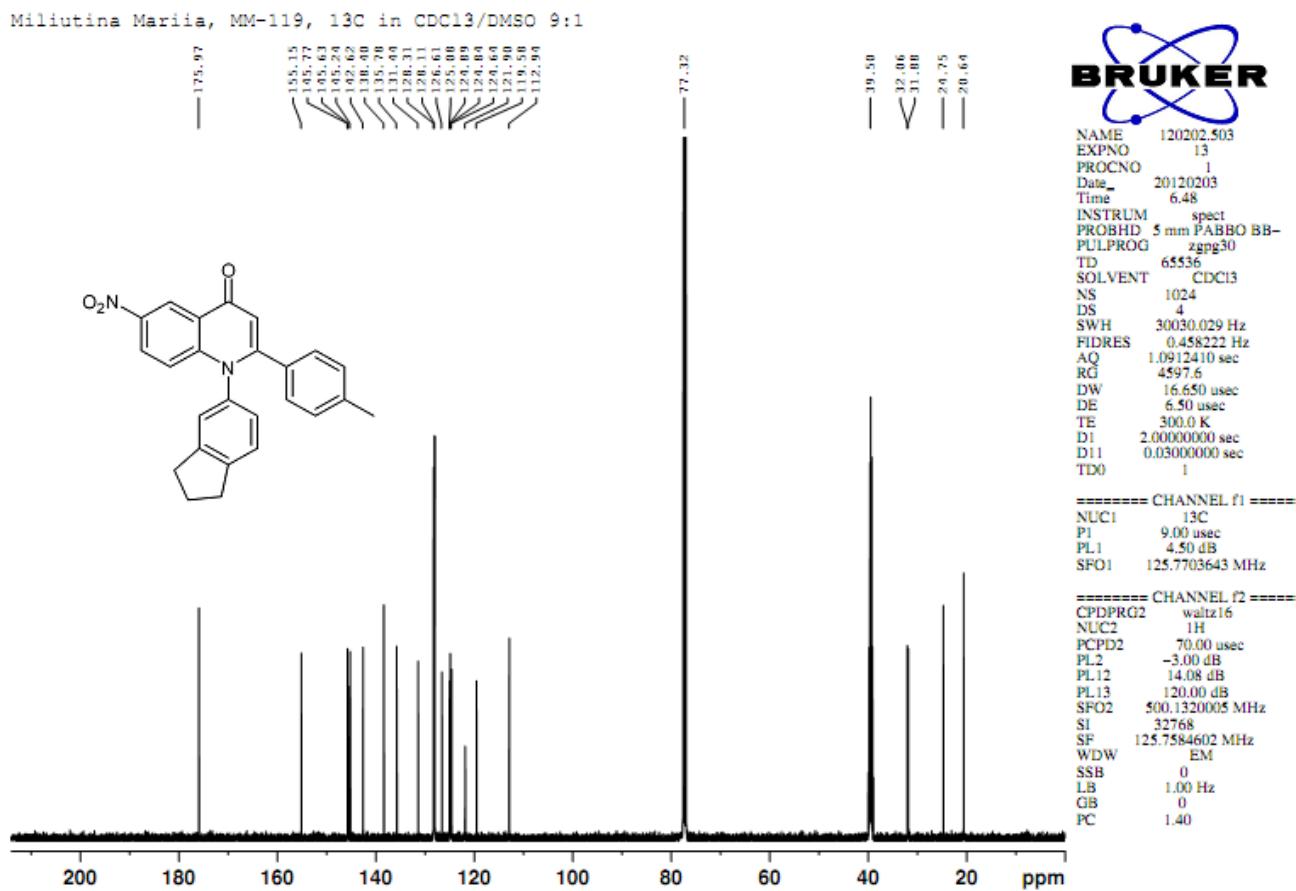
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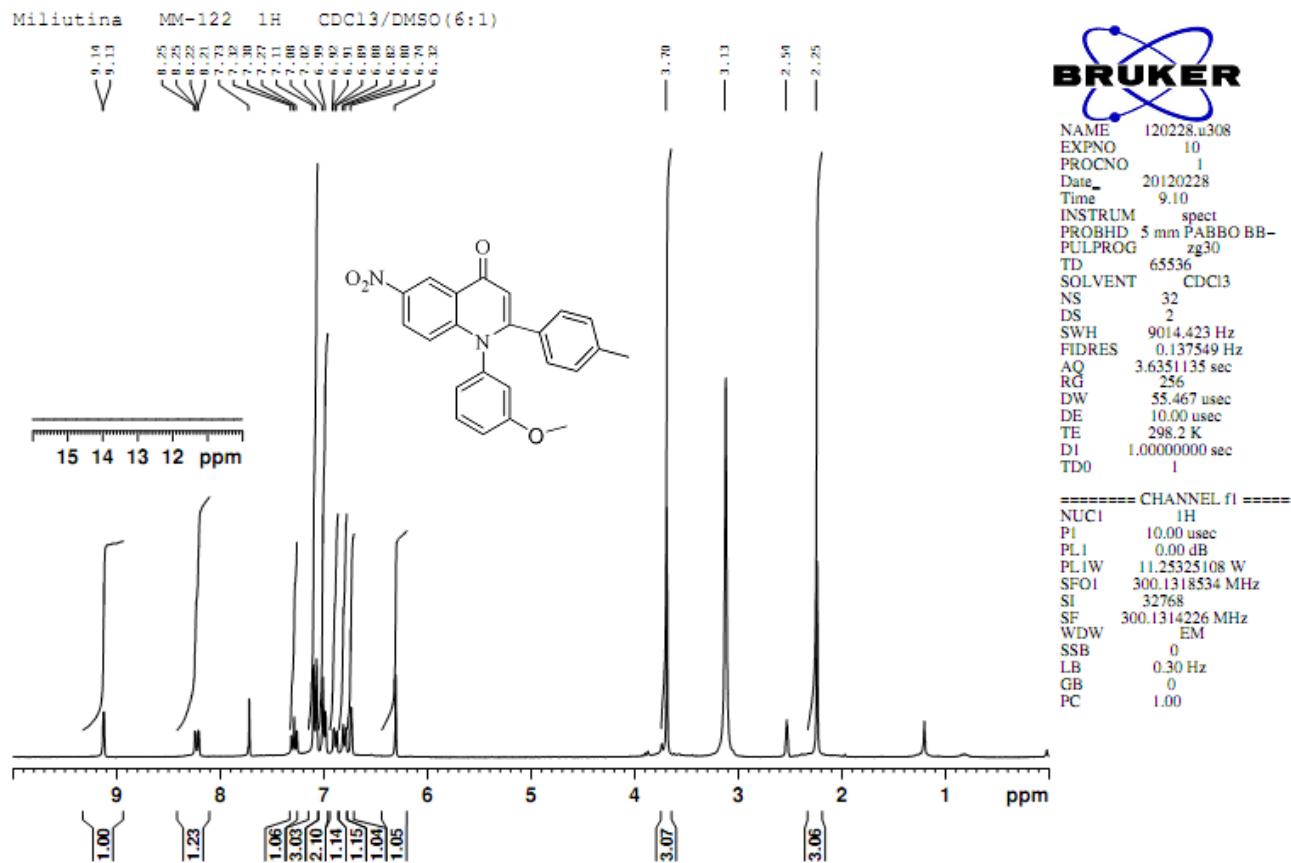
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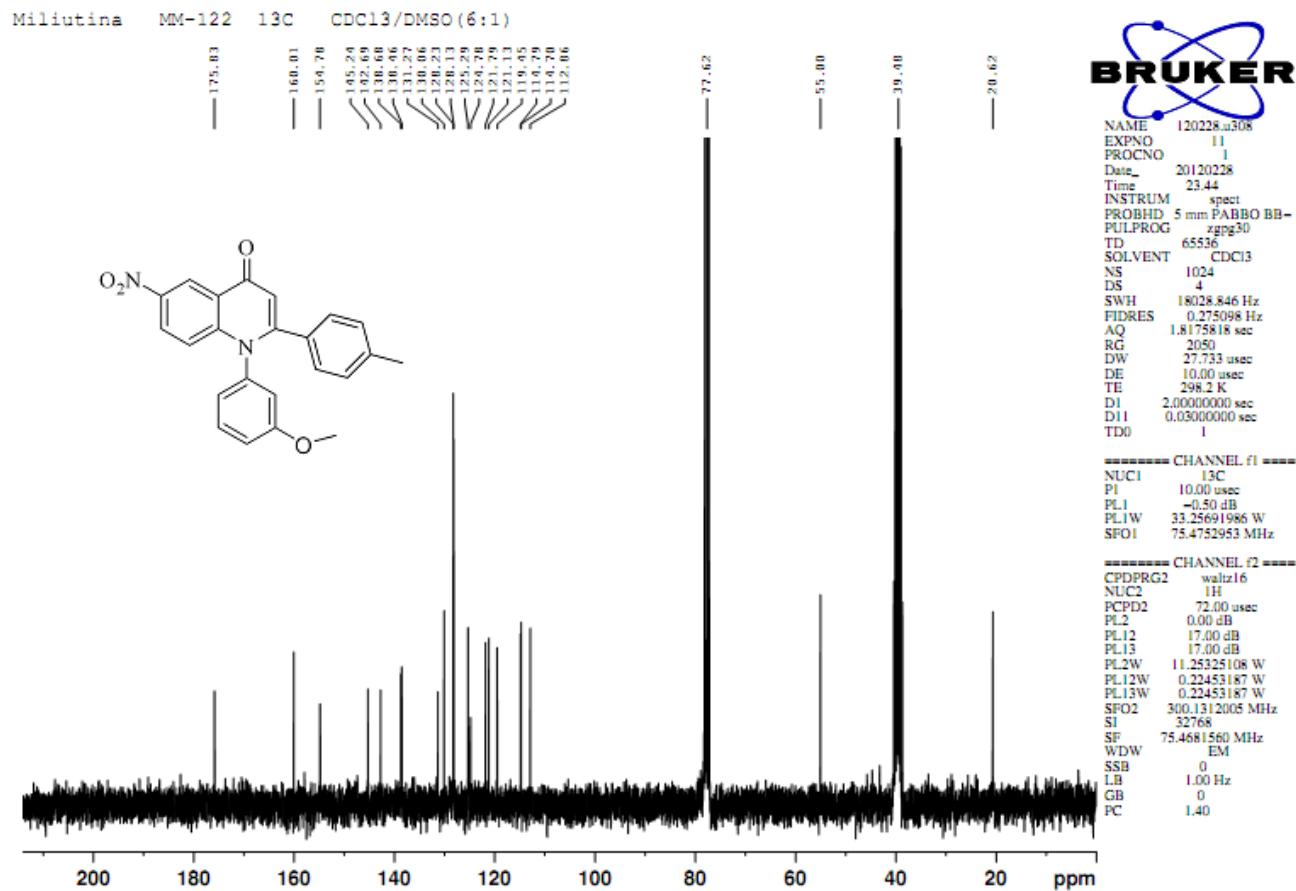
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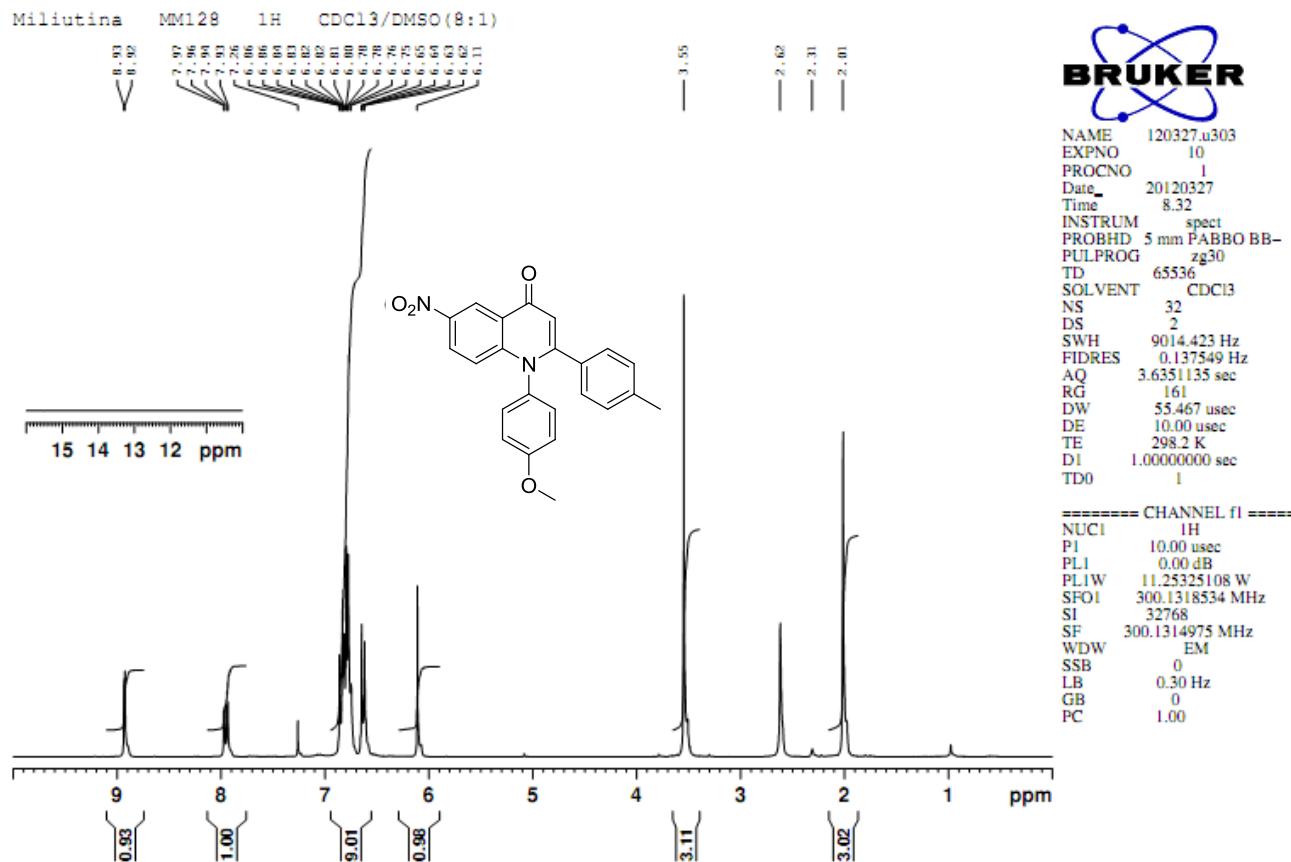
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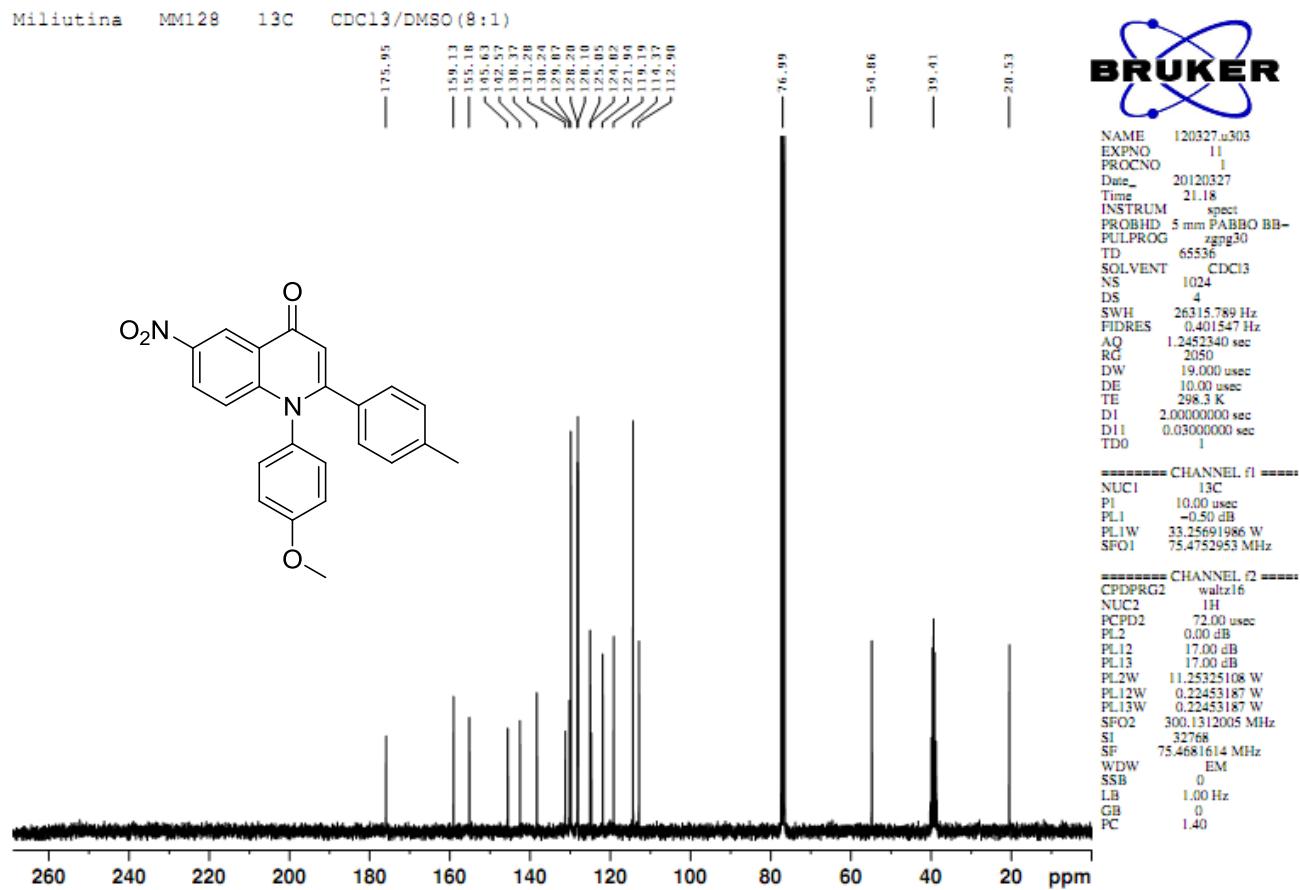
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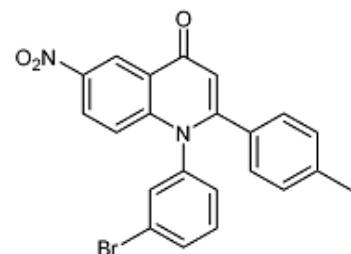
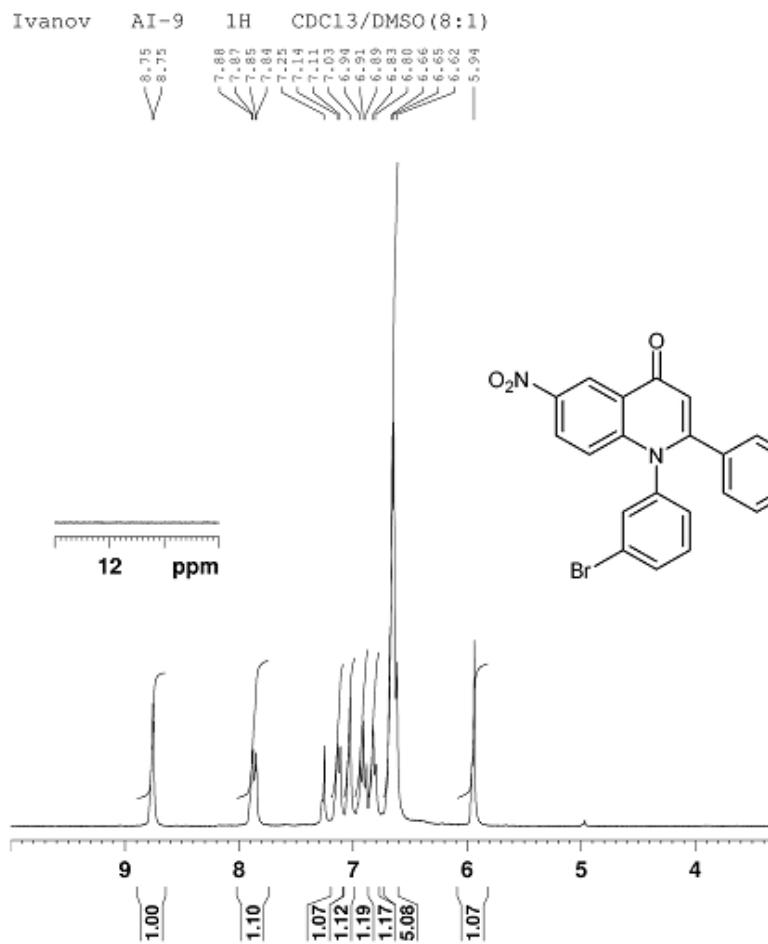
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1-(4-Methoxyphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7ap).



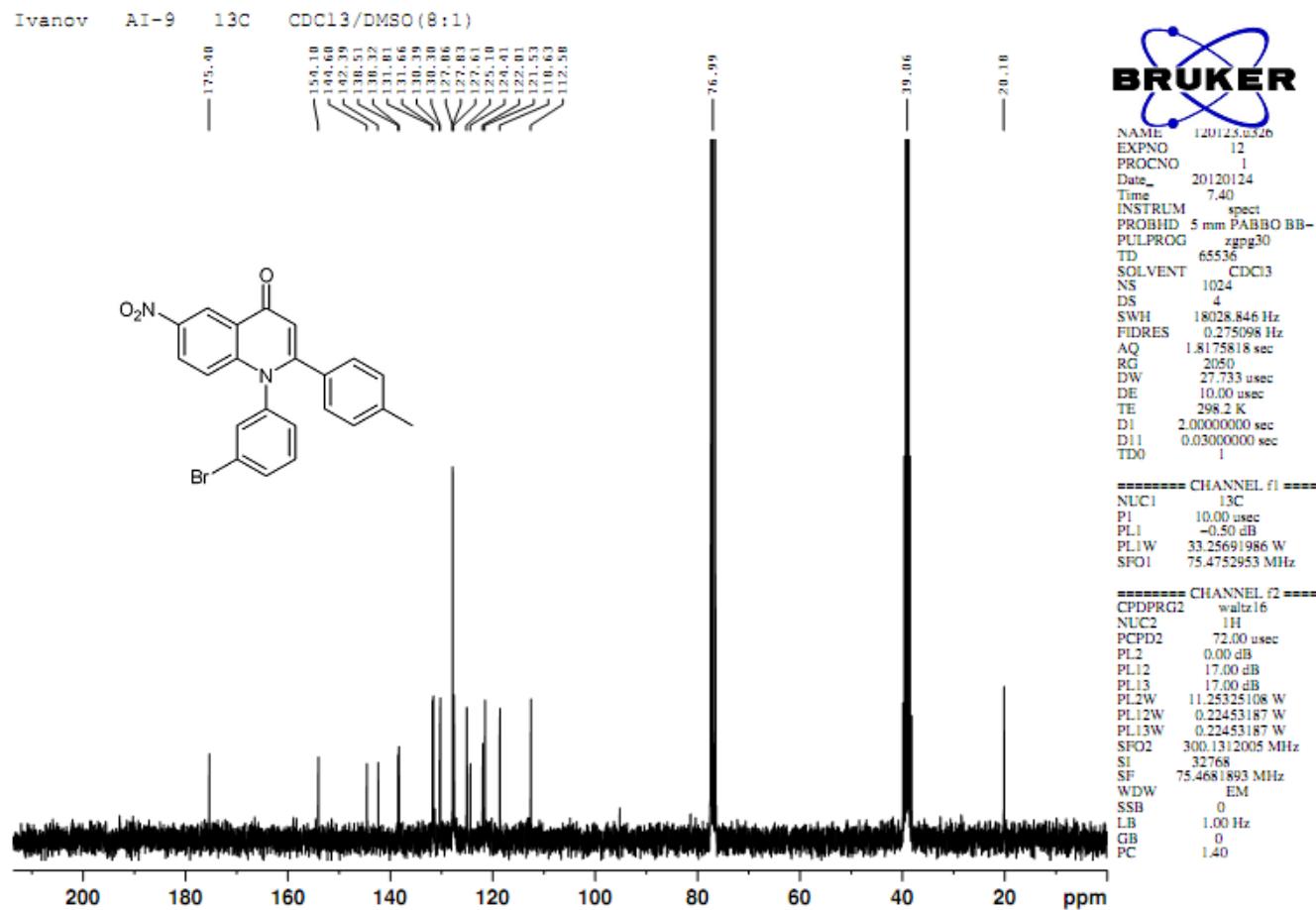
6-Nitro-1-(3-bromophenyl)-2-p-tolyl-4-quinolone (7aq).



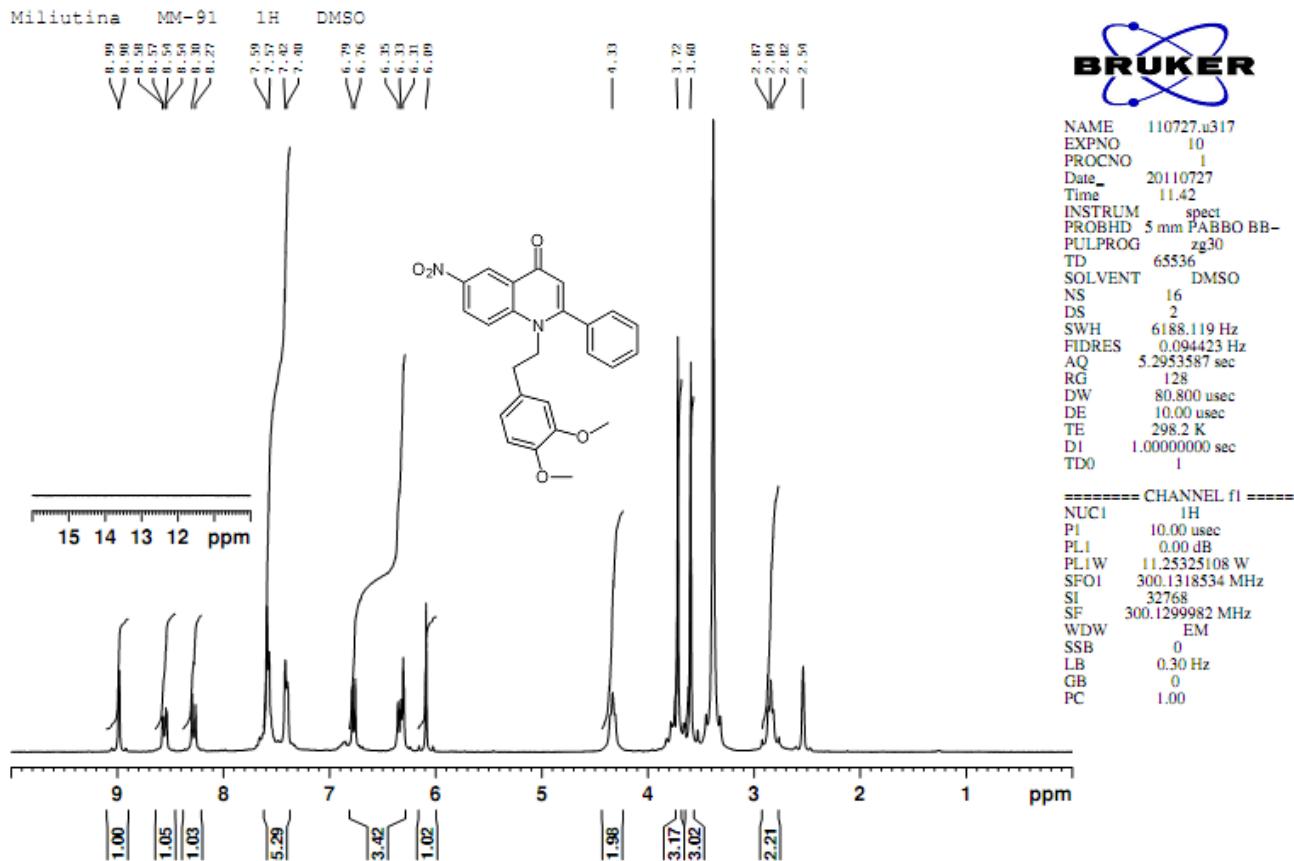
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FIDRES 0.114441 Hz
AQ 4.3691168 sec
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DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
PI 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
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SSB 0
LB 0.30 Hz
GB 0
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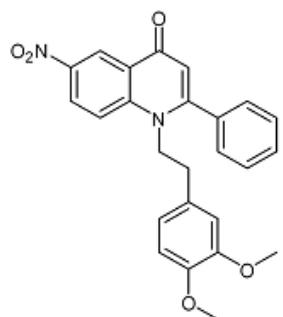
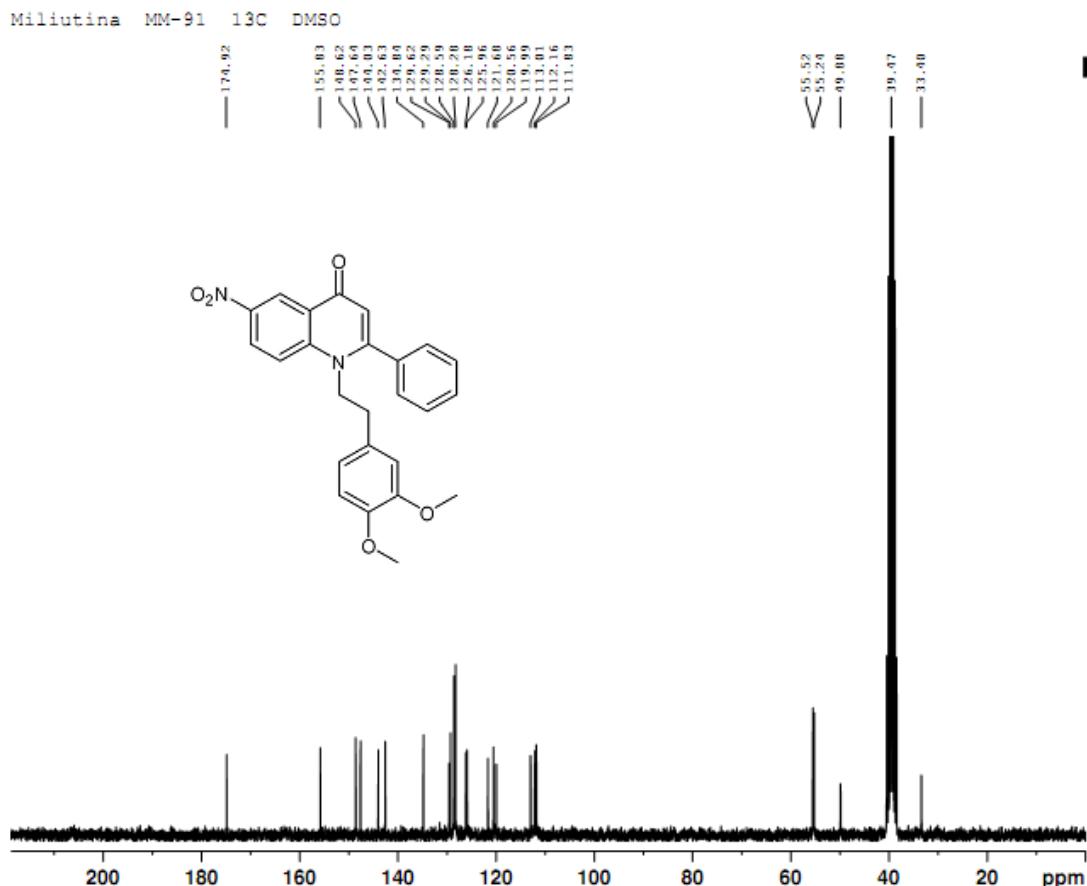
6-Nitro-1-(3-bromophenyl)-2-p-tolyl-4-quinolone (7aq).



1-(3,4-Dimethoxyphenethyl)-6-nitro-2-phenylquinolin-4(1H)-one (7ba).



1-(3,4-Dimethoxyphenethyl)-6-nitro-2-phenylquinolin-4(1*H*)-one (7ba).



BRUKER

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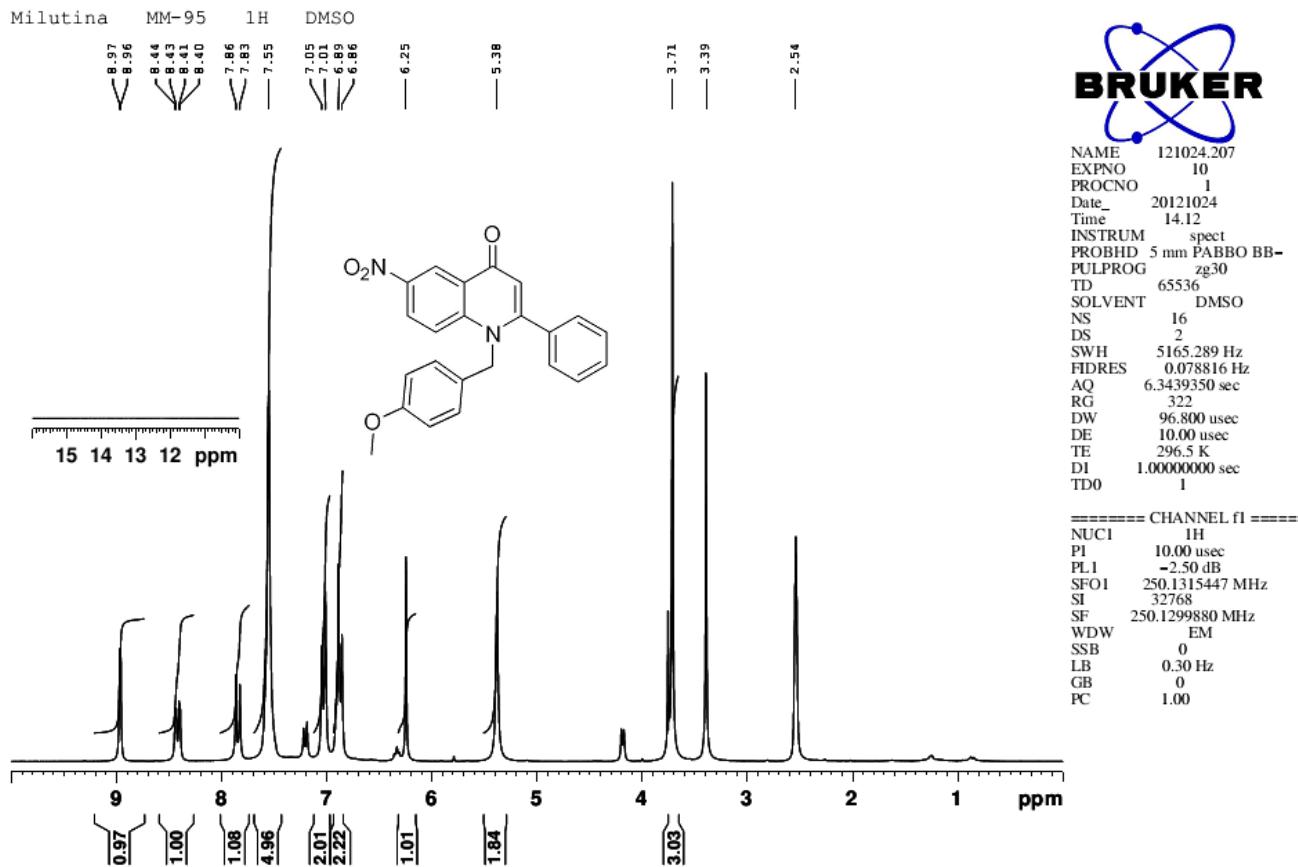
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FIDRES   0.228882 Hz
AQ        2.1845834 sec
RG          2050
DW        33.333 usec
DE         10.00 usec
TE        298.8 K
D1      2.0000000 sec
D11     0.03000000 sec
DELTA    1.89999998 sec
TDO      1

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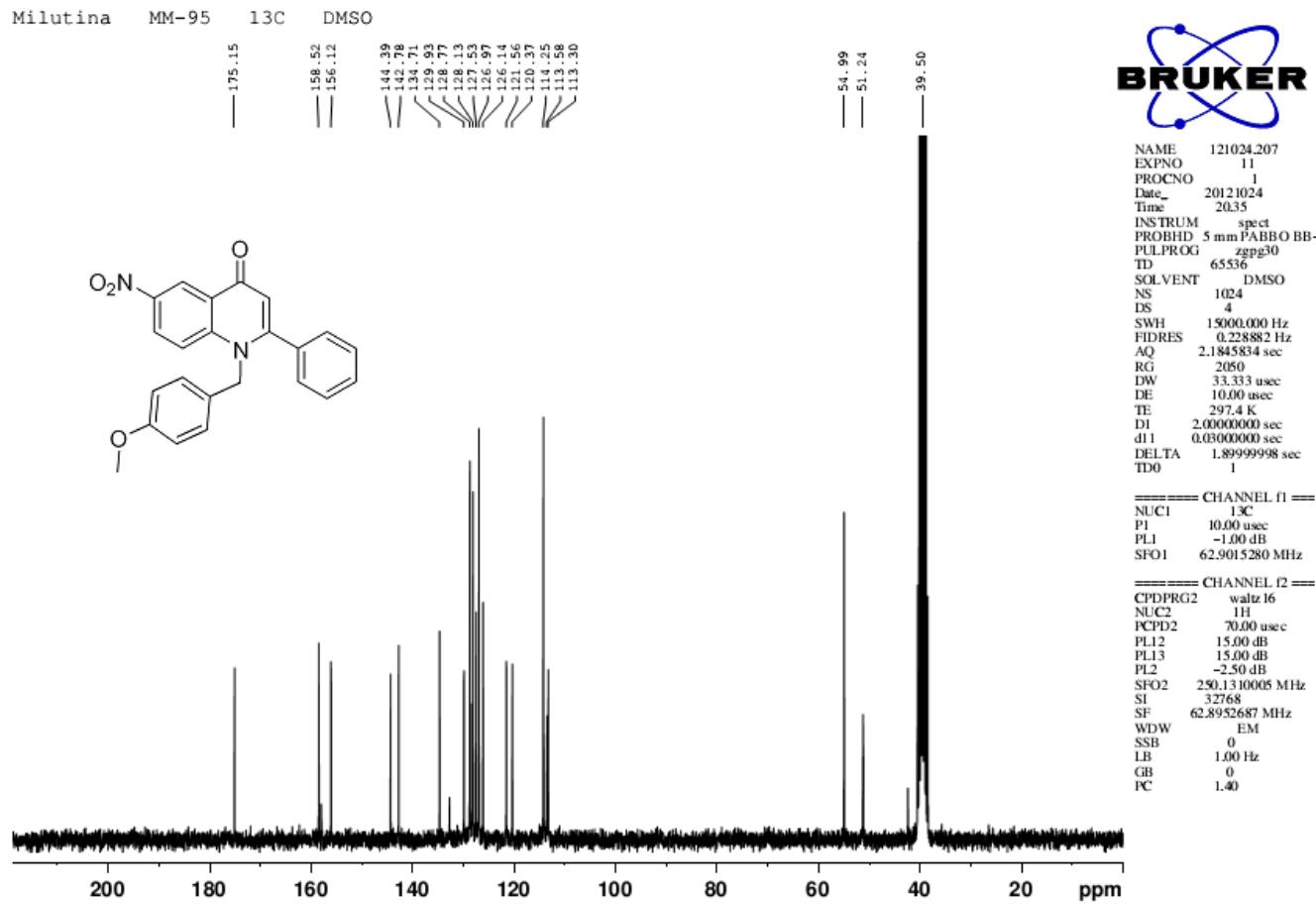
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P1 10.00 usec
PL1 -1.00 dB
SEQ1 67.8015280 MHz

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NUC2       1H
PCPD2     70.00 usec
PL12      15.00 dB
PL13      15.00 dB
PL2       -2.50 dB
SFO2     250.1310005 MHz
SI        32768
SF      62.8952704 MHz
WDW      EM
SSB      0
LB       1.00 Hz
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BC      1.40
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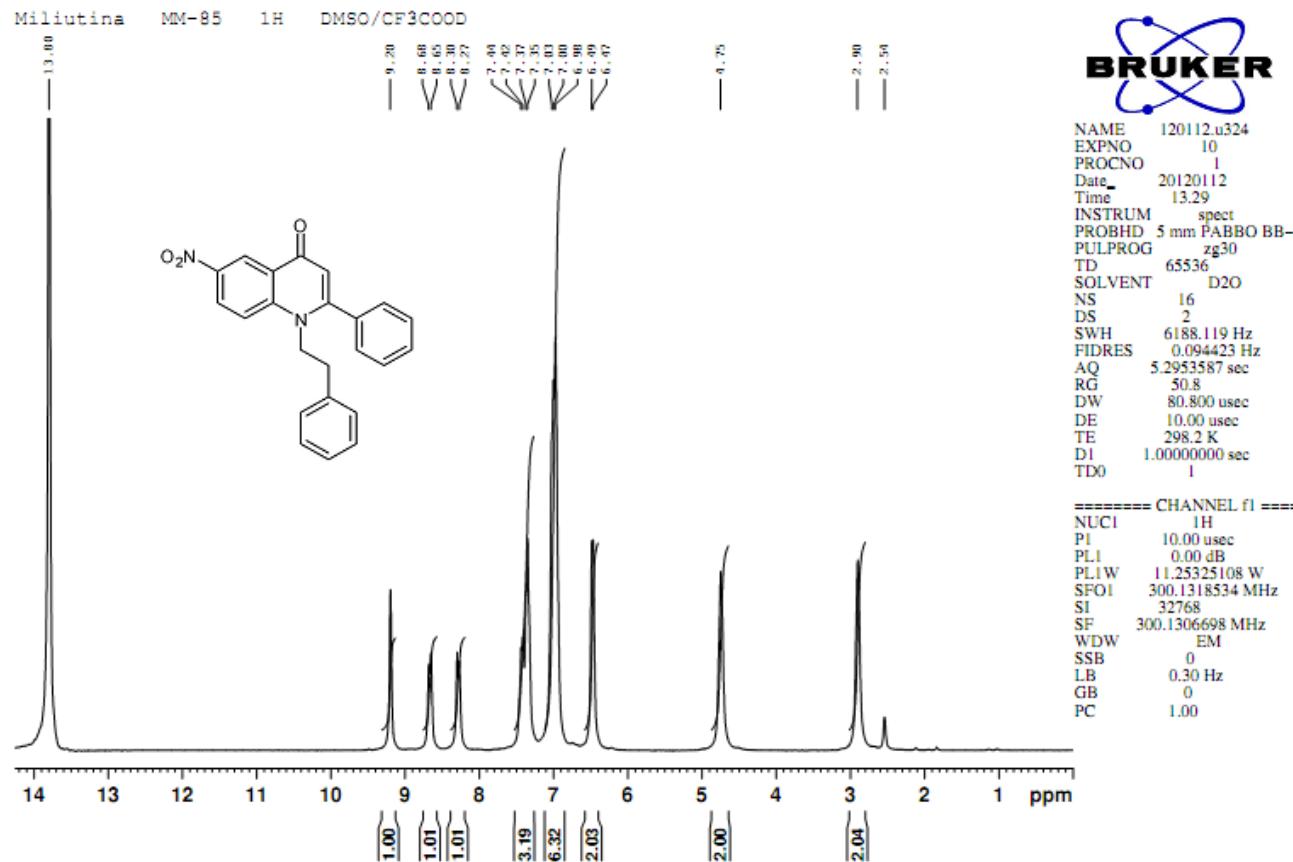
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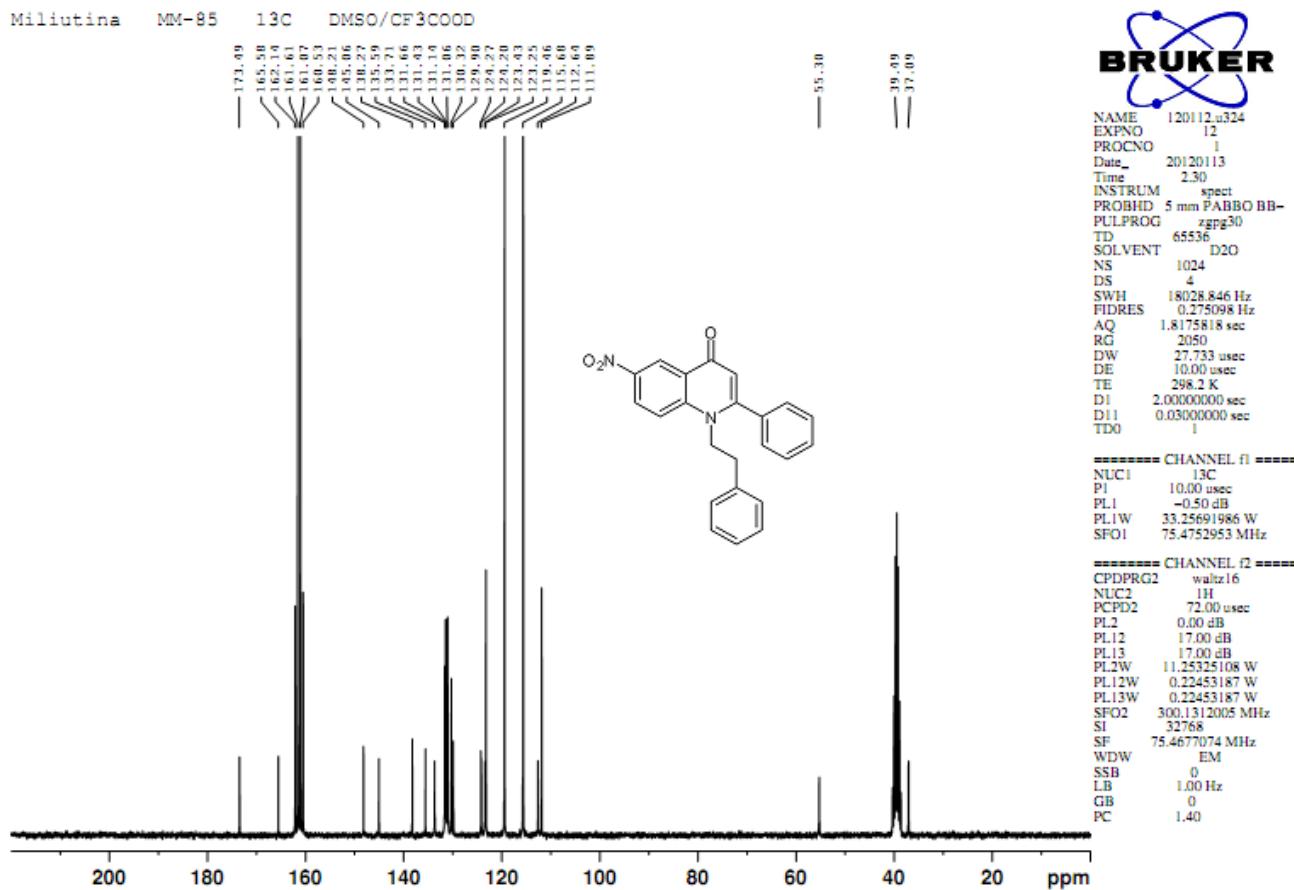
1-(4-Methoxybenzyl)-6-nitro-2-phenylquinolin-4(1H)-one (7bb).



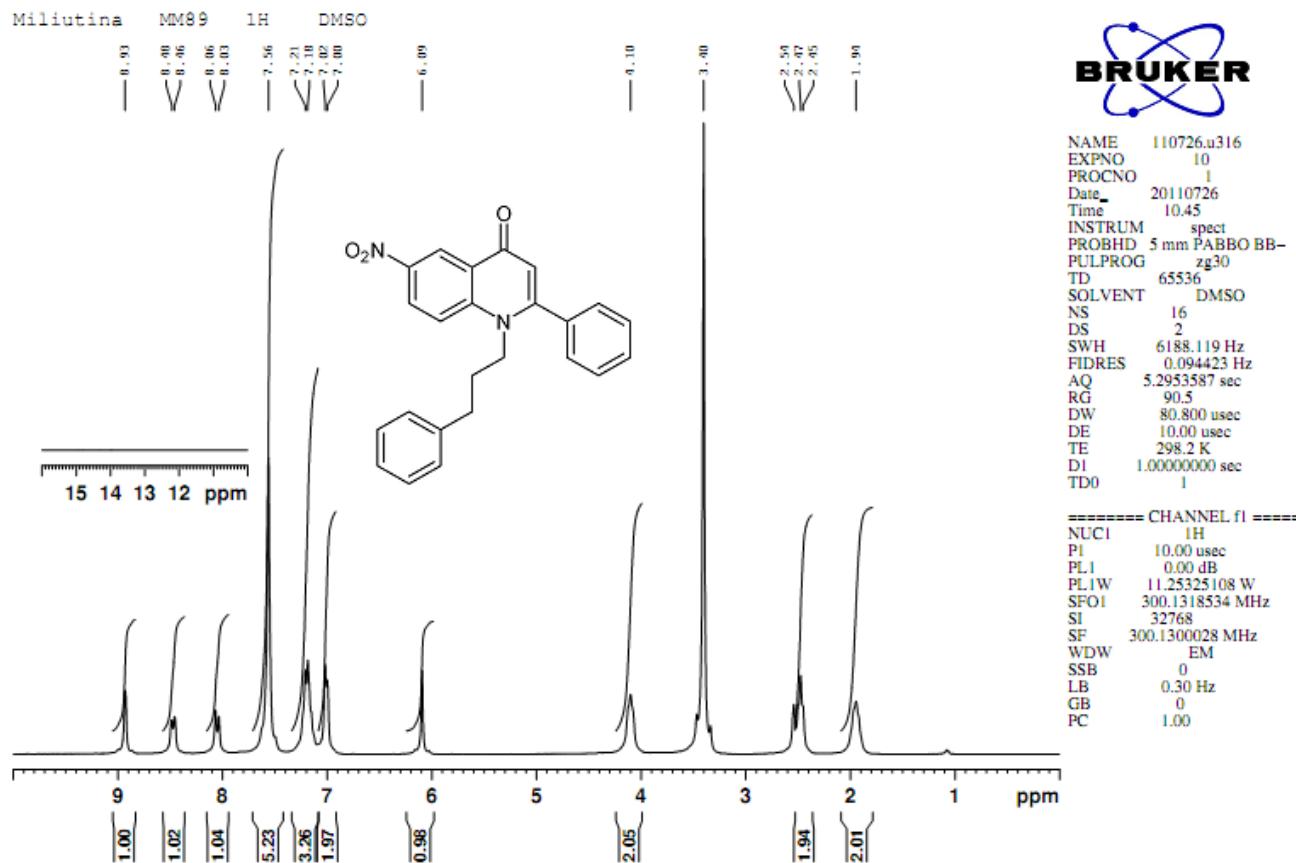
6-Nitro-1-phenethyl-2-phenylquinolin-4(1H)-one (7bc).



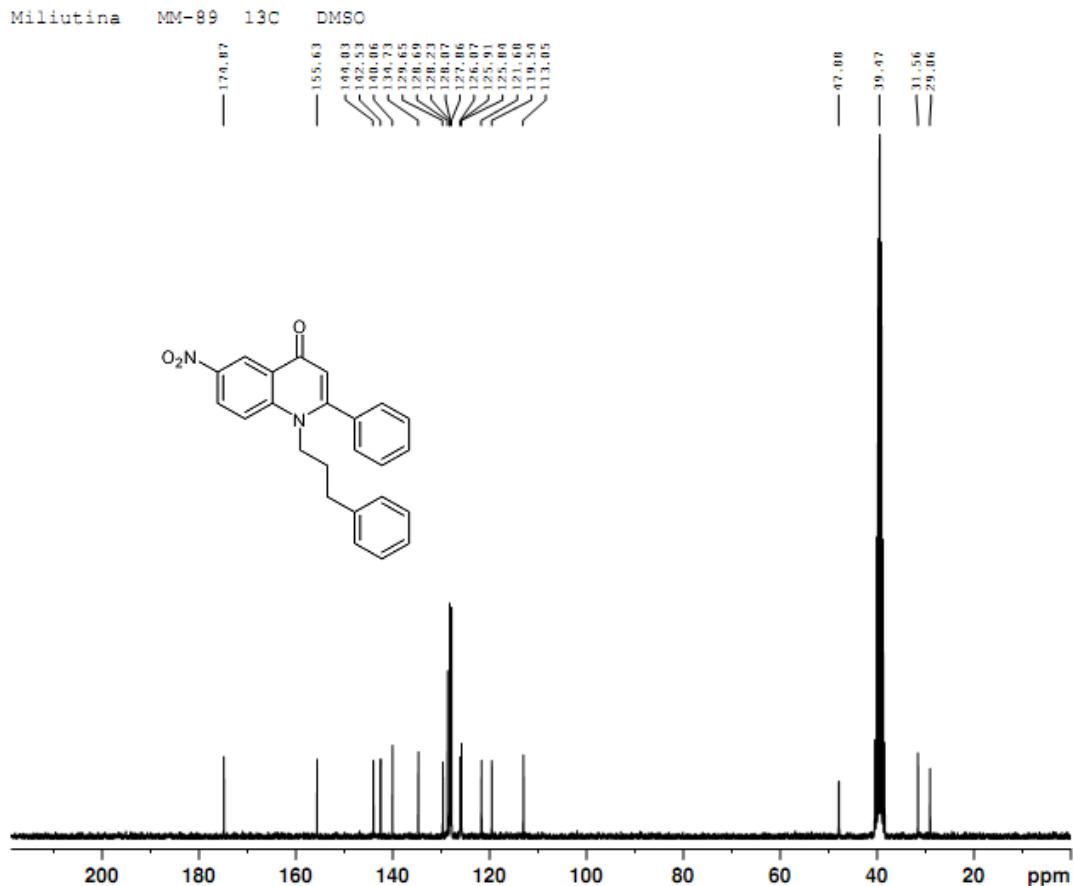
6-Nitro-1-phenethyl-2-phenylquinolin-4(1H)-one (7bc).



6-Nitro-4-oxo-2-phenyl-1-(3-phenylpropyl)quinoline (7bd).



6-Nitro-4-oxo-2-phenyl-1-(3-phenylpropyl)quinoline (7bd).

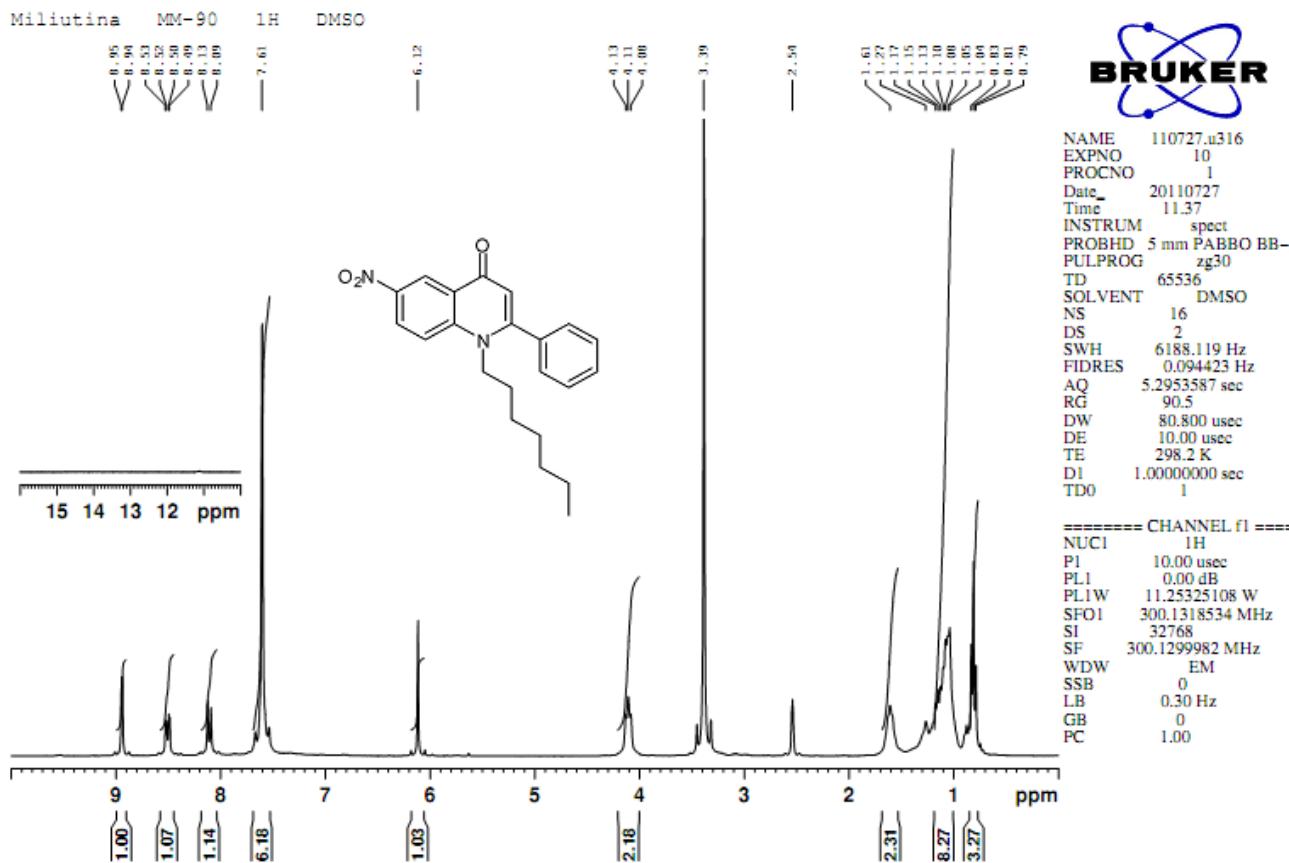


NAME 110726.206
EXPNO 10
PROCNO 1
Date 20110726
Time 18.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.2 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TD0 1

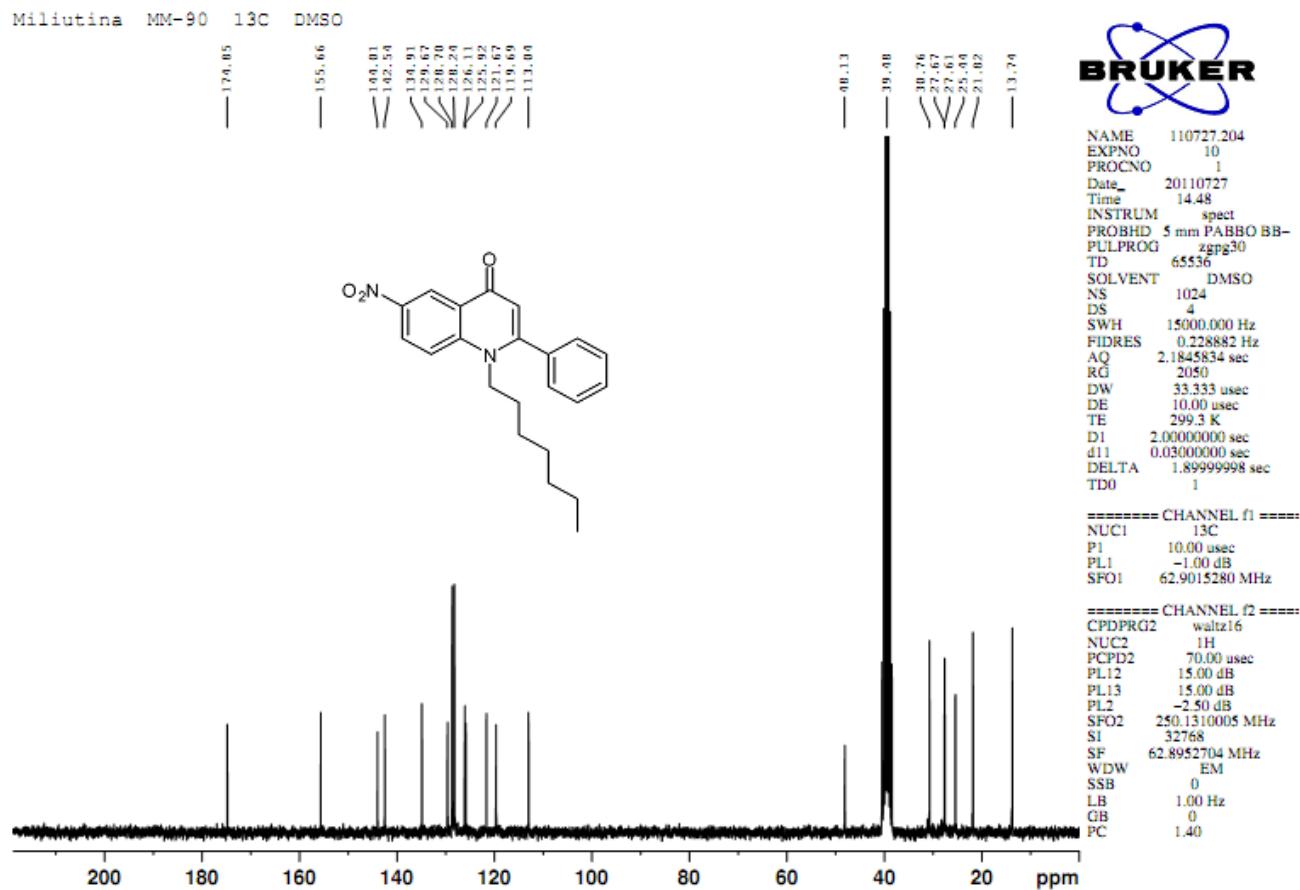
===== CHANNEL f1 =====
NUC1 ^{13}C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ^1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

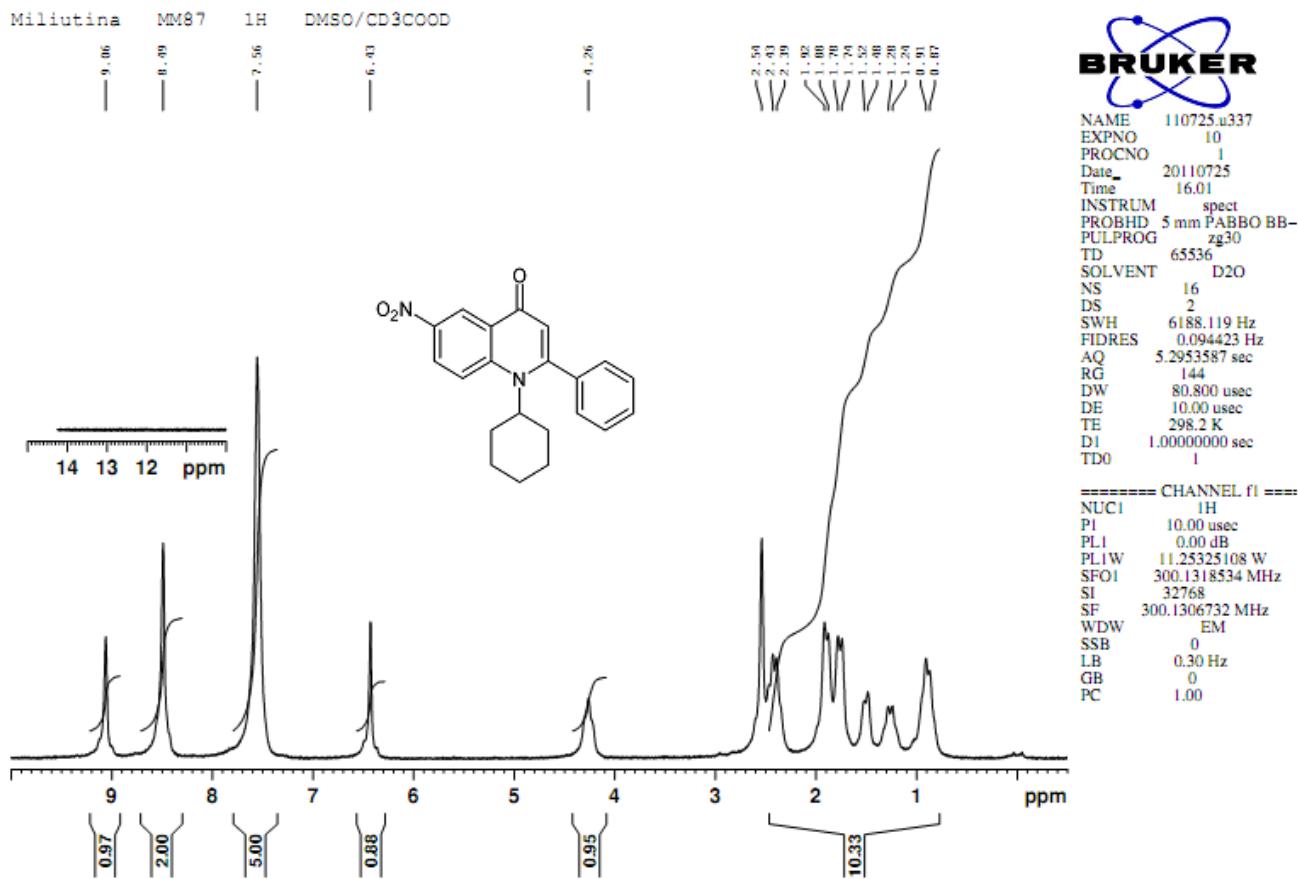
1-Heptyl-6-nitro-2-phenylquinolin-4(1H)-one (7be).



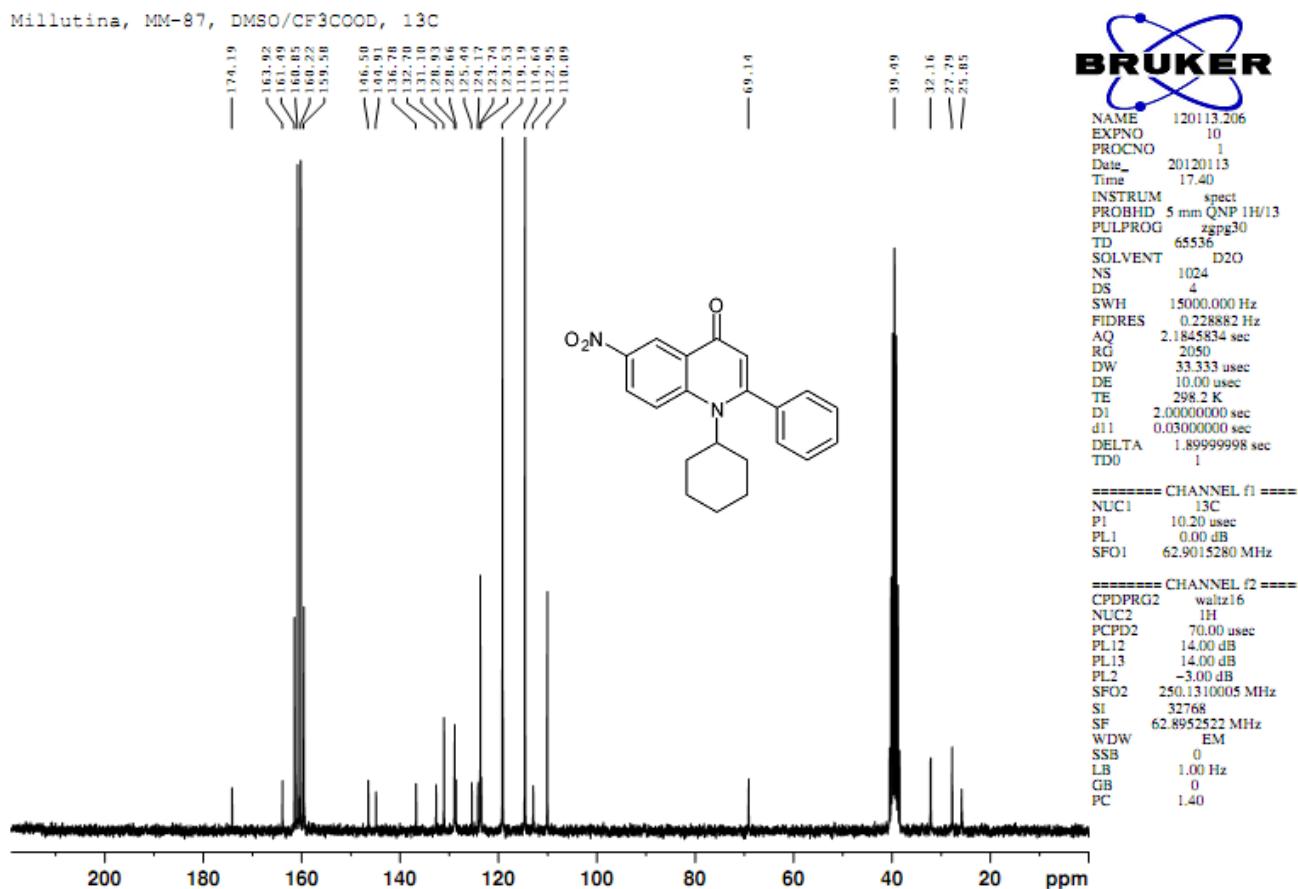
1-Heptyl-6-nitro-2-phenylquinolin-4(1H)-one (7be).



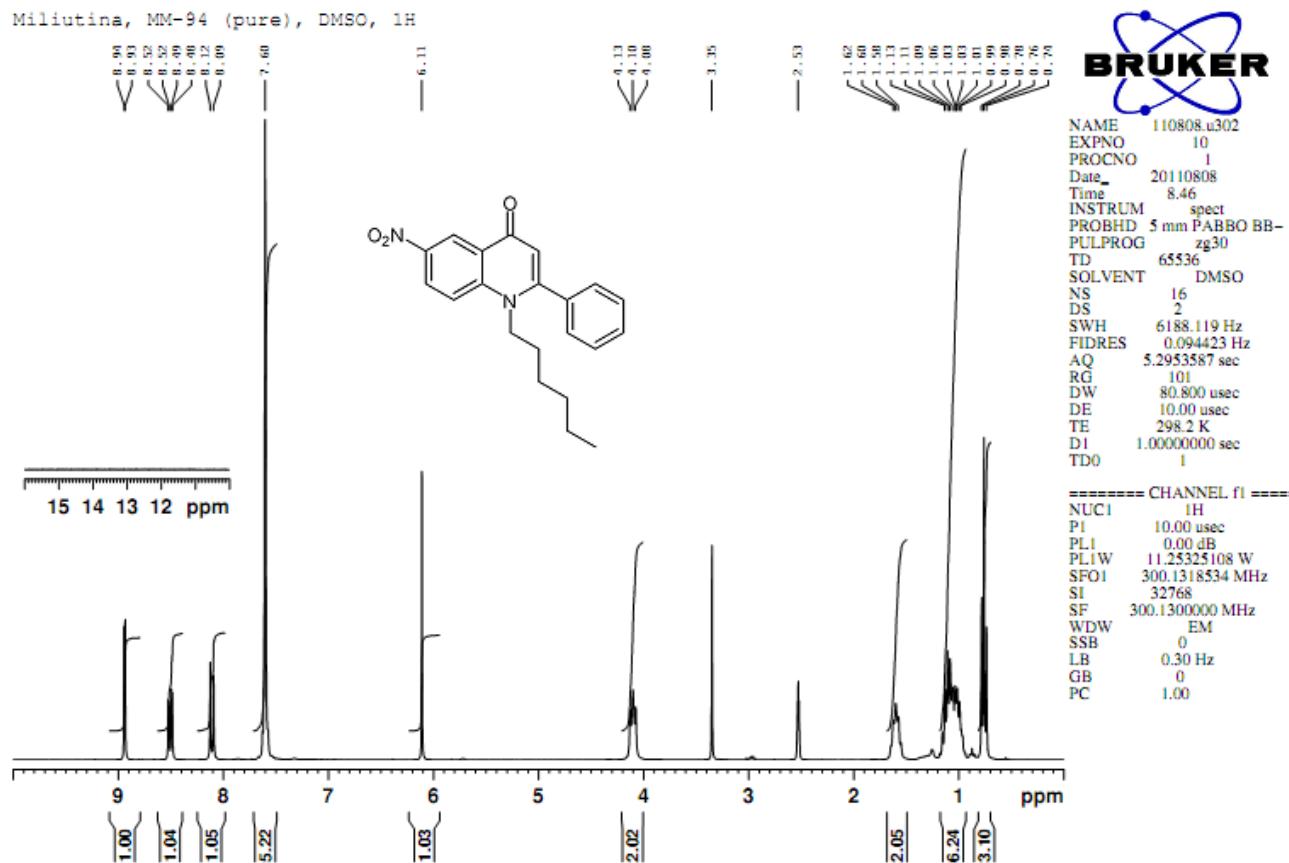
1-cyclohexane-6-nitro-4-oxo-2-phenylquinoline (7bf).



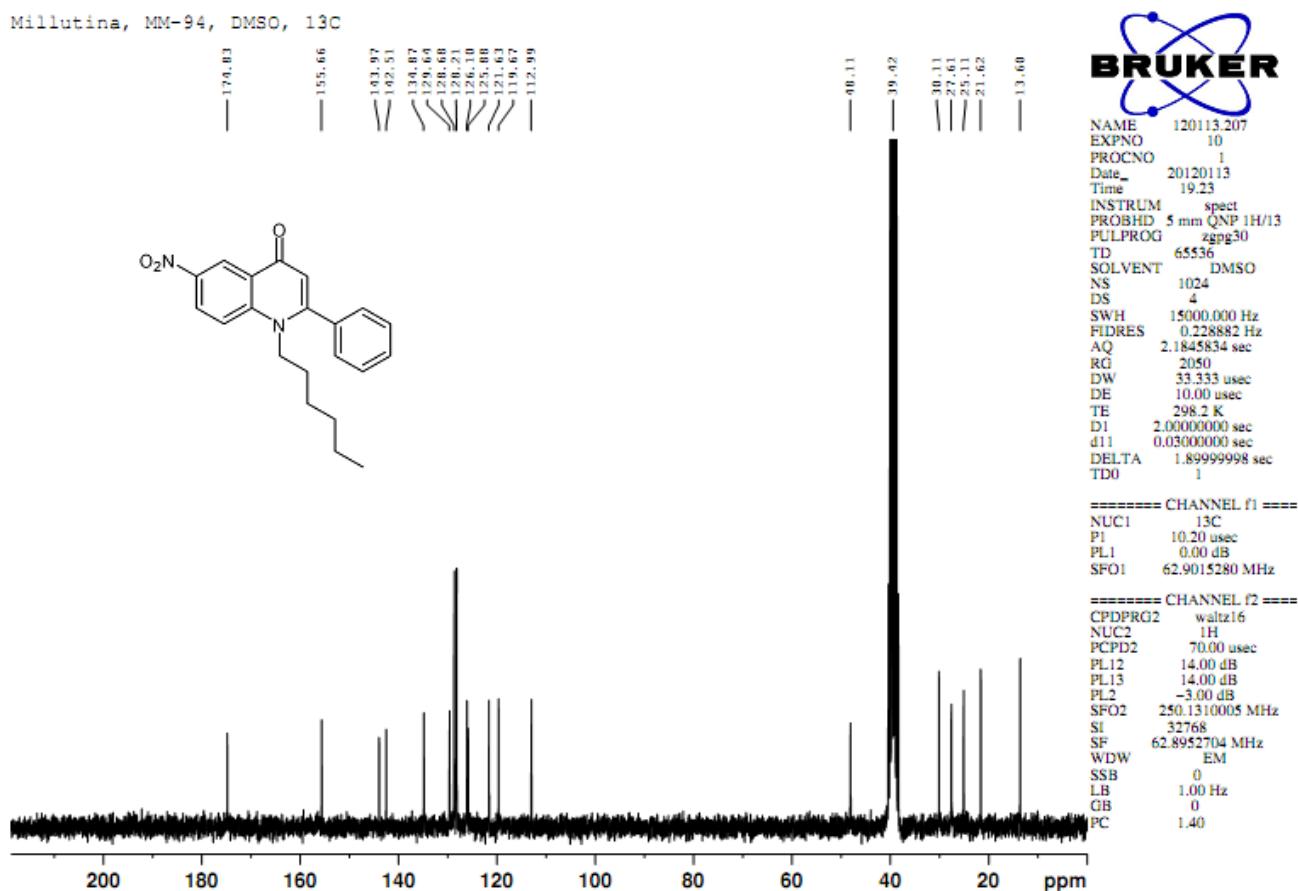
1-cyclohexane-6-nitro-4-oxo-2-phenylquinoline (7bf).



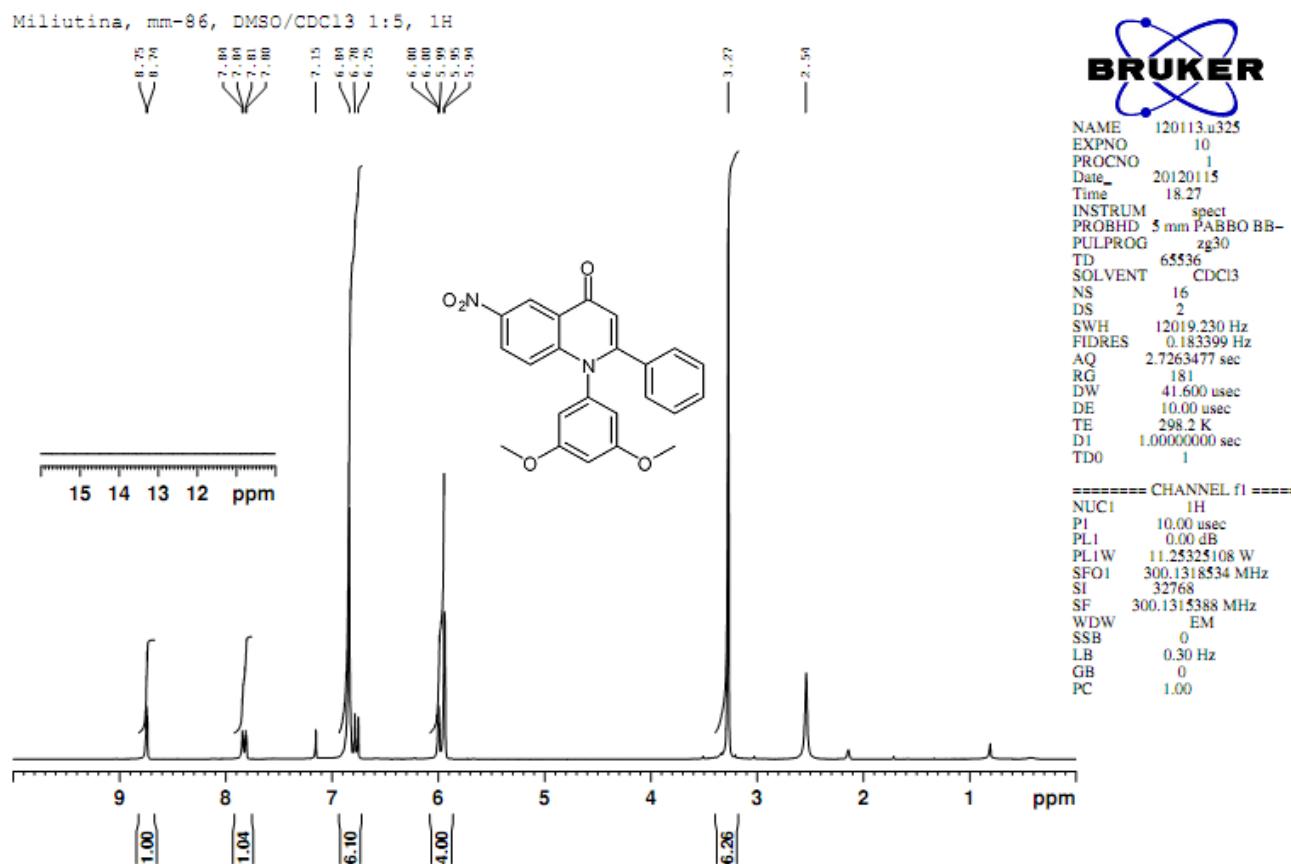
1-Hexyl-6-nitro-2-phenylquinolin-4(1H)-one (7bg).



1-Hexyl-6-nitro-2-phenylquinolin-4(1*H*)-one (7bg).



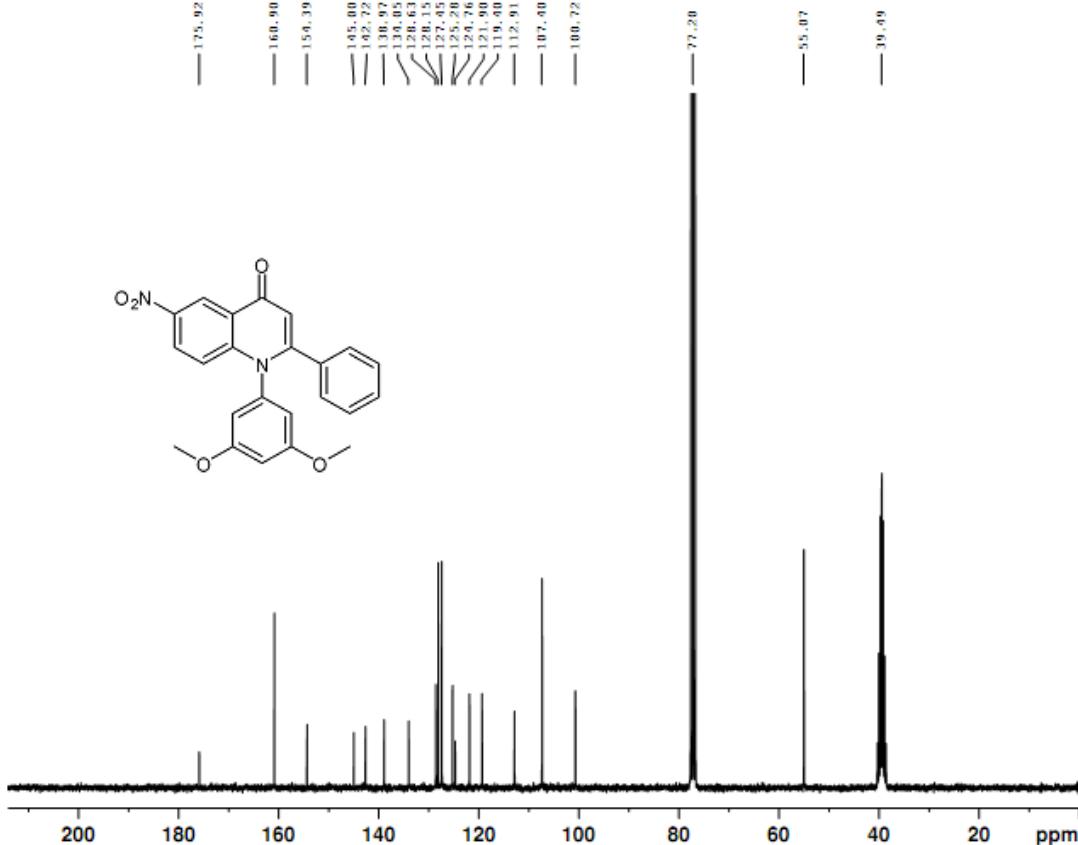
1-(3,5-dimethoxybenzen)-6-nitro-4-oxo-2-phenylquinoline (7bh).



1-(3,5-dimethoxybenzen)-6-nitro-4-oxo-2-phenylquinoline (7bh).

Miliutina, mm-86, DMSO/CDCl₃ 1:5, ¹³C

The chemical structure shows a quinoline ring system substituted at position 1 with a 3,5-dimethoxyphenyl group, at position 2 with a phenyl group, and at position 6 with a nitro group.

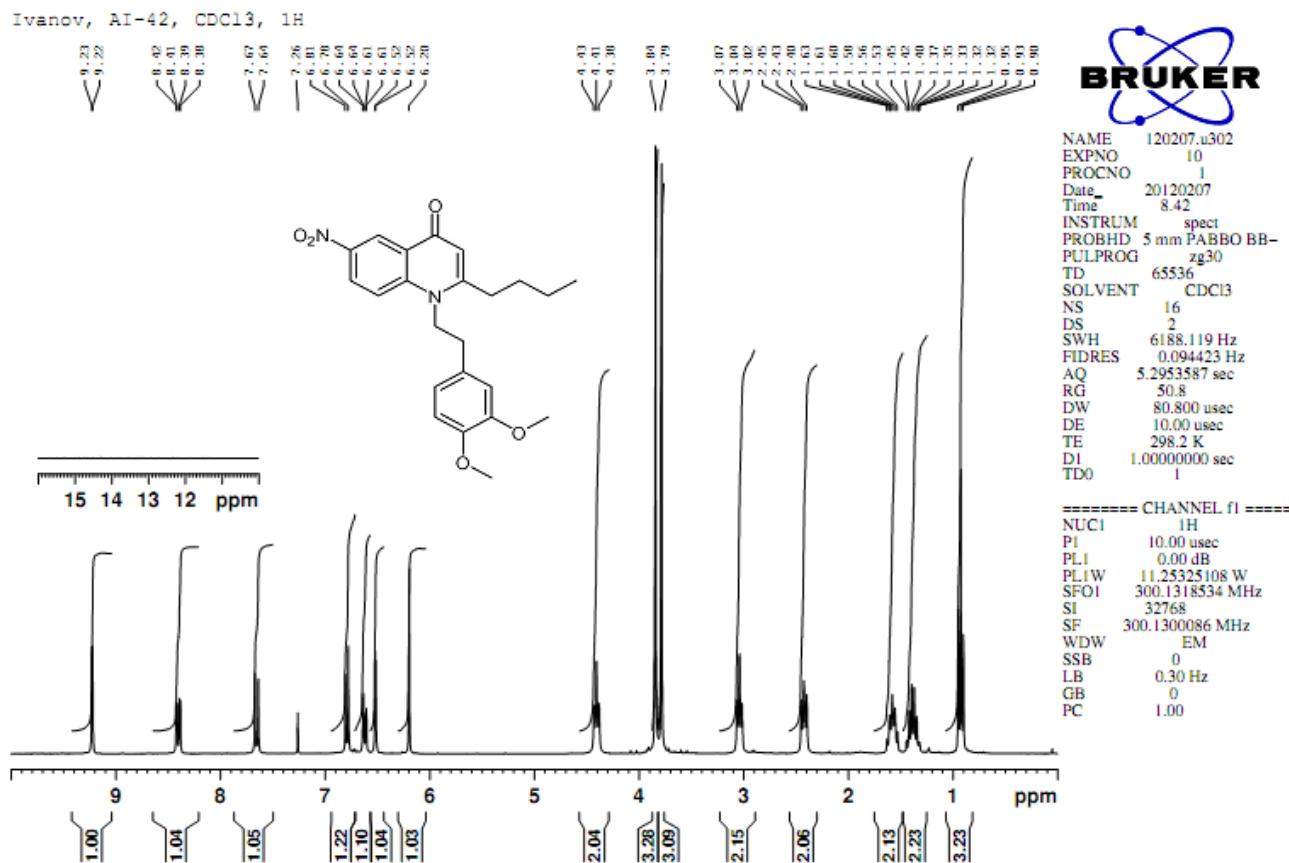


NAME 120113.u325
EXPNO 11
PROCNO 1
Date_ 20120115
Time 20.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

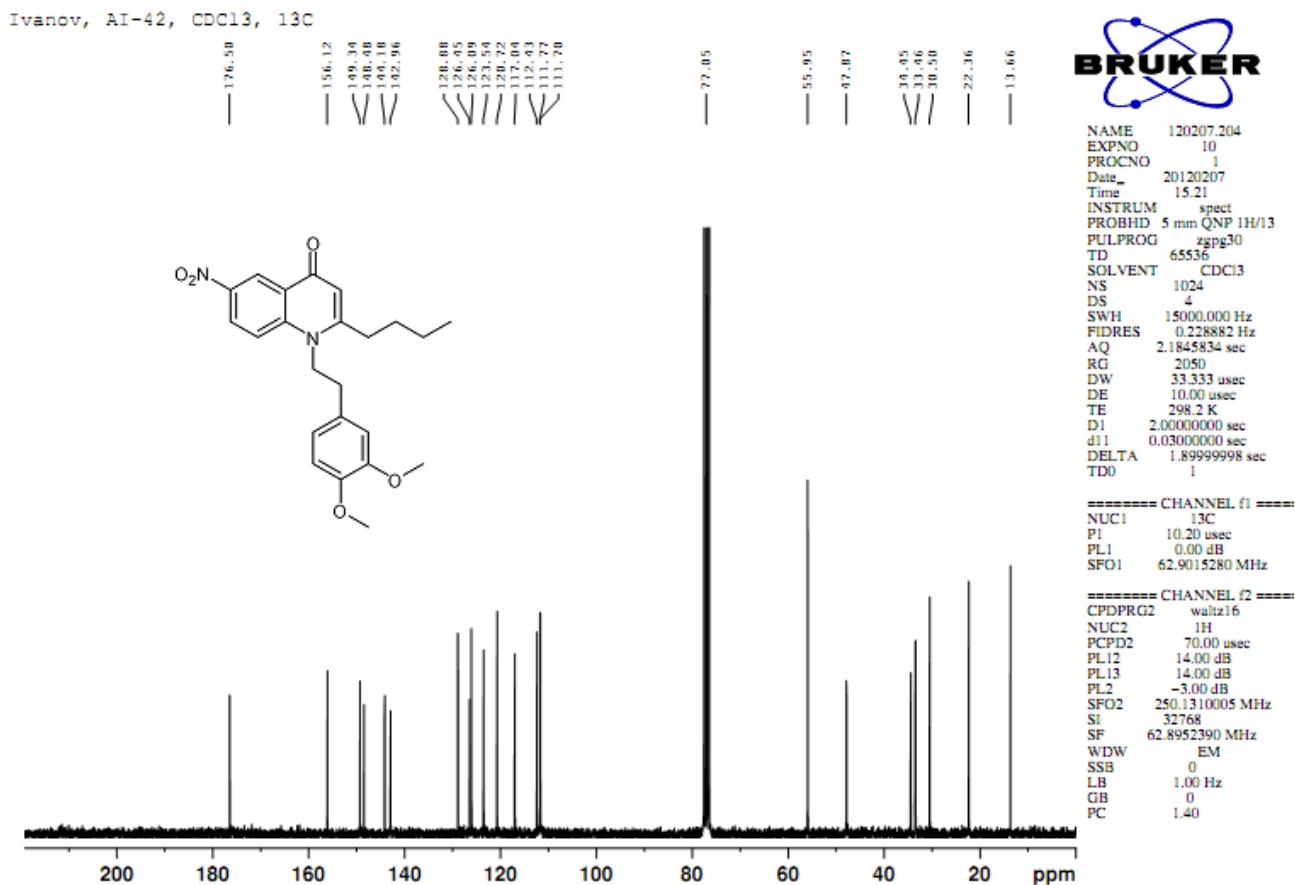
===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 -0.50 dB
PL1 W 33.25691986 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 ¹H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4681550 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

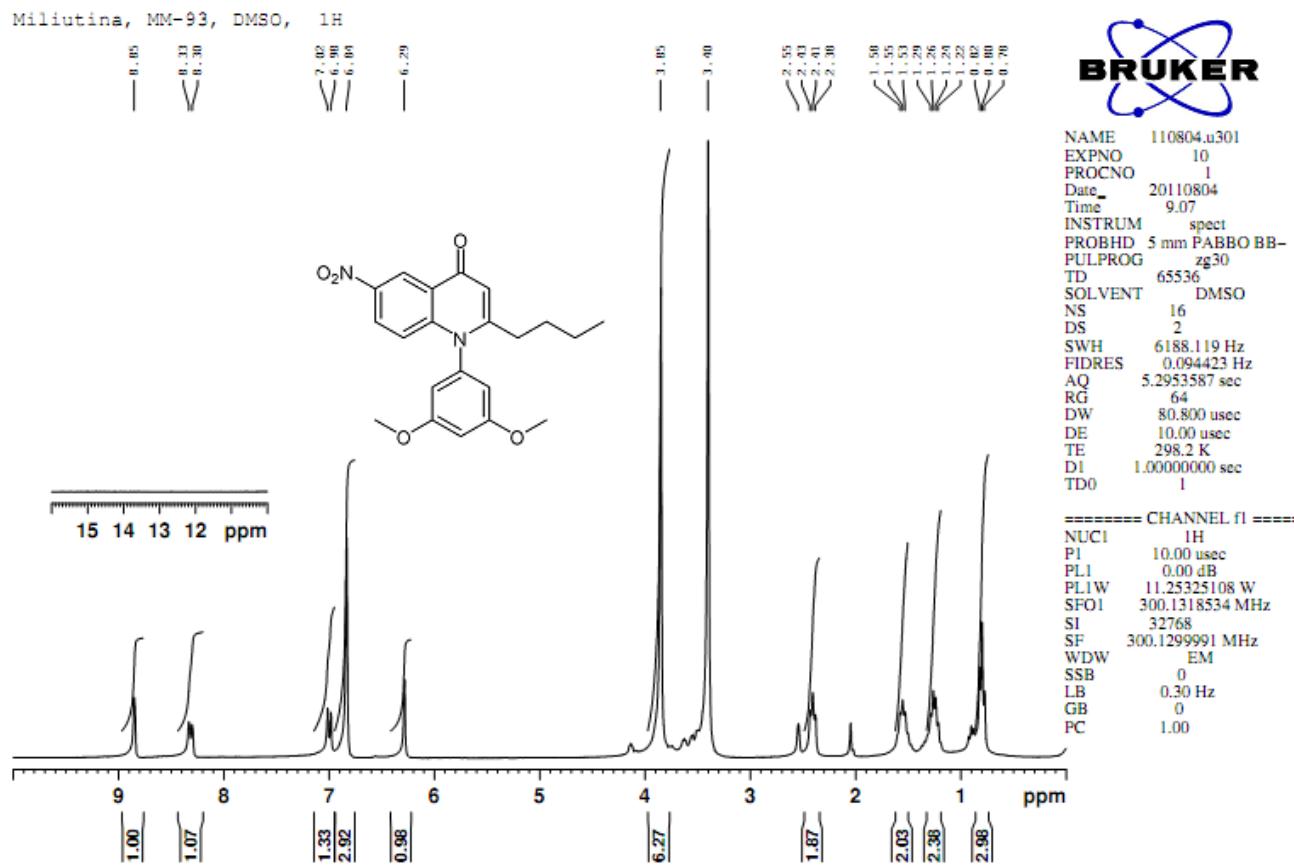
6-Nitro-1-(3,4-dimethoxyphenethyl)-2-p-tolyl-4-quinolone (7ca).



6-Nitro-1-(3,4-dimethoxyphenethyl)-2-p-tolyl-4-quinolone (7ca).

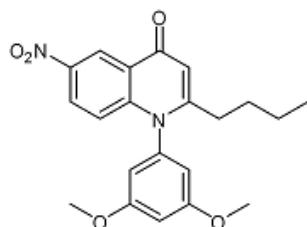
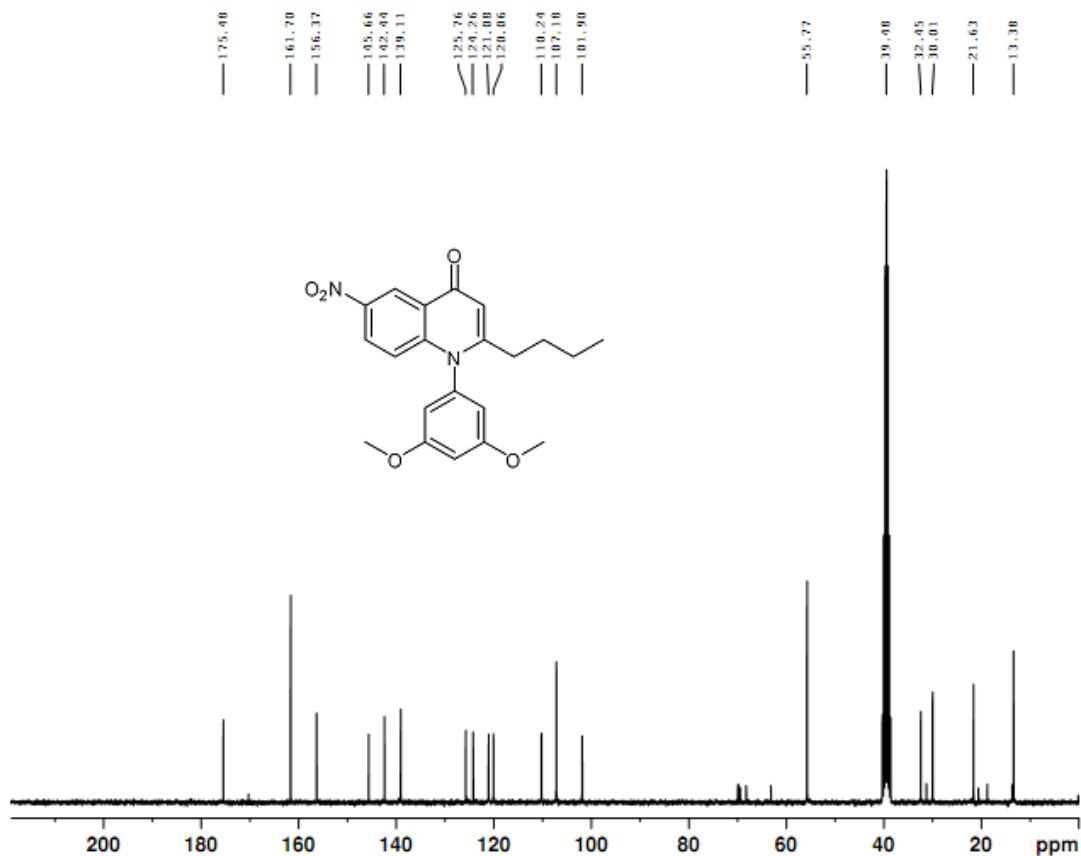


2-Butyl-1-(3,5-dimethoxyphenyl)-6-nitroquinolin-4(1H)-one (7cb).



2-Butyl-1-(3,5-dimethoxyphenyl)-6-nitroquinolin-4(1H)-one (7cb).

Miliutina, MM-93, DMSO, ^{13}C



```

NAME 110809.u316
EXPNO 10
PROCNO 1
Date 20110809
Time 23.34
INSTRUM spect
PROBID 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SF01 75.4752953 MHz

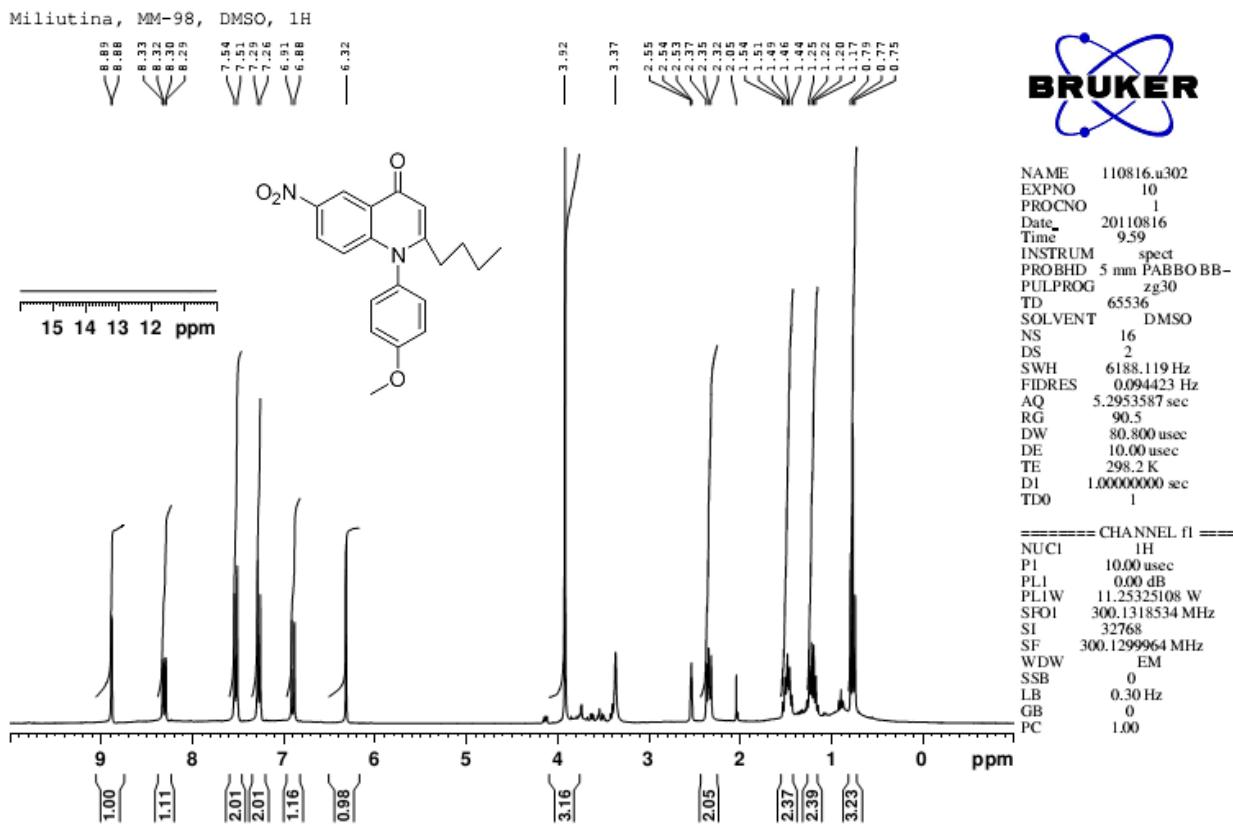
```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SF02 300.1312005 MHz
SI 32768
SF 75.4677864 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

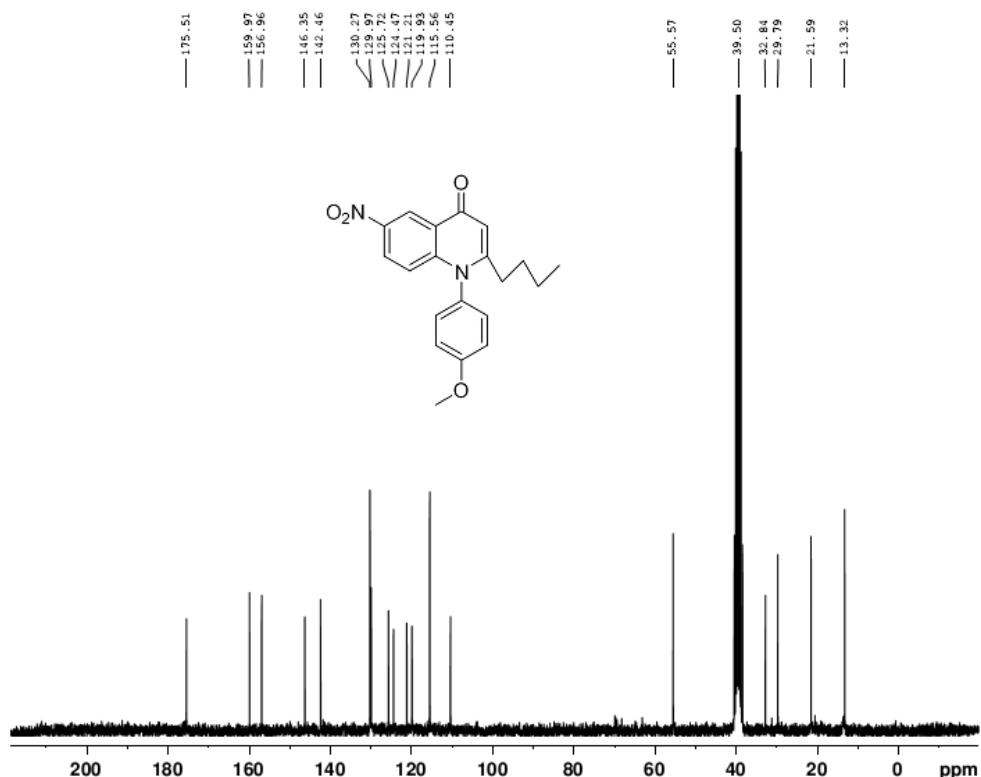
```

2-Butyl-1-(4-methoxyphenyl)-6-nitroquinolin-4(1H)-one (7cc).



2-Butyl-1-(4-methoxyphenyl)-6-nitroquinolin-4(1H)-one (7cc).

Miliutina, MM-98, DMSO, ^{13}C



NAME 110818.202
 EXPNO 10
 PROCN0 1
 Date 20110818
 Time 12.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 1620
 DW 33.333 usc
 DE 10.00 usc
 TE 297.9 K
 DI 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 T0 1

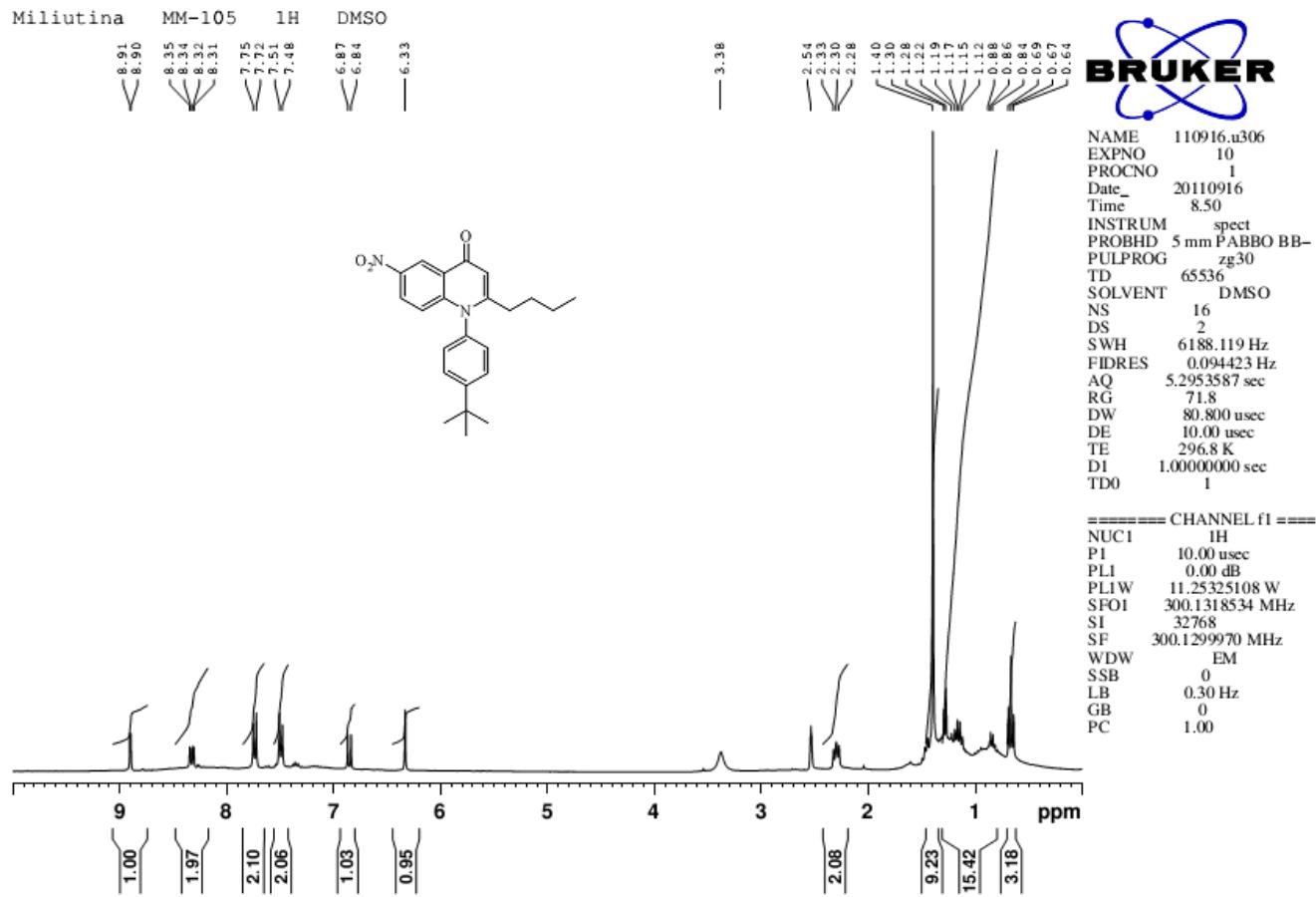
===== CHANNEL f1 =====

NUC1	^{13}C
P1	10.00 usc
PL1	-1.00 dB
SFO1	62.9015280 MHz

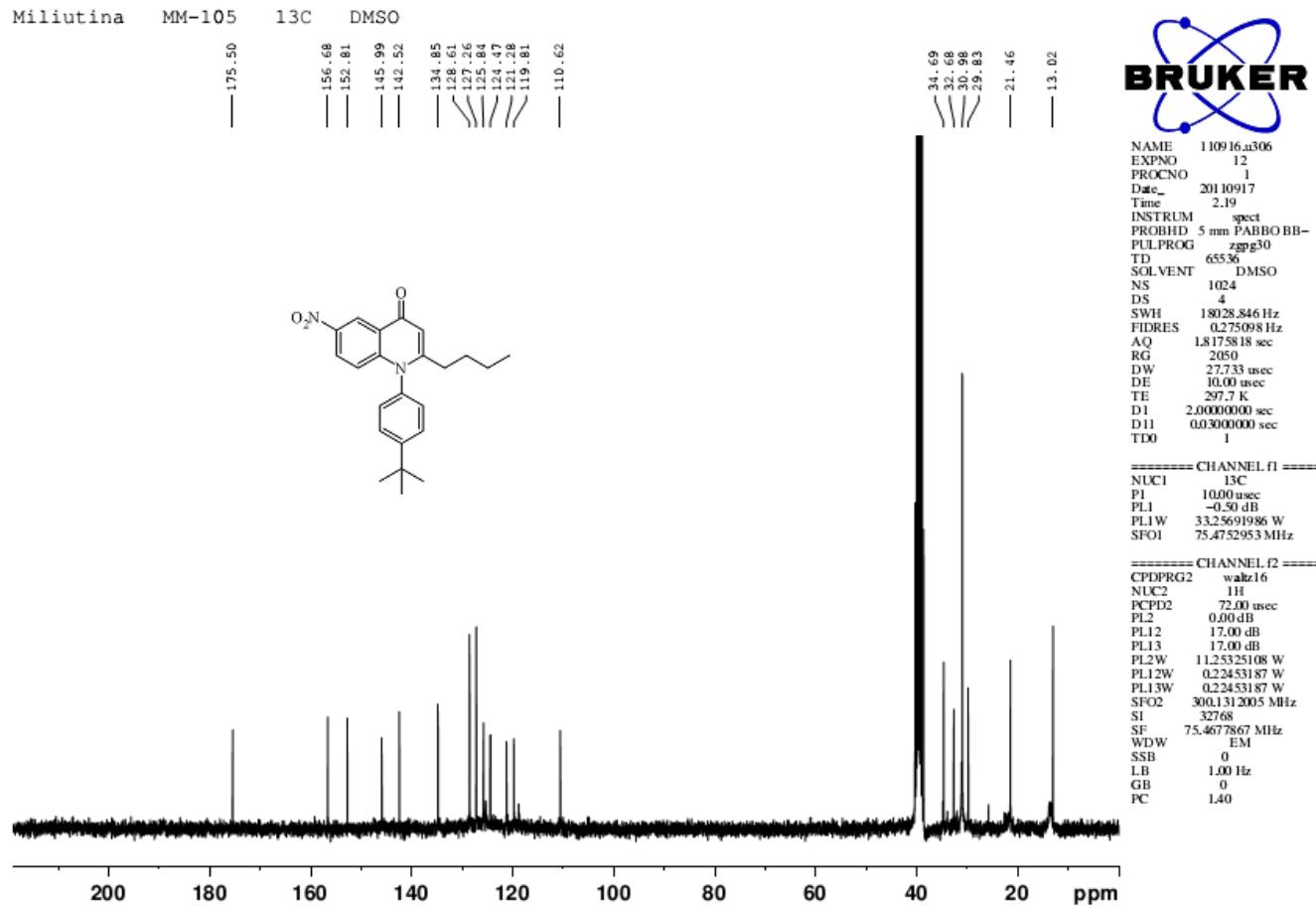
===== CHANNEL f2 =====

CPDPG2	walzt16
NUC2	^1H
PCPD2	70.00 usc
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz
SI	32768
SF	62.8952692 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

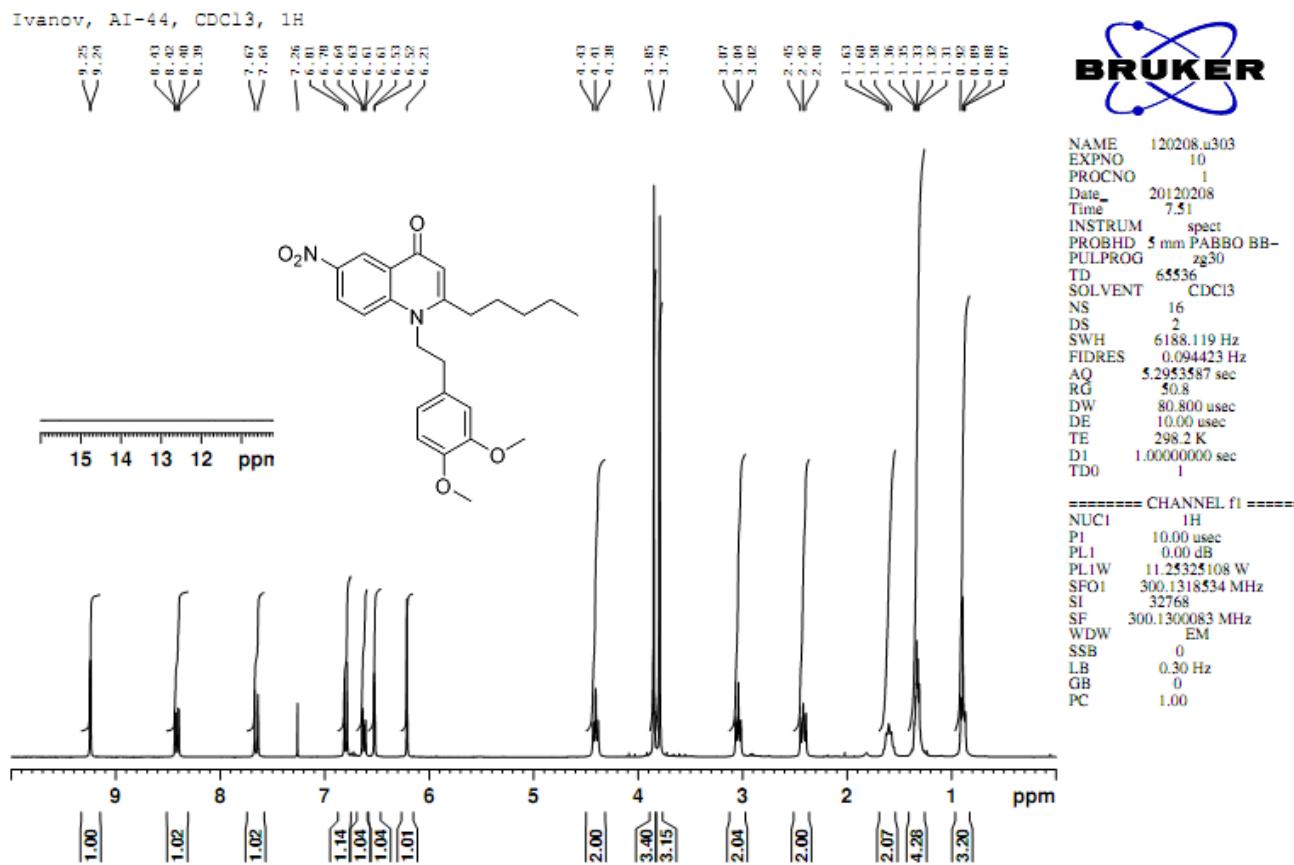
2-Butyl-1-(4-*tert*-butylphenyl)-6-nitroquinolin-4(1*H*)-one (7cd).



2-Butyl-1-(4-*tert*-butylphenyl)-6-nitroquinolin-4(1*H*)-one (7cd).



6-Nitro-(3,4-dimethoxyphenethyl)-2-pentyl-4-quinolone (7da).

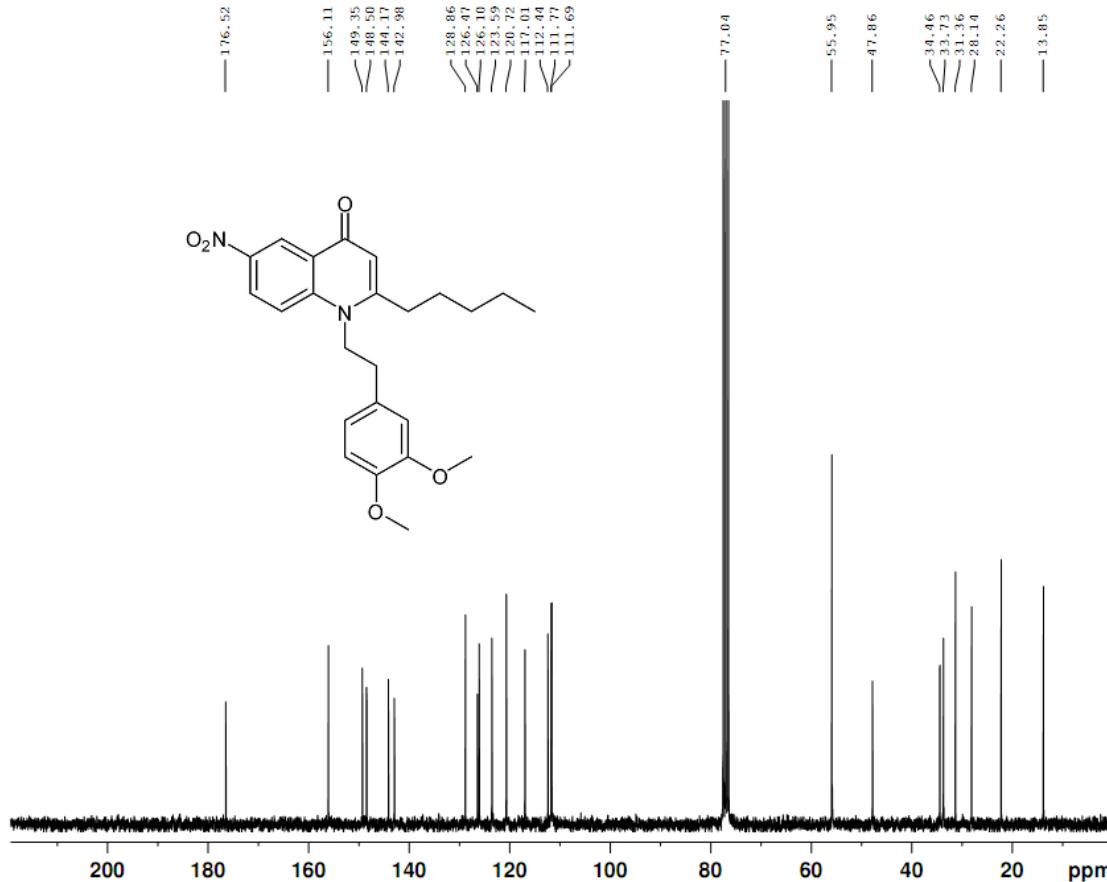


NAME 120208.u303
 EXPNO 10
 PROCNO 1
 Date_ 20120208
 Time 7.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 50.8
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0.00 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz
 SI 32768
 SF 300.1300083 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

6-Nitro-(3,4-dimethoxyphenethyl)-2-pentyl-4-quinolone (7da).

Ivanov, AI-44, CDCl_3 , ^{13}C

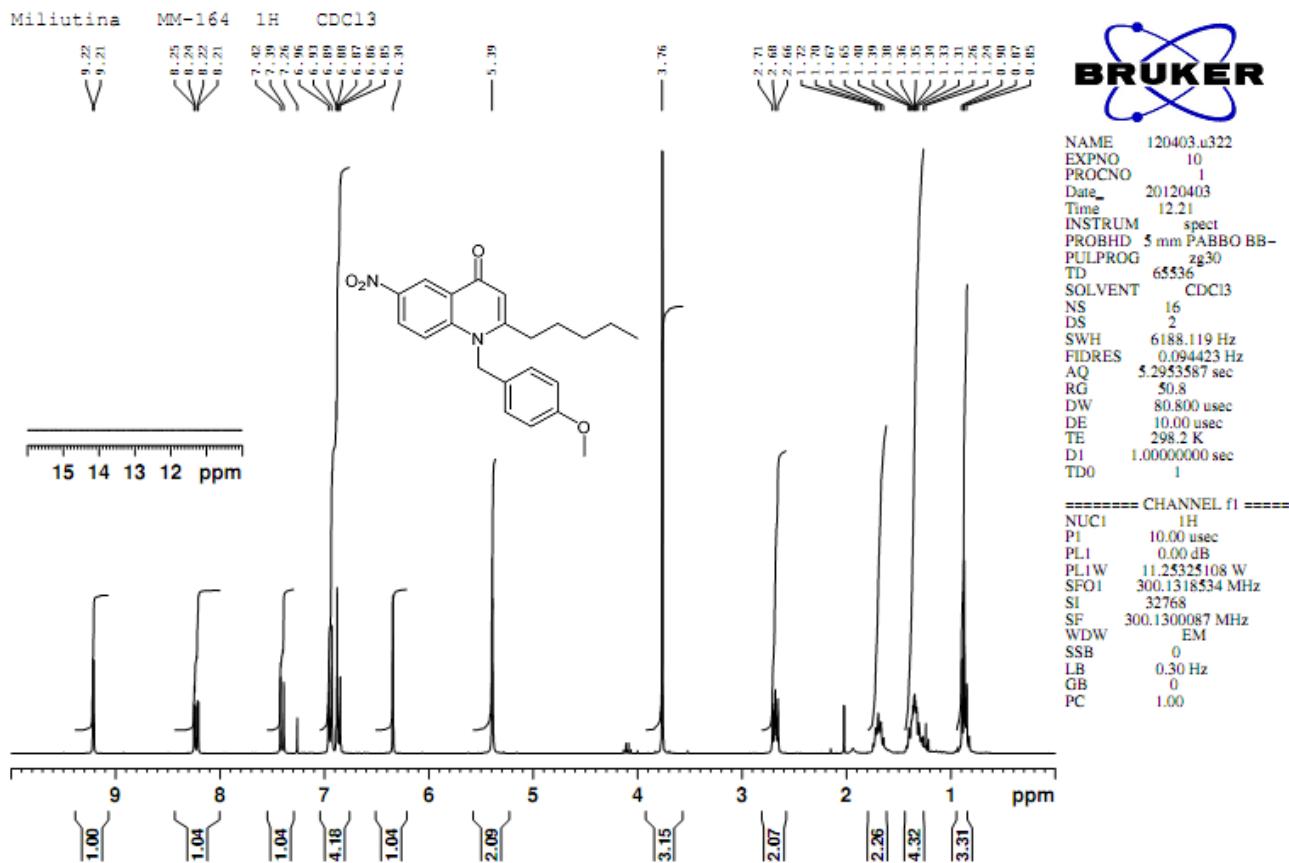


NAME 120208.203
 EXPNO 10
 PROCNO 1
 Date_ 20120208
 Time 12.38
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpp30
 TD 65536
 SOLVENT CDCl_3
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TDO 1

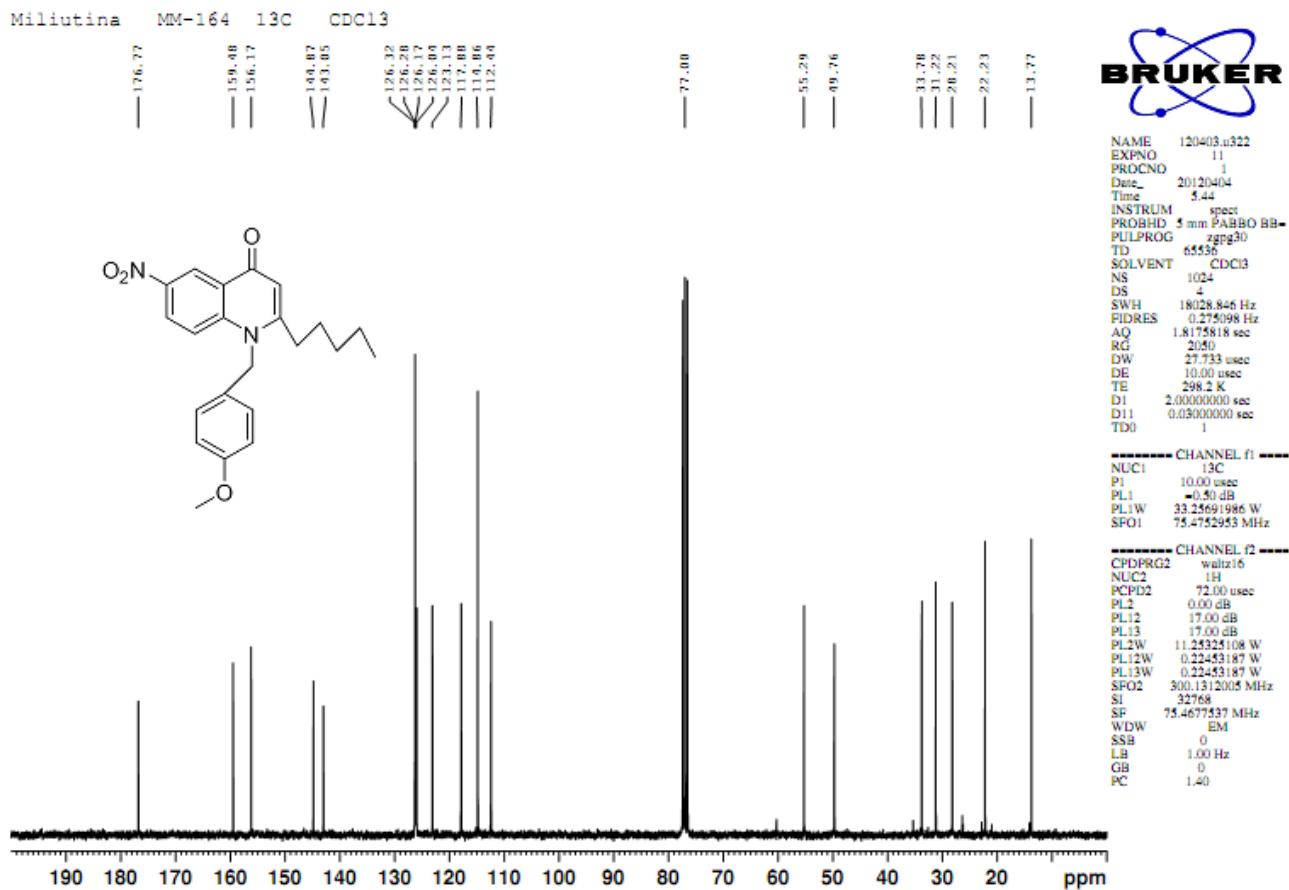
===== CHANNEL f1 =====
 NUC1 ^{13}C
 PI 10.20 usec
 PL1 0.00 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^1H
 PCPD2 70.00 usec
 PL12 14.00 dB
 PL13 14.00 dB
 PL2 -3.00 dB
 SFO2 250.1310005 MHz
 SI 32768
 SF 62.8952390 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

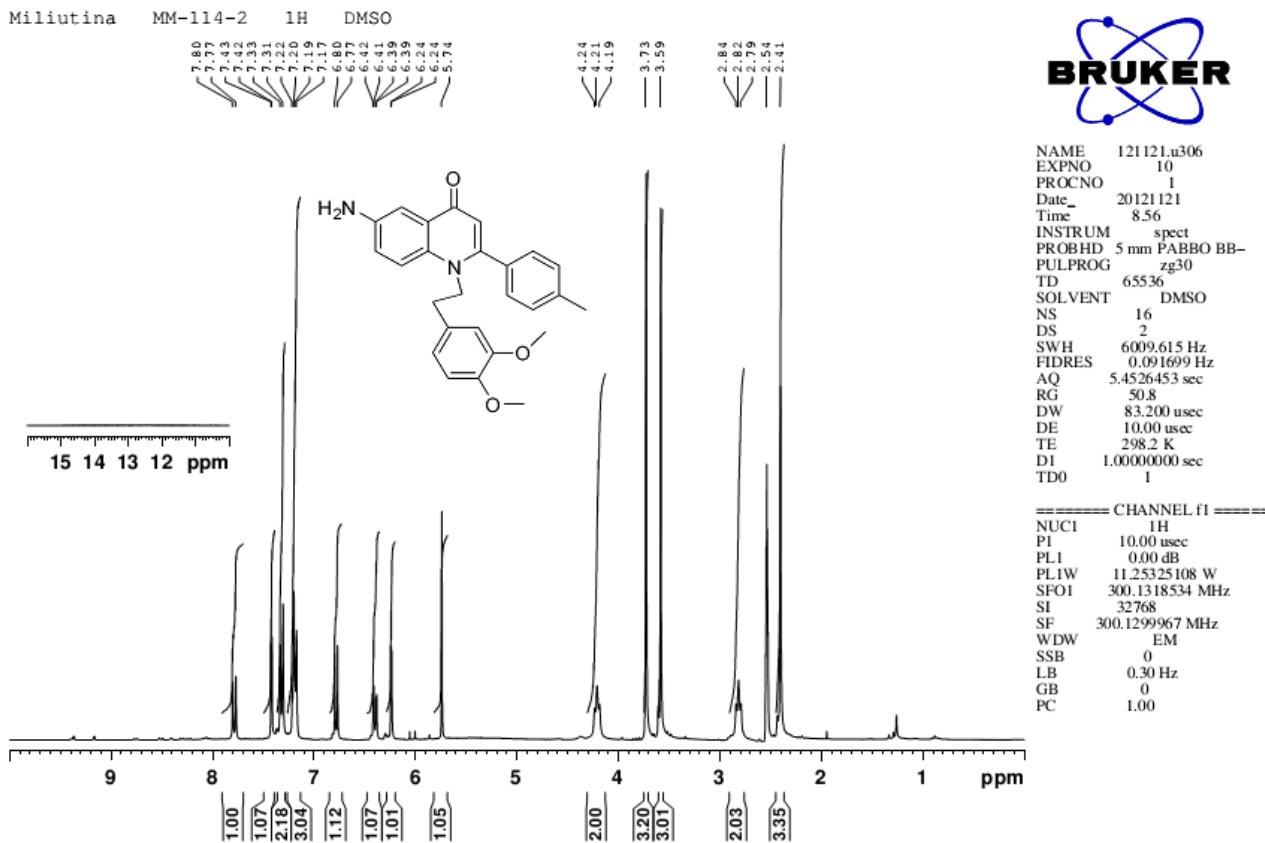
1-(4-Methoxybenzyl)-6-nitro-2-pentylquinolin-4(1H)-one (7db).



1-(4-Methoxybenzyl)-6-nitro-2-pentylquinolin-4(1H)-one (7db).

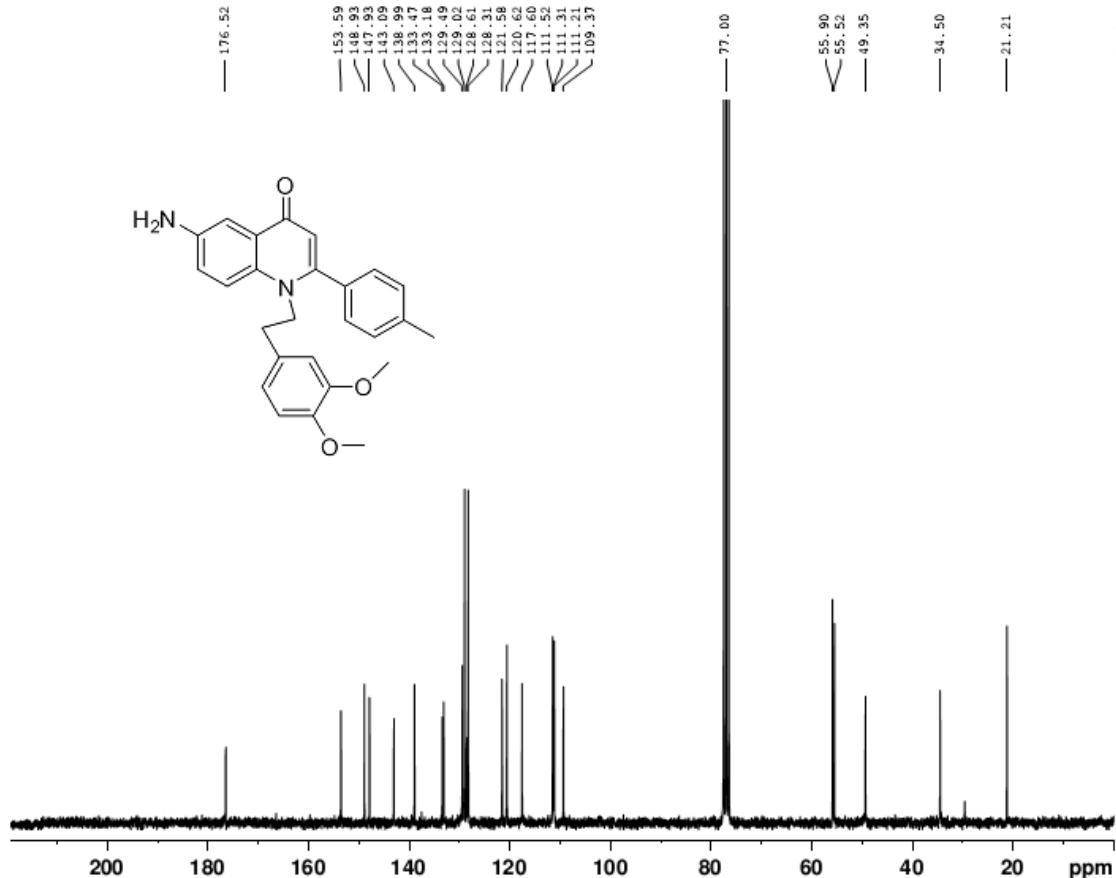


| **6-Amino-1-(3,4-dimethoxyphenethyl)-2-p-tolylquinolin-4(1*H*)-one (8aa).**



| **6-Amino-1-(3,4-dimethoxyphenethyl)-2-p-tolylquinolin-4(1H)-one (8aa).**

Miliutina, MM-114-2, CDCl_3 , ^{13}C



```

NAME      120706.203
EXPNO     10
PROCNO    1
Date:    20120706
Time:   22.36
INSTRUM  spect
PROBHD  5 mm PABBO BB-
PULPROG zpgg30
TD        65536
SOLVENT   CDCl3
NS        2048
DS         4
SWH       15000.000 Hz
FIDRES   0.228882 Hz
AQ        2.1845834 sec
RG        2050
DW        33.333 usec
DE        10.00 usec
TE        298.6 K
D1        2.0000000 sec
d11      0.03000000 sec
DELTA    1.89999998 sec
TD0          1

```

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===== CHANNEL f1 =====
NUC1      13C
PI        10.00 usec
PL1      -1.00 dB
SFO1     62.9015280 MHz

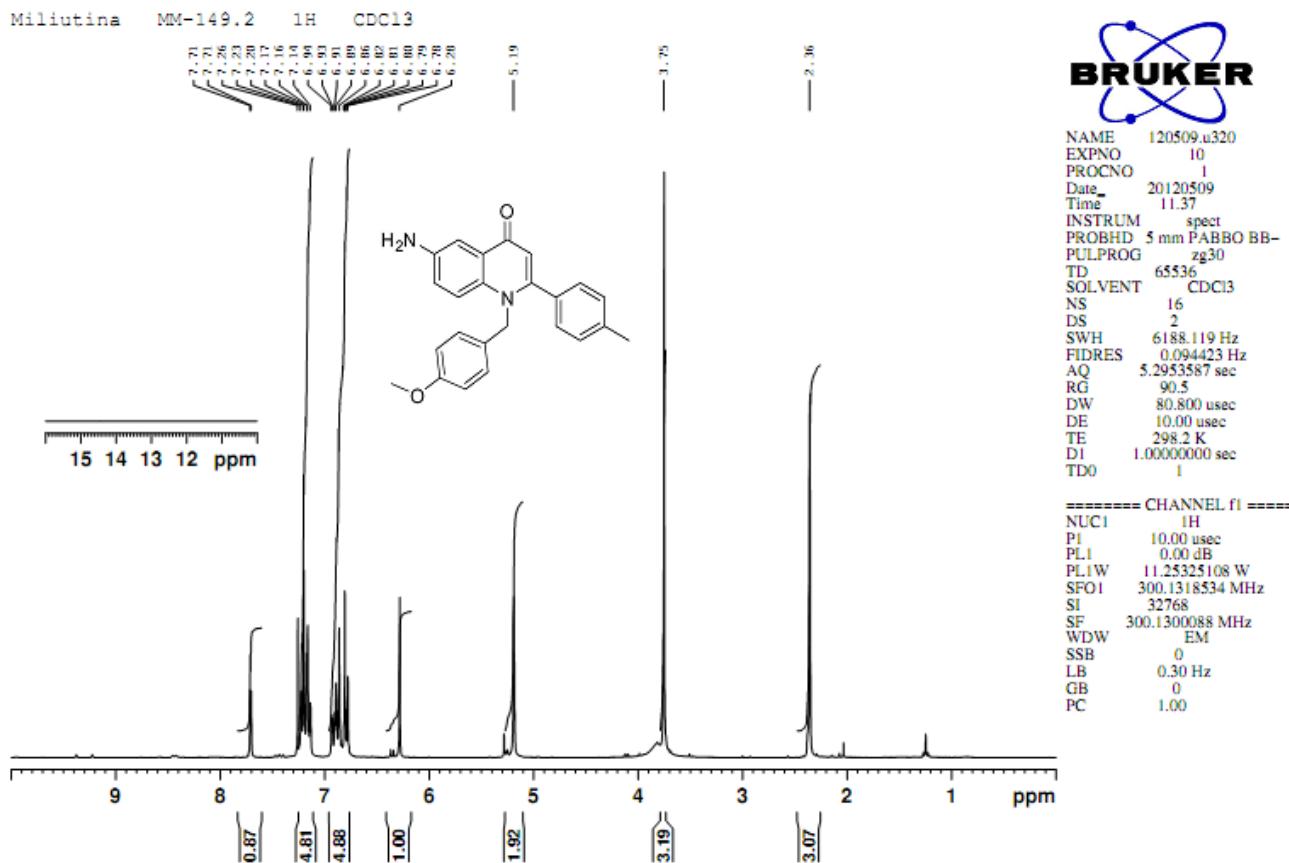
```

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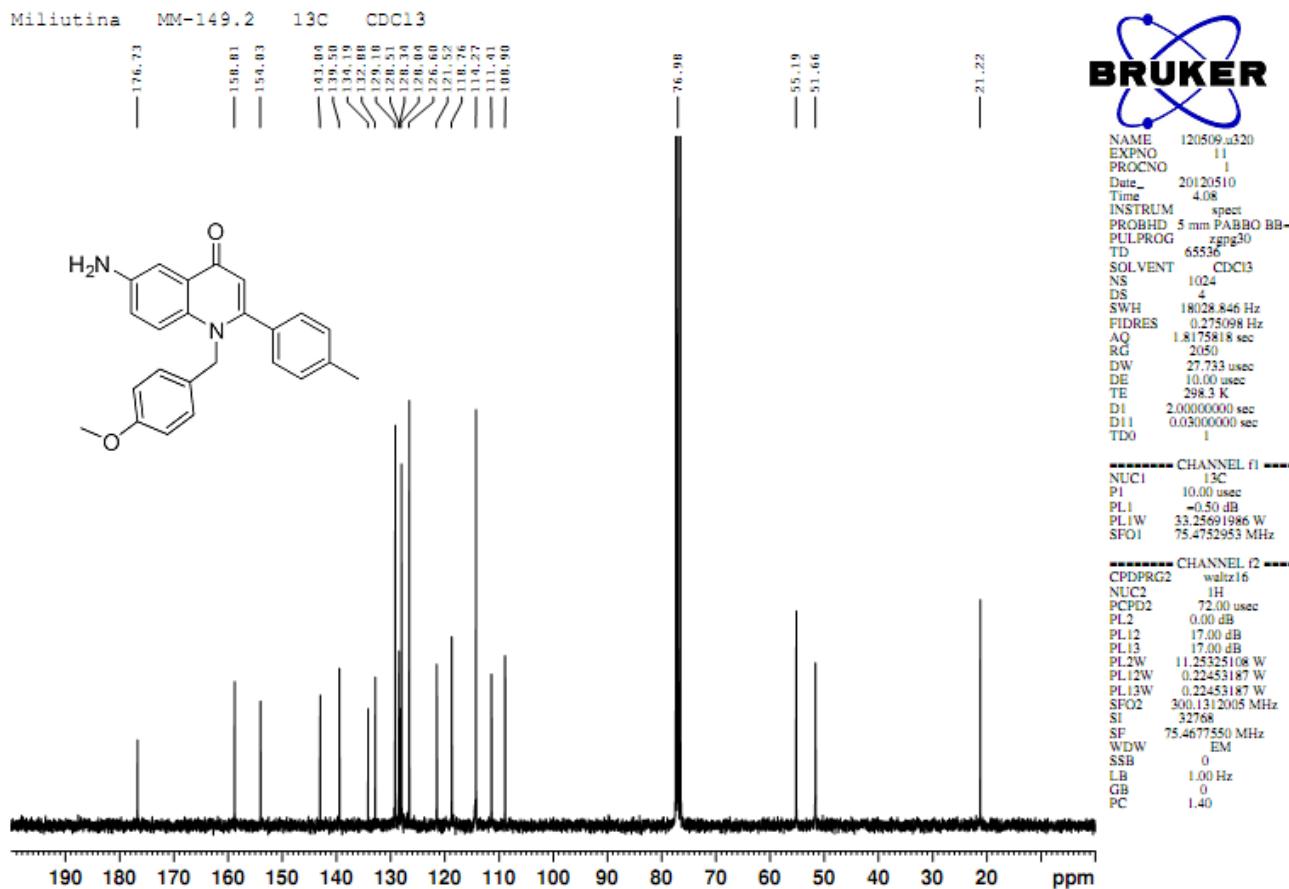
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2     70.00 usec
PL12     15.00 dB
PL13     15.00 dB
PL2      -2.50 dB
SFO2     250.1310005 MHz
SI        32768
SF       62.8952423 MHz
WDW        EM
SSB        0
LB        1.00 Hz
GB        0
PC        1.40

```

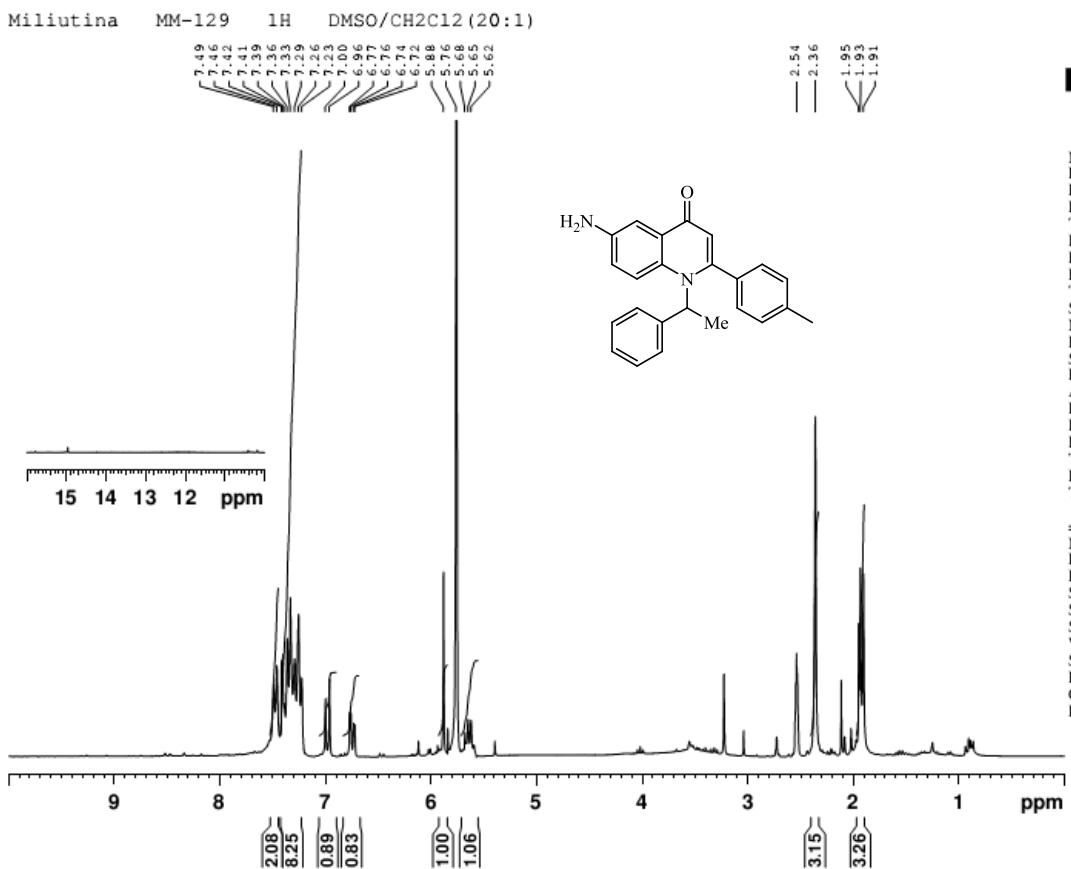
| 6-Amino-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (8ab).



| 6-Amino-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (8ab).



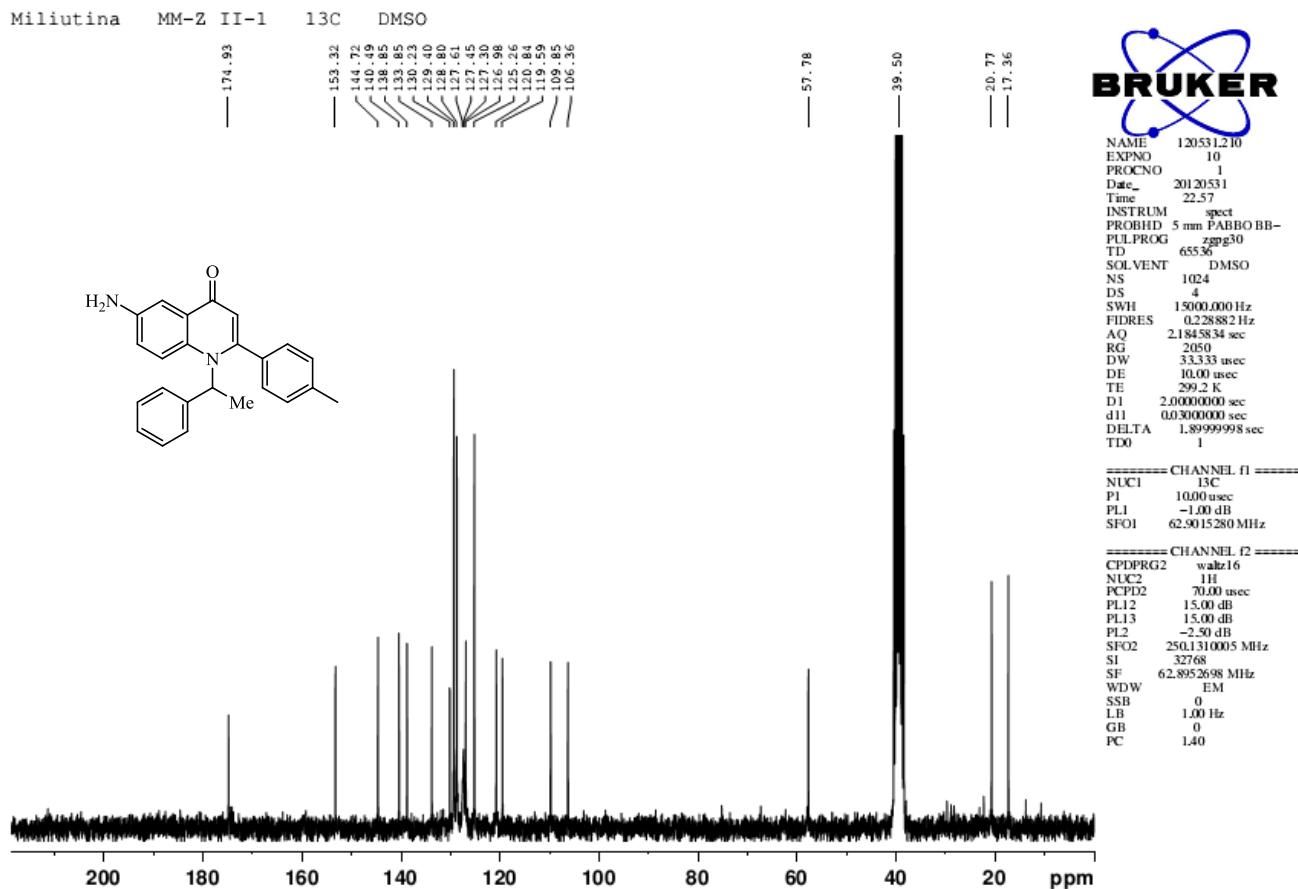
| 6-Amino-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (**8ac**).



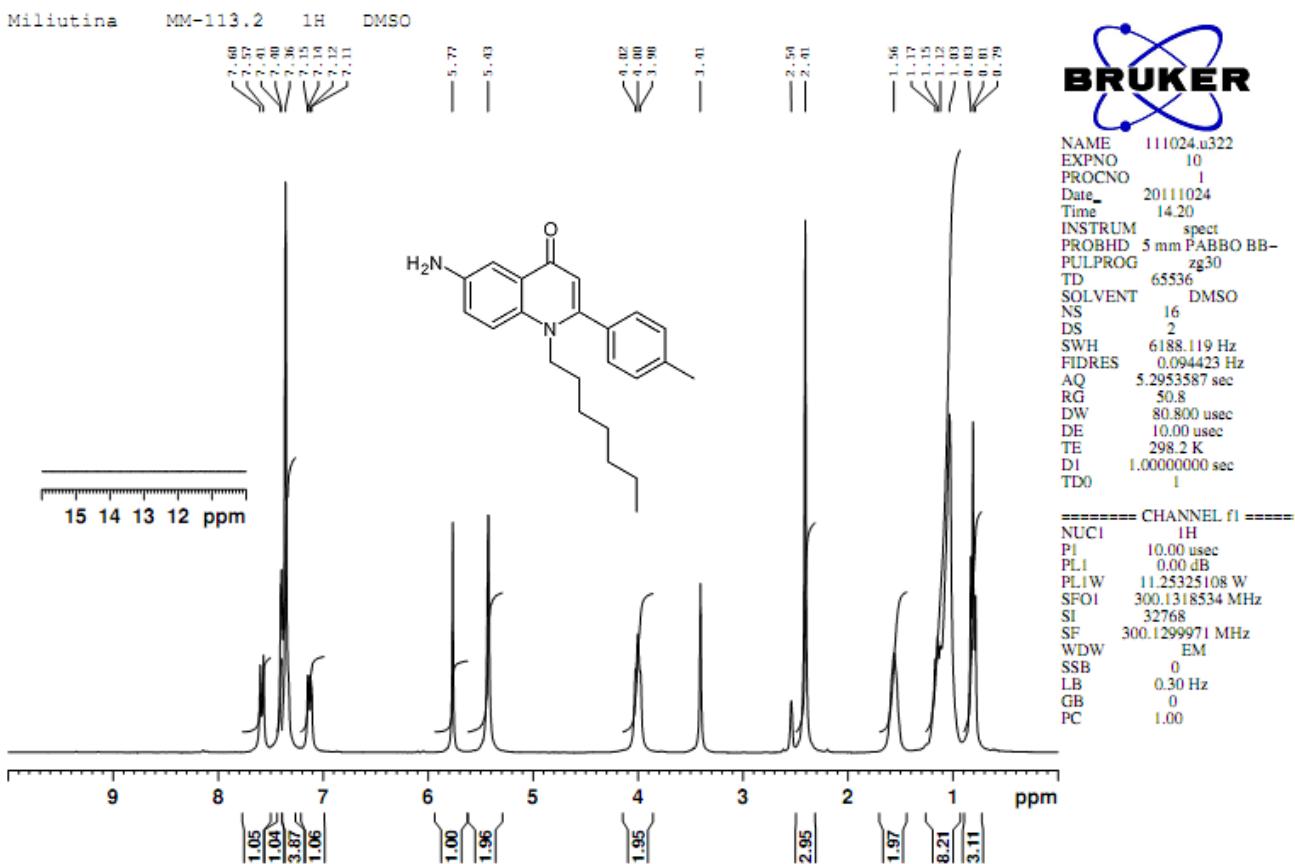
NAME 121217.205
EXPNO 10
PROCNO 1
Date_ 20121217
Time 14.03
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 161
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUCI 1H
PI 11.40 usec
PL1 -3.00 dB
SF01 250.1315447 MHz
SI 32768
SF 250.1299838 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

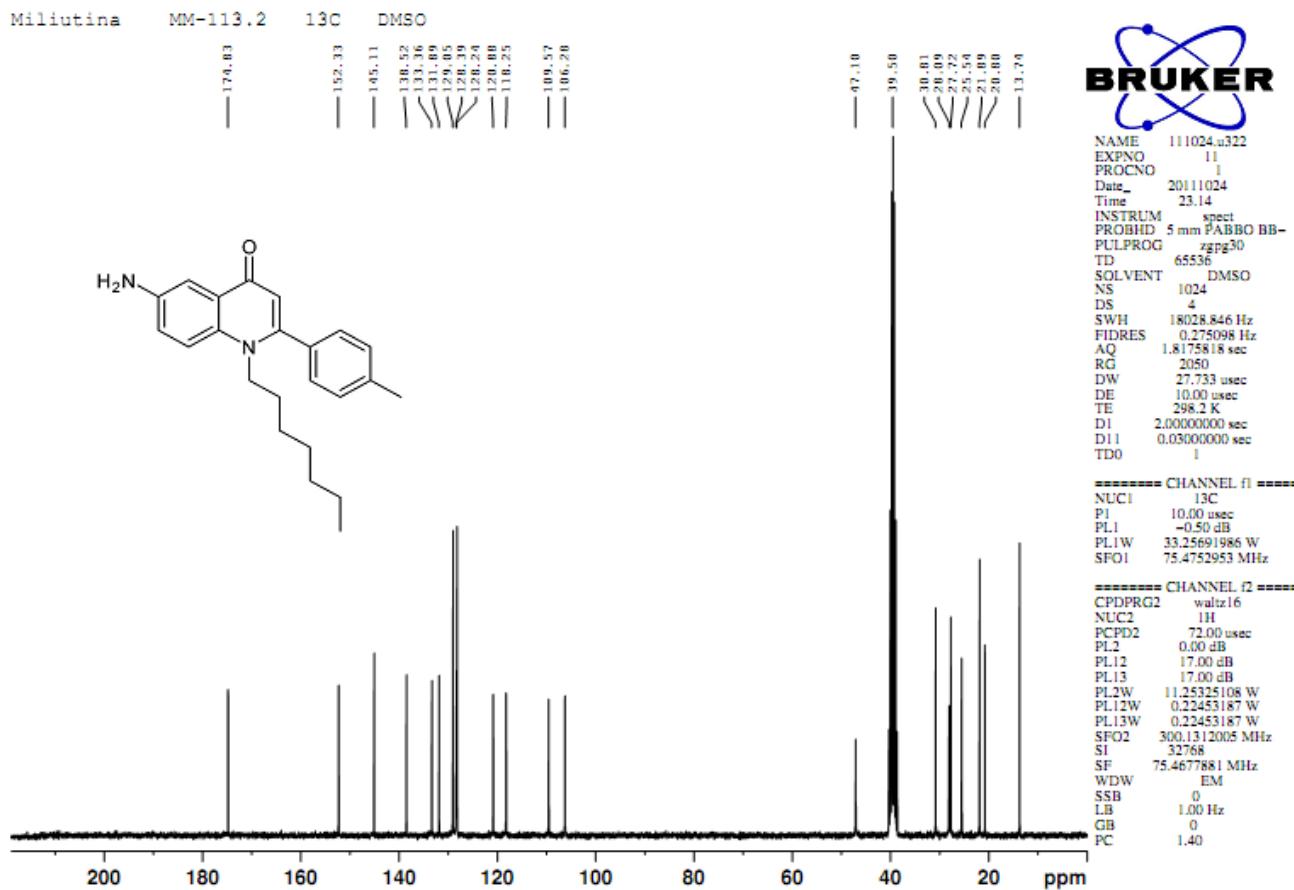
| **6-Amino-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (8ac).**



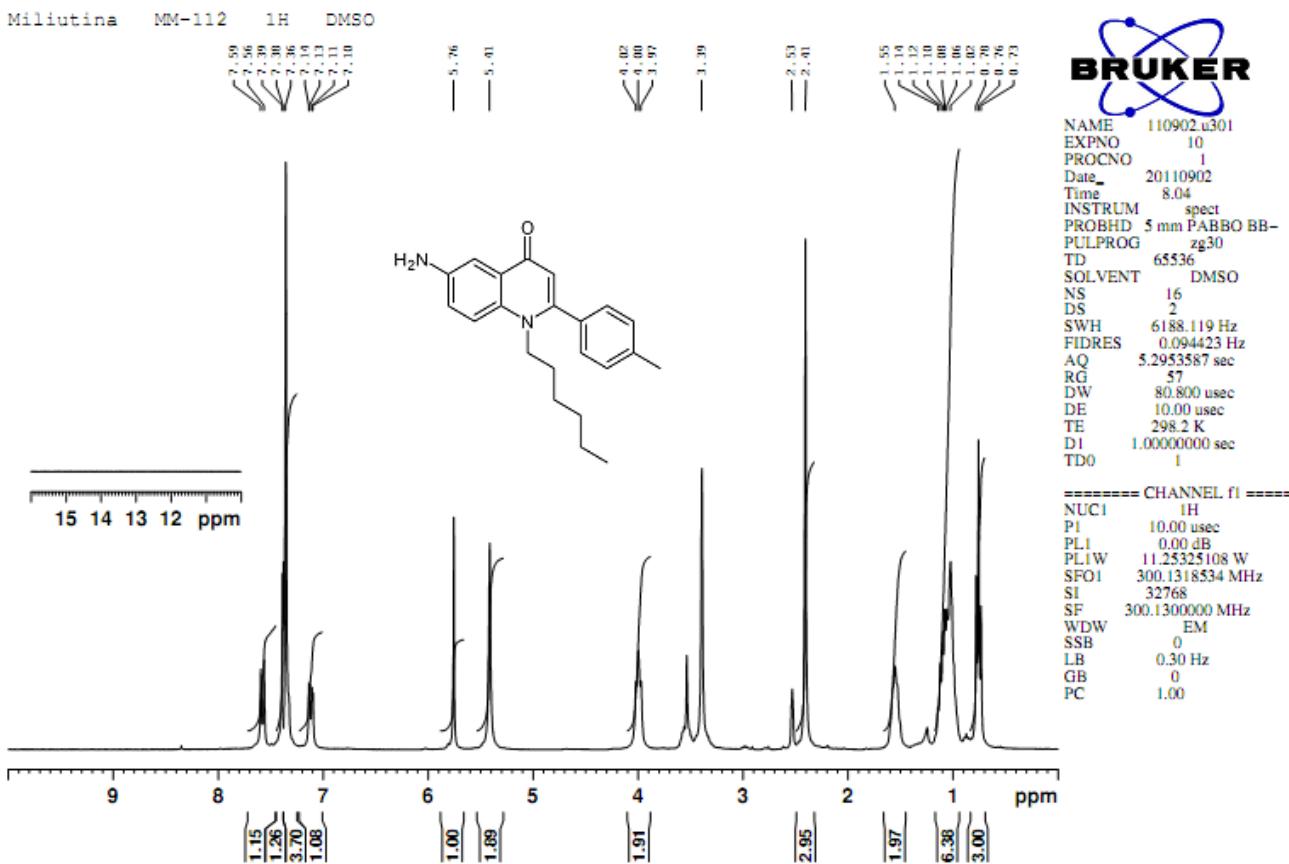
6-Amino-1-heptyl-2-*p*-tolylquinolin-4(1*H*)-one (8ad).



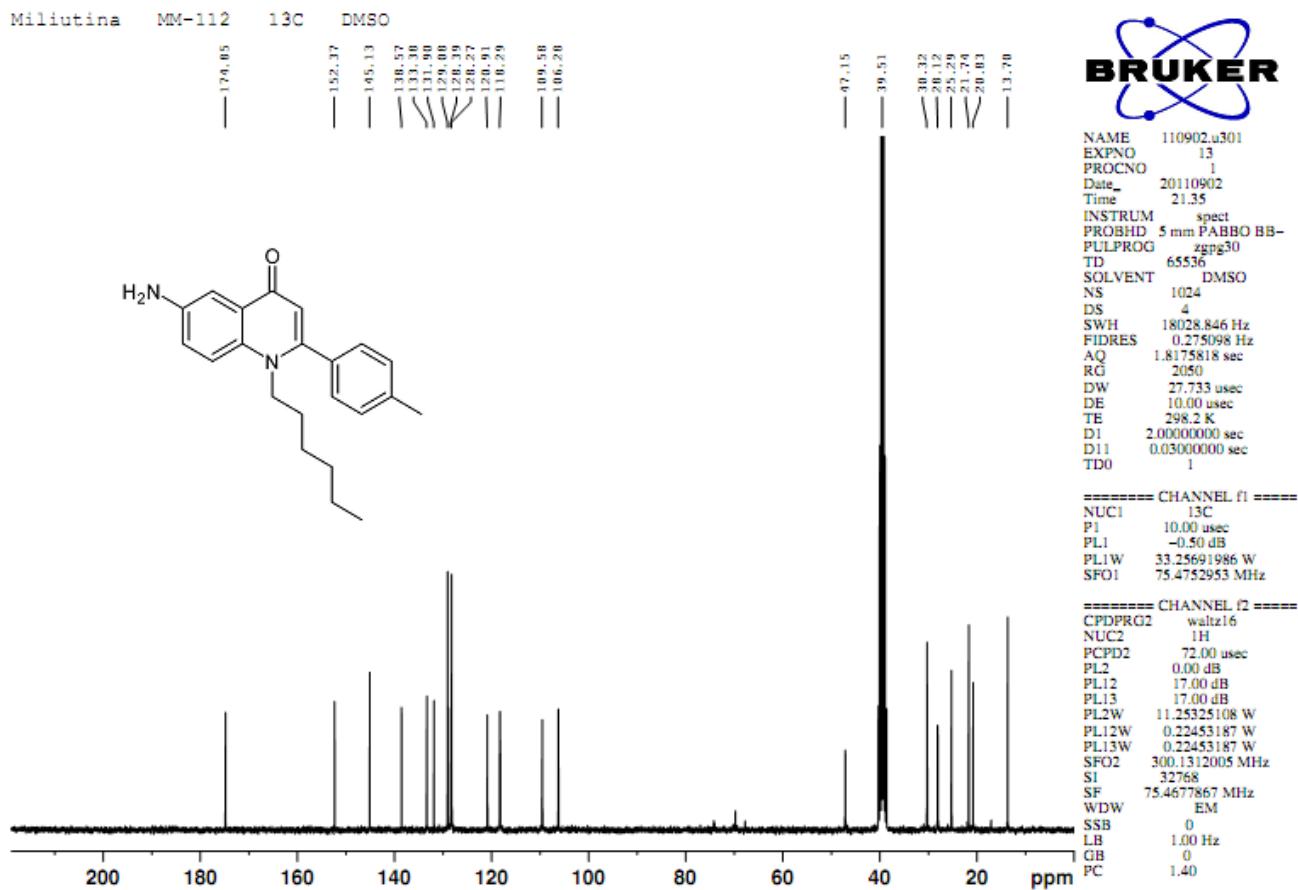
| 6-Amino-1-heptyl-2-p-tolylquinolin-4(1H)-one (8ad).



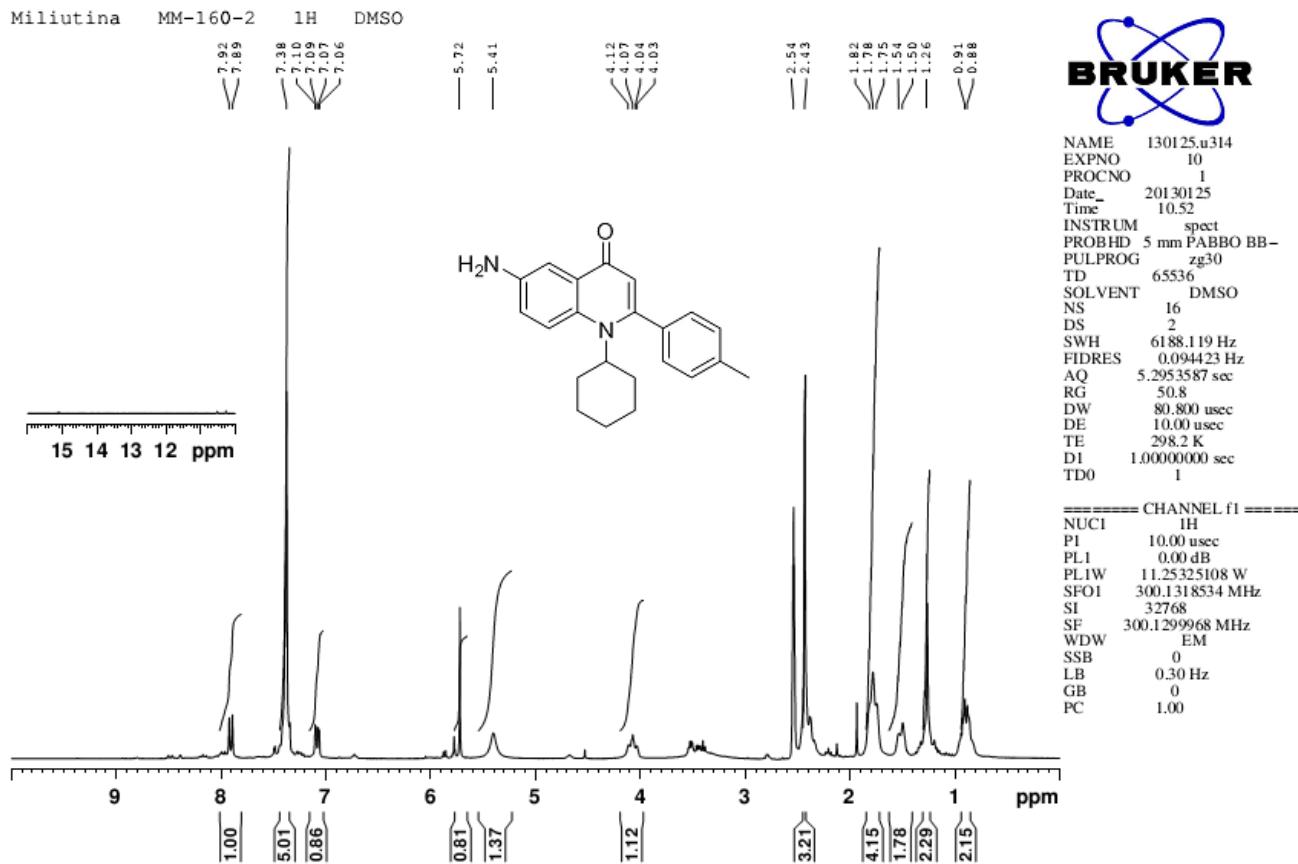
| **6-Amino-1-hexyl-2-p-tolylquinolin-4(1H)-one (8ae).**



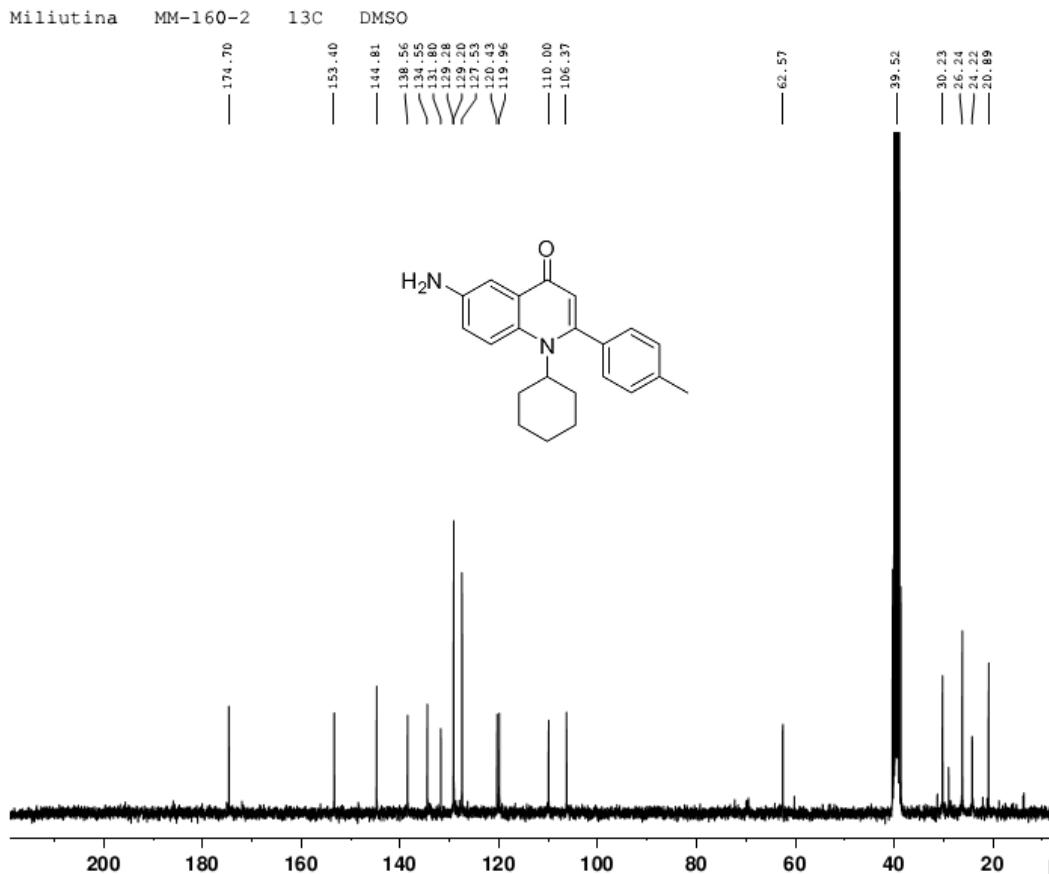
| **6-Amino-1-hexyl-2-p-tolylquinolin-4(1H)-one (8ae).**



Formatiert: Englisch (USA)

6-Amino-1-cyclohexyl-2-p-tolylquinolin-4(1H)-one (8af).

| **6-Amino-1-cyclohexyl-2-p-tolylquinolin-4(1H)-one (8af).**

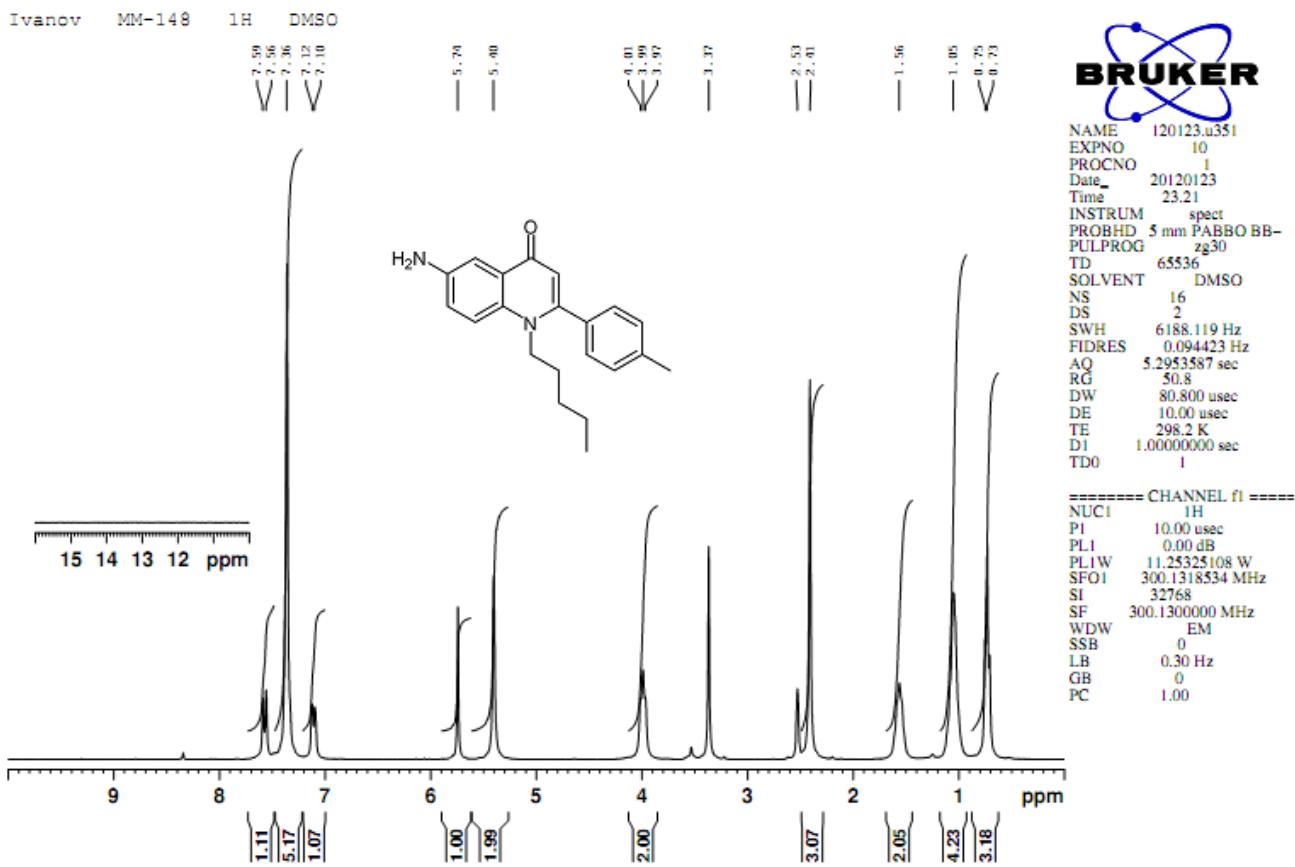


NAME 130125a314
EXPNO 11
PROCNO 1
Date 20130125
Time 22:03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.2750981 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

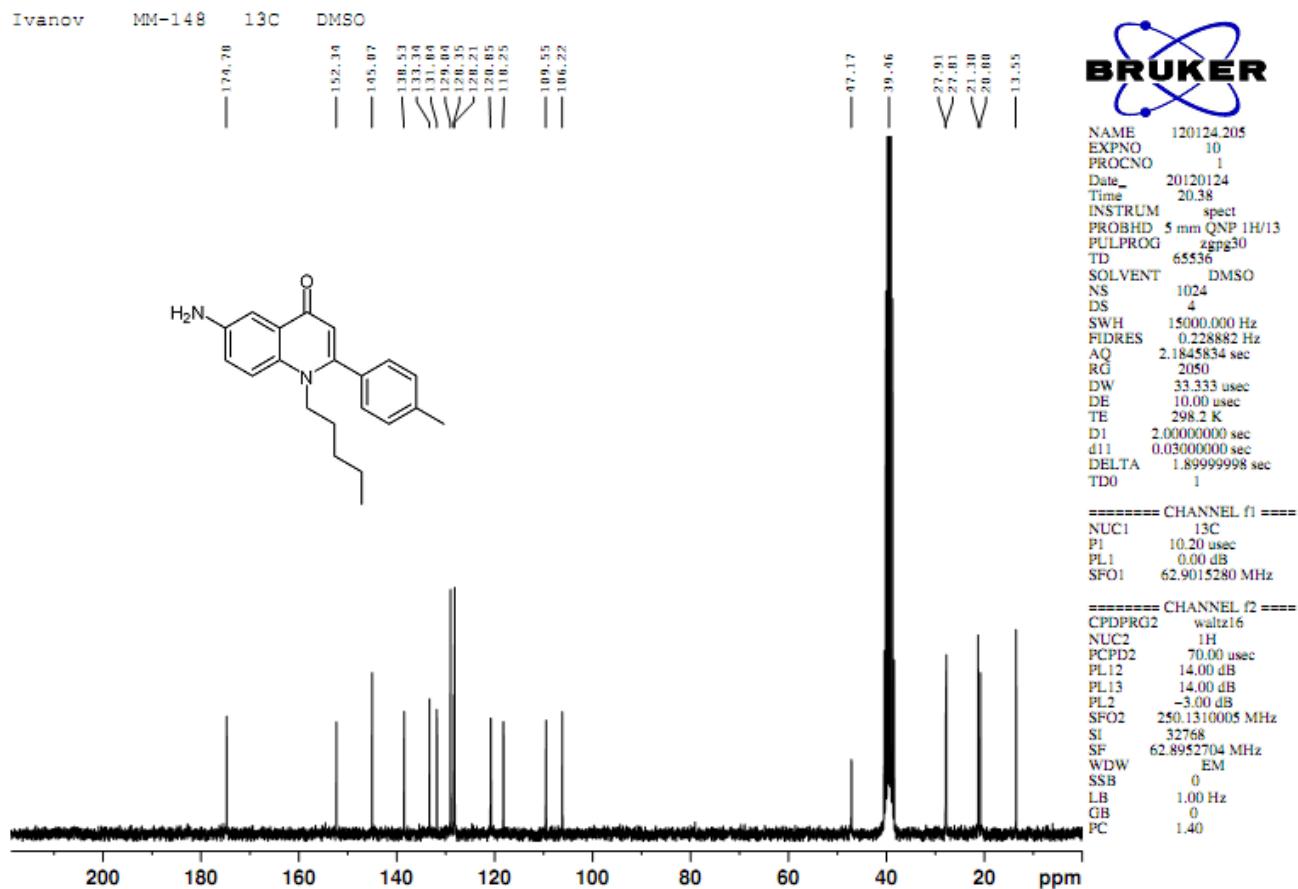
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

===== CHANNEL d =====
CPDPG2 walkz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32.768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

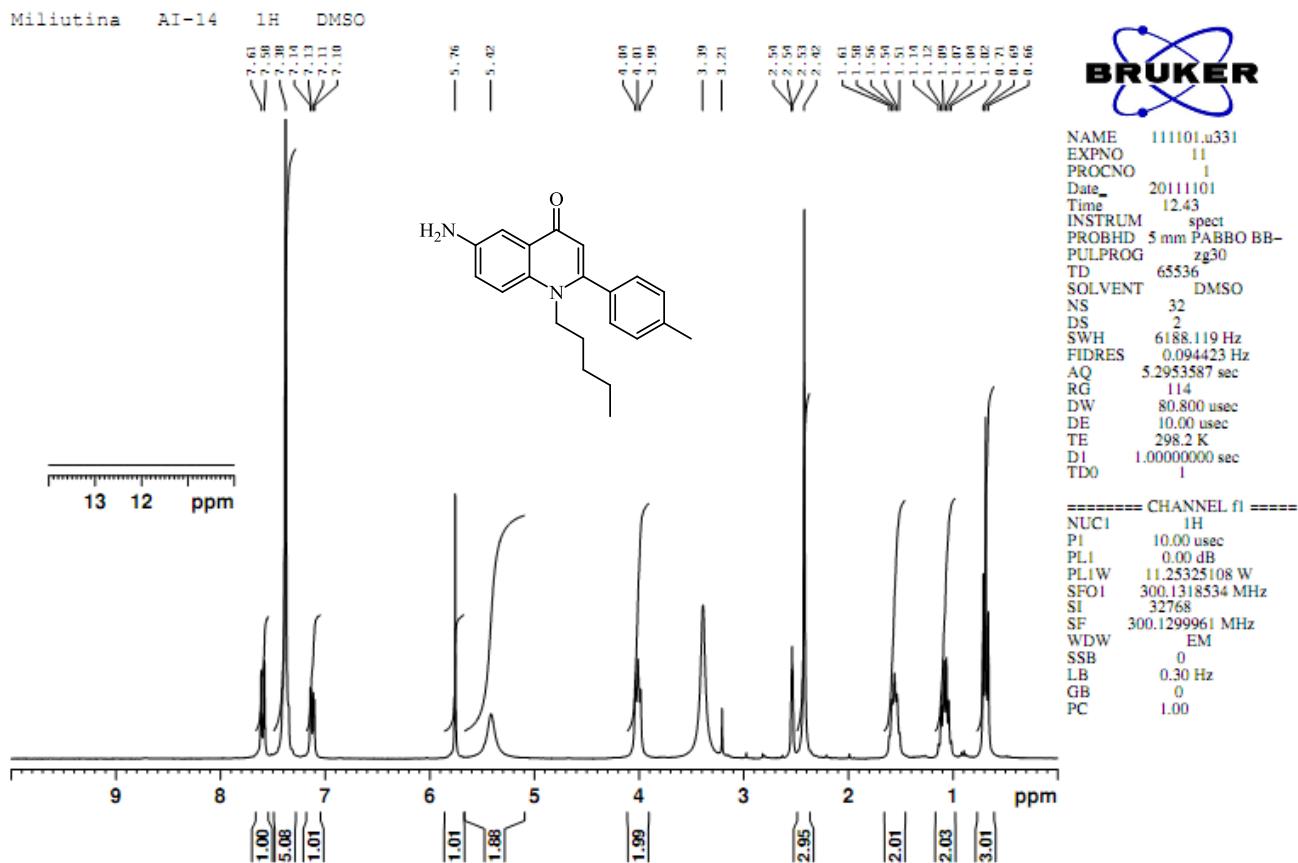
| 6-Amino-1-pentyl-2-*p*-tolylquinolin-4(1*H*)-one (**8ag**).



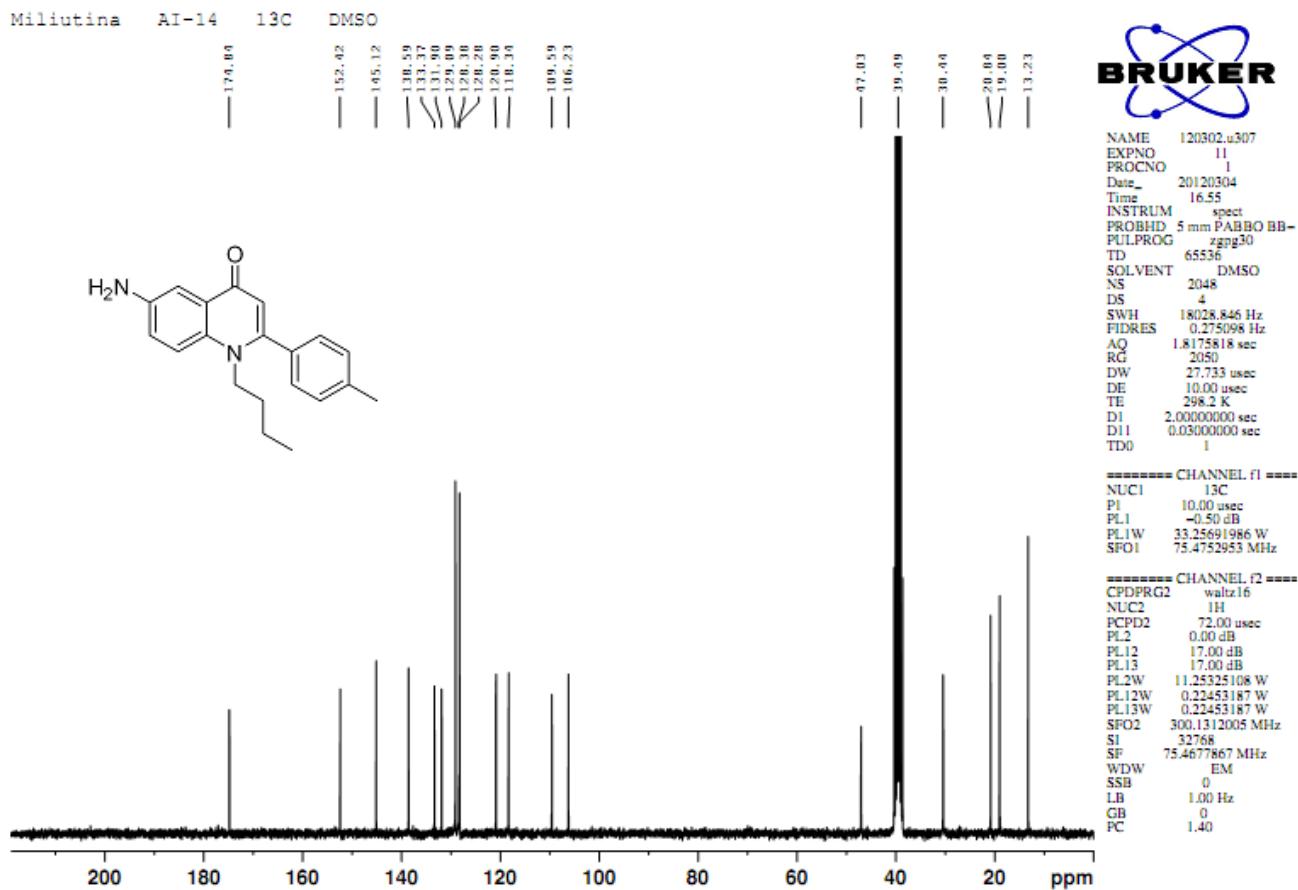
6-Amino-1-pentyl-2-*p*-tolylquinolin-4(1*H*)-one (8ag).



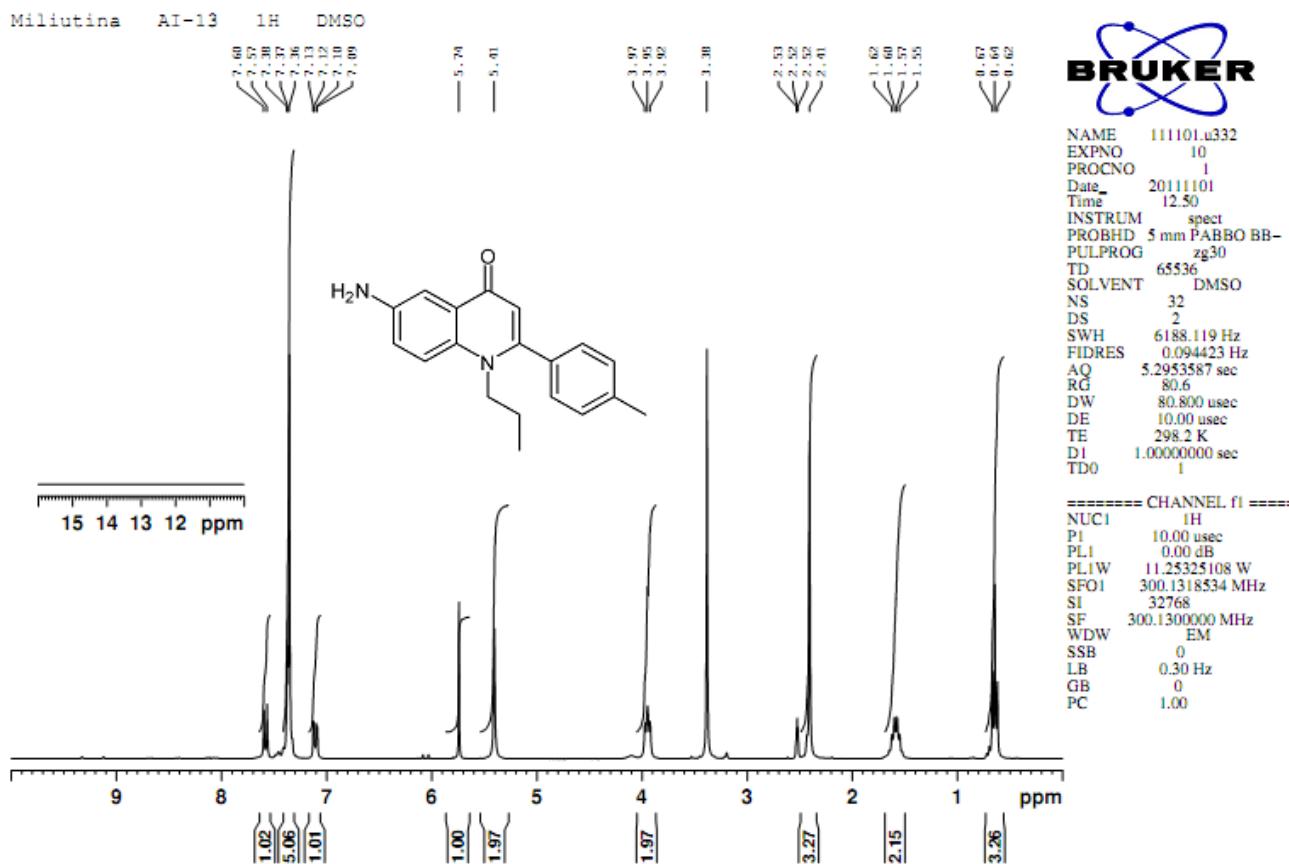
6-Amino-1-*n*-butyl-2-*p*-tolyl-4-quinolone (**8ah**).



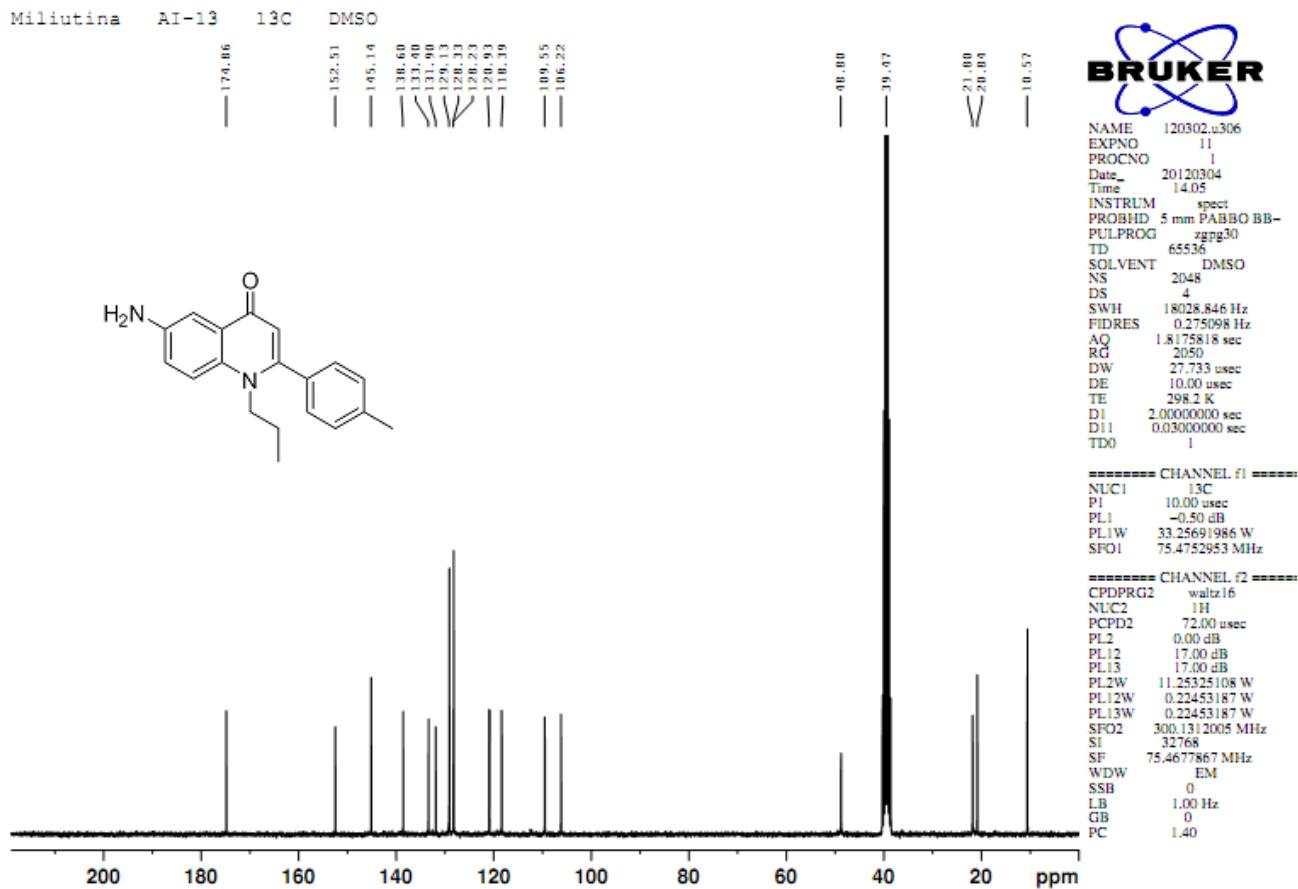
| **6-Amino-1-*n*-butyl-2-*p*-tolyl-4-quinolone (8ah).**



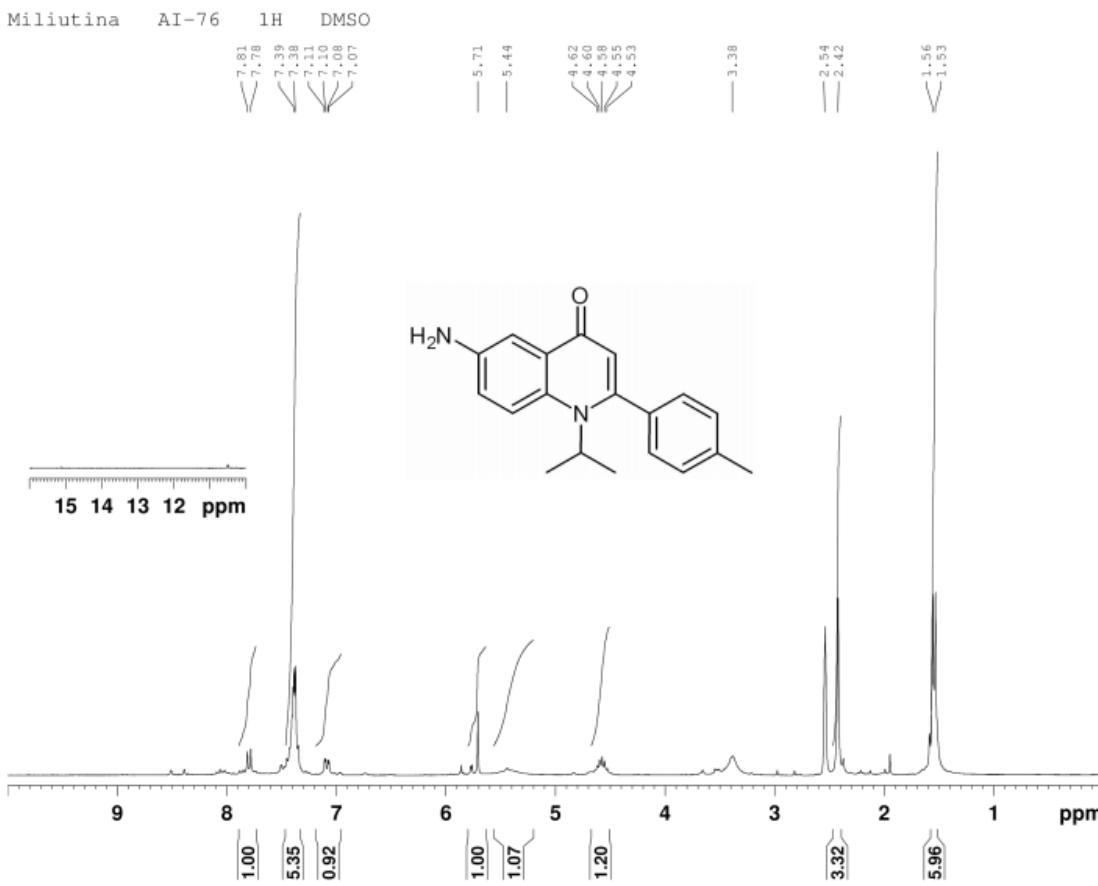
| **6-Amino-1-*n*-propyl-2-*p*-tolyl-4-quinolone (8ai).**



| 6-Amino-1-*n*-propyl-2-*p*-tolyl-4-quinolone (**8ai**).



| **6-Amino-1-isopropyl-2-p-tolylquinolin-4(1H)-one (8aj).**



```

NAME 130123.u315
EXPNO 10
PROCNO 1
Date_ 20130123
Time 13.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

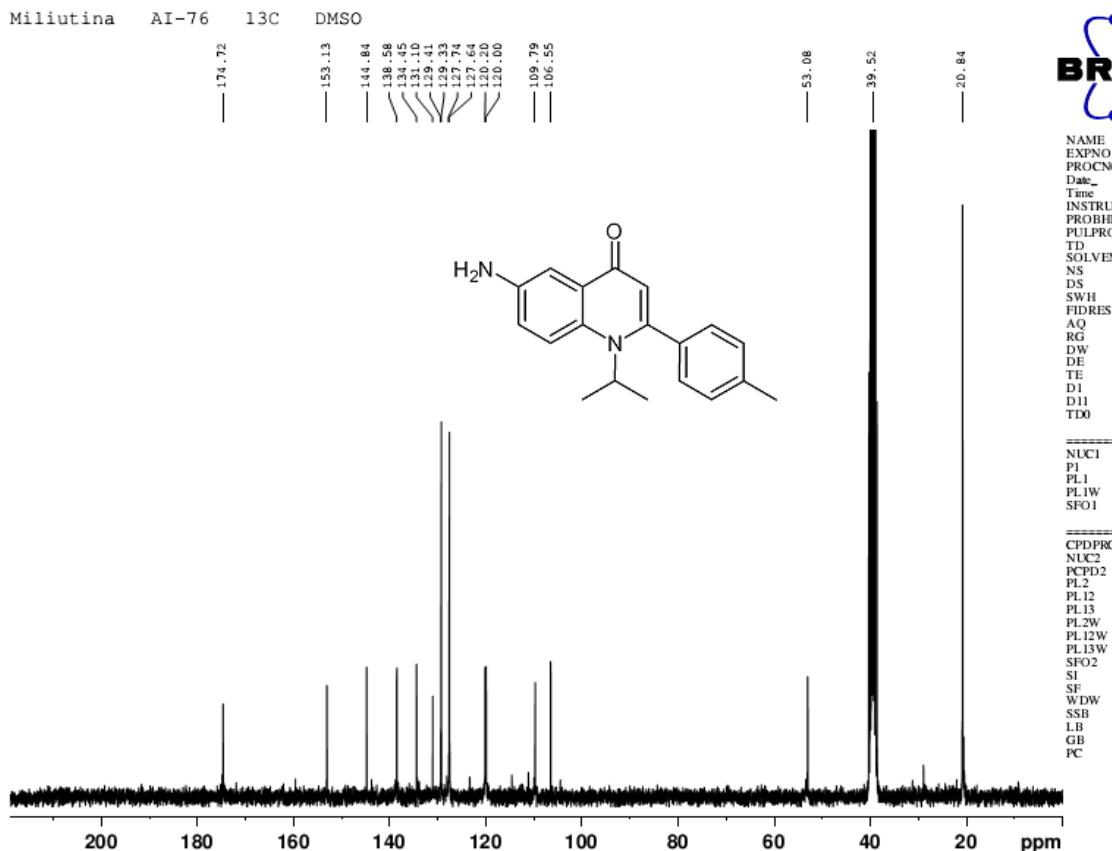
```

```

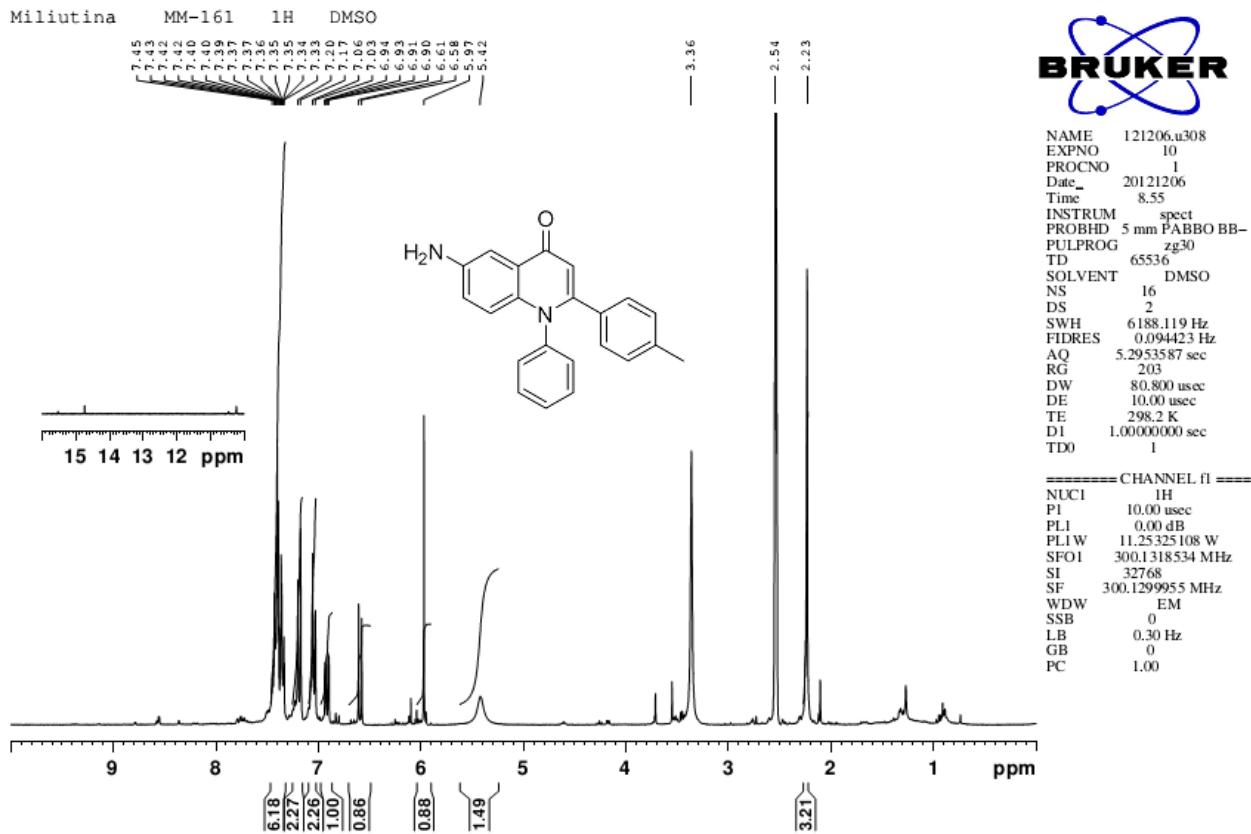
===== CHANNEL f1 ====
NUC1 1H
PI 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299976 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

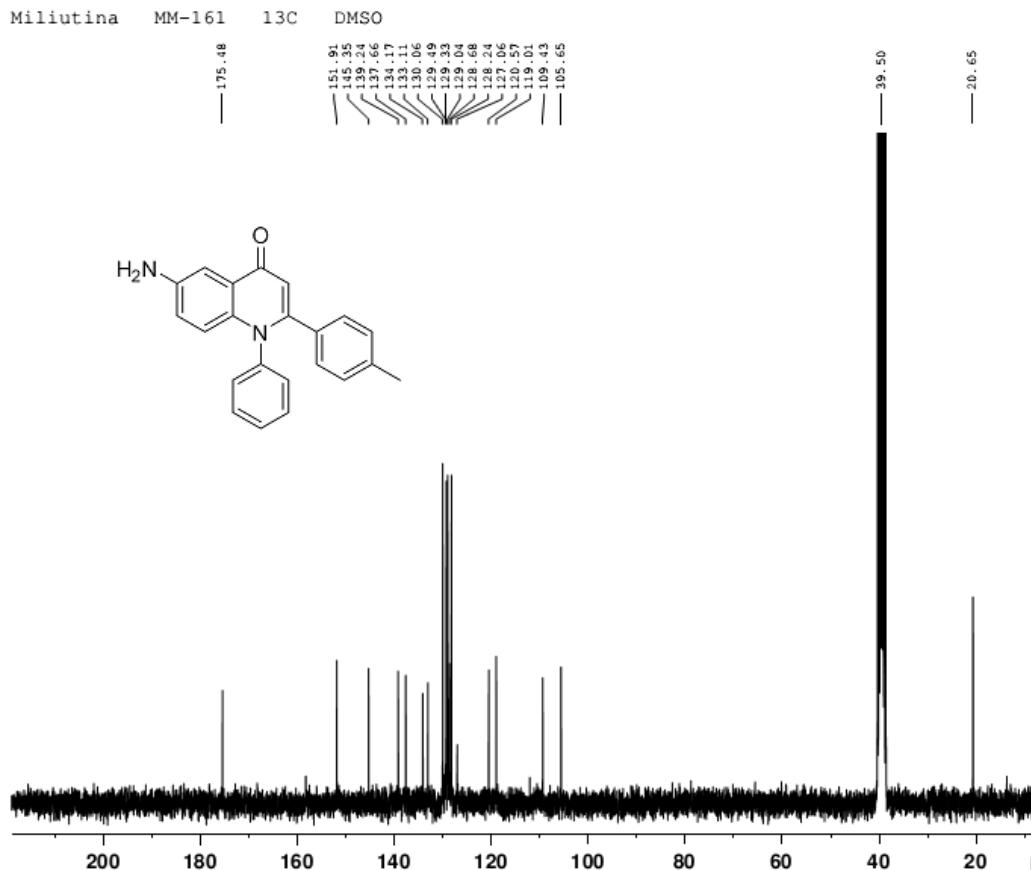
| **6-Amino-1-isopropyl-2-p-tolylquinolin-4(1H)-one (8aj).**



| 6-Amino-1-phenyl-2-p-tolylquinolin-4(1H)-one (**8ak**).



| **6-Amino-1-phenyl-2-p-tolylquinolin-4(1H)-one (8ak).**



```

NAME 121207.u319
EXPNO 10
PROCNO 1
Date 20121208
Time 15.56
INSTRUM spect
PROBID 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

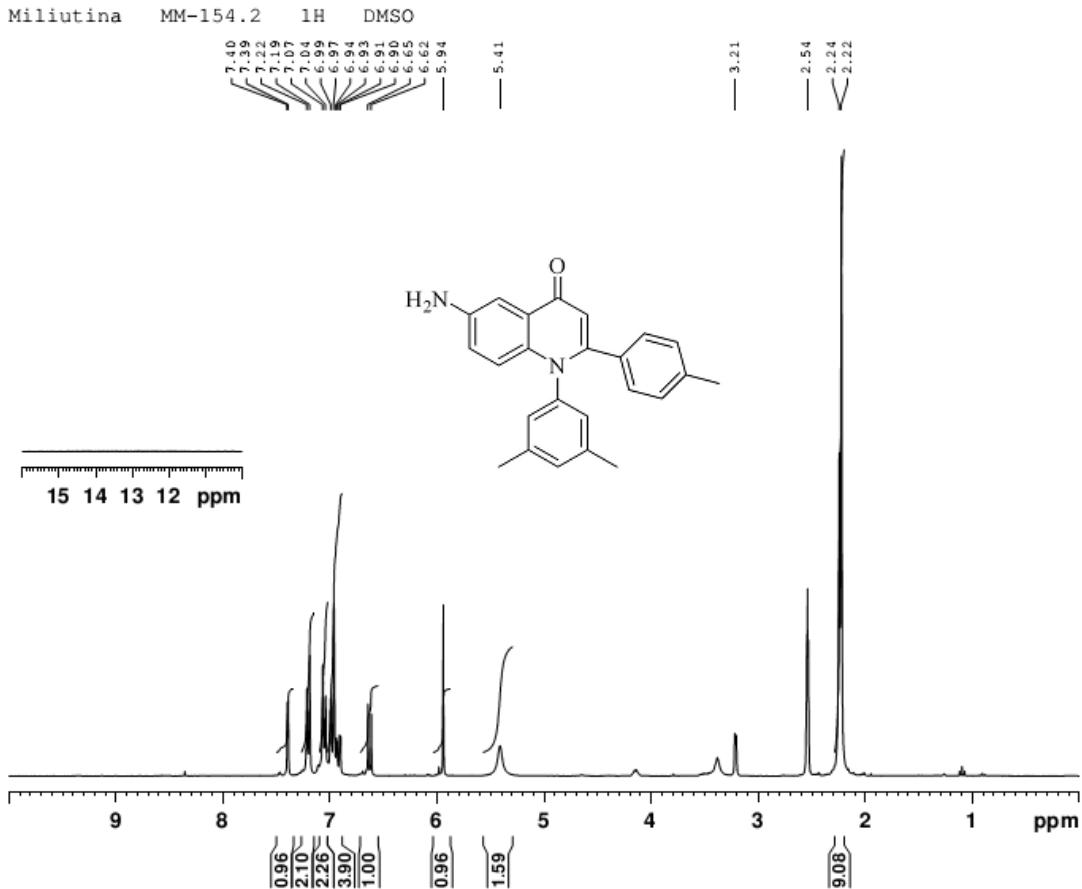
```

```

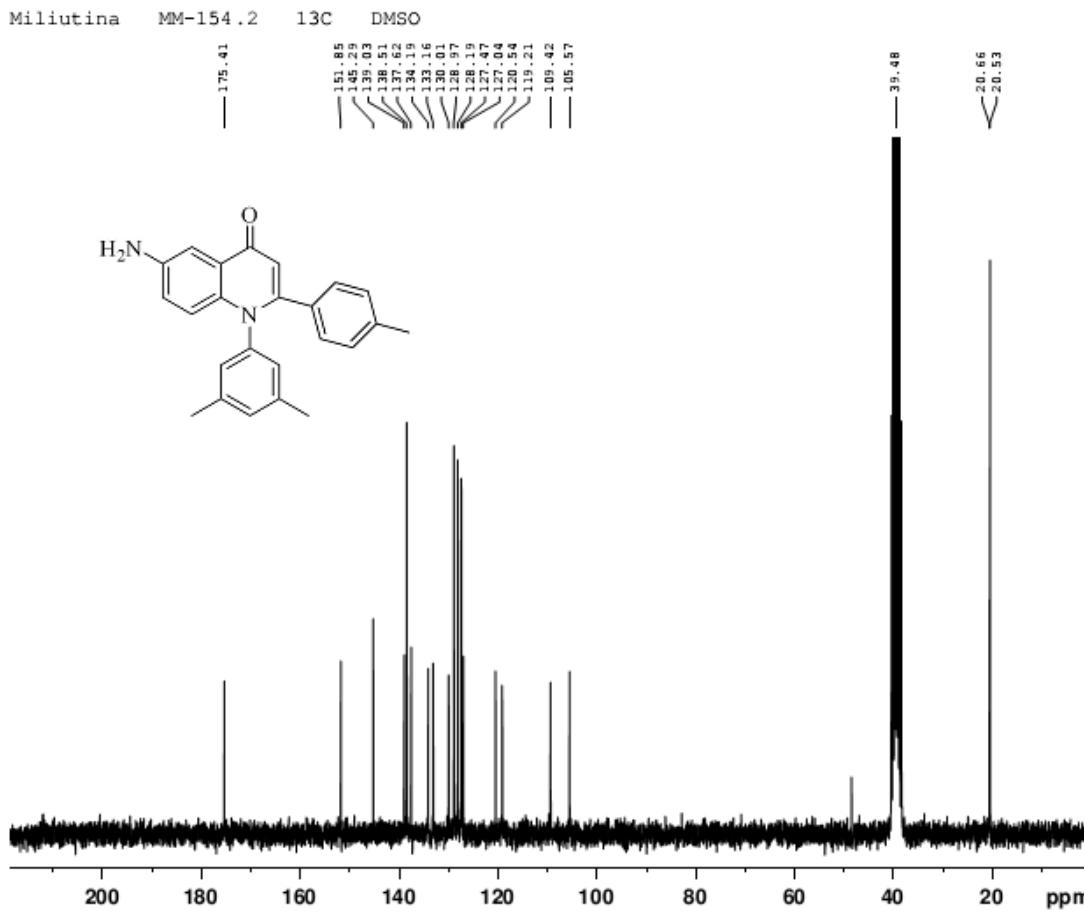
===== CHANNEL f2 =====
CPDPRG2 walkz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677879 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

| **6-Amino-1-(3,5-dimethylphenyl)-2-p-tolylquinolin-4(1H)-one (**8am**).**



| **6-Amino-1-(3,5-dimethylphenyl)-2-p-tolylquinolin-4(1H)-one (**8am**l).**



```

NAME 121122.211
EXPNO 10
PROCNO 1
Date_ 20121122
Time 23.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 10.20 usec
PL1 0.00 dB
SFO1 62.9015280 MHz

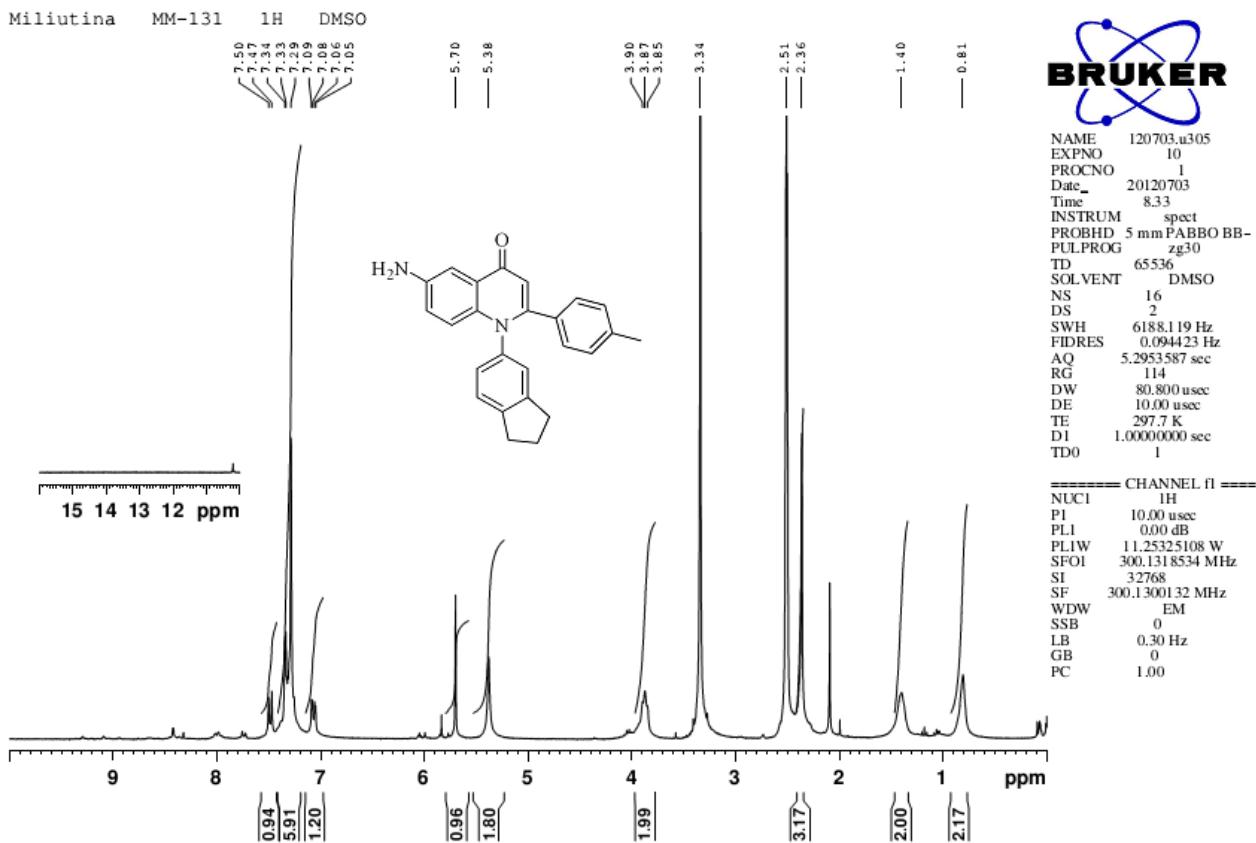
```

```

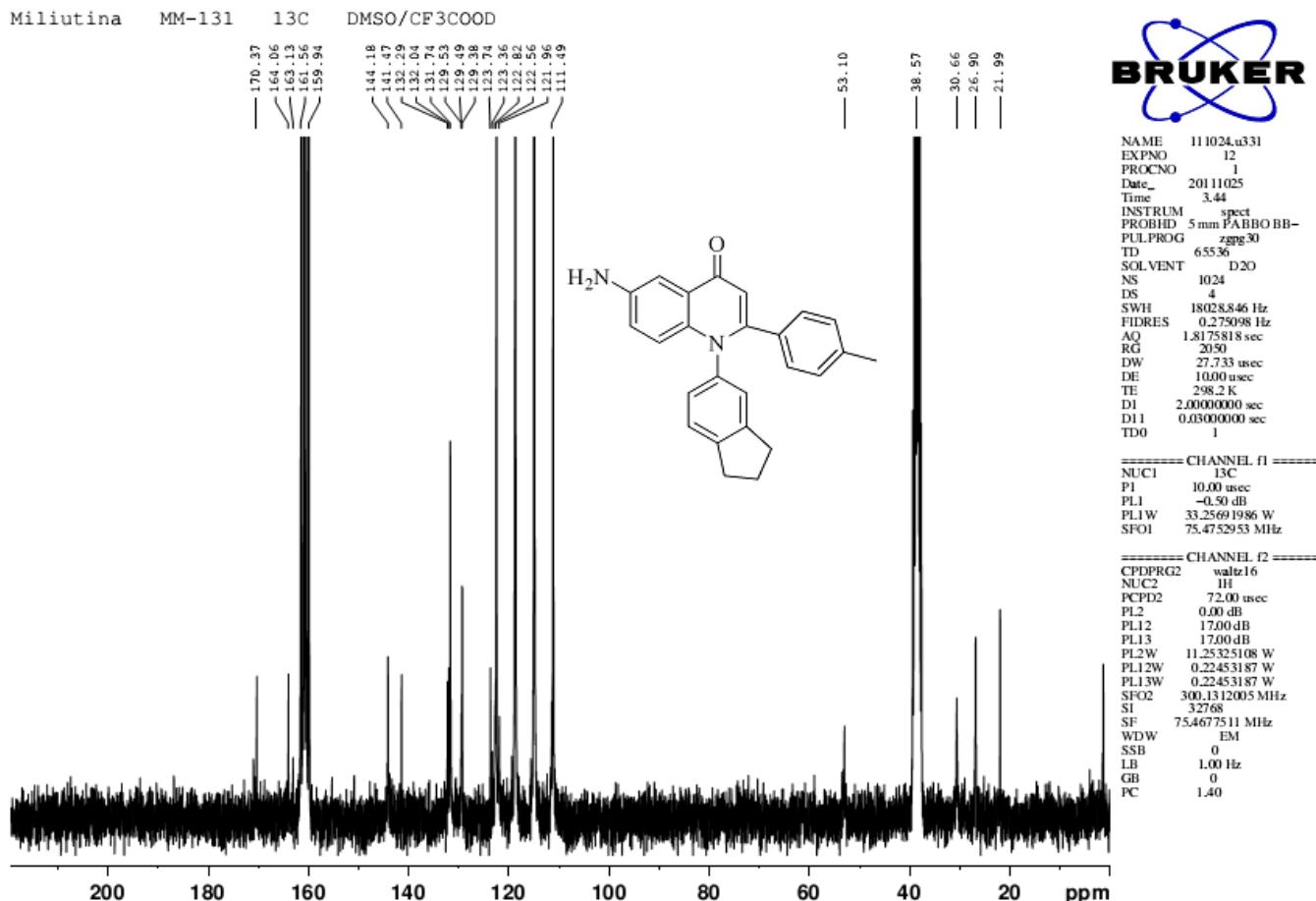
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952692 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

| 6-Amino-1-(2,3-dihydro-1*H*-inden-5-yl)-2-*p*-tolylquinolin-4(*1H*)-one (**8ann**).

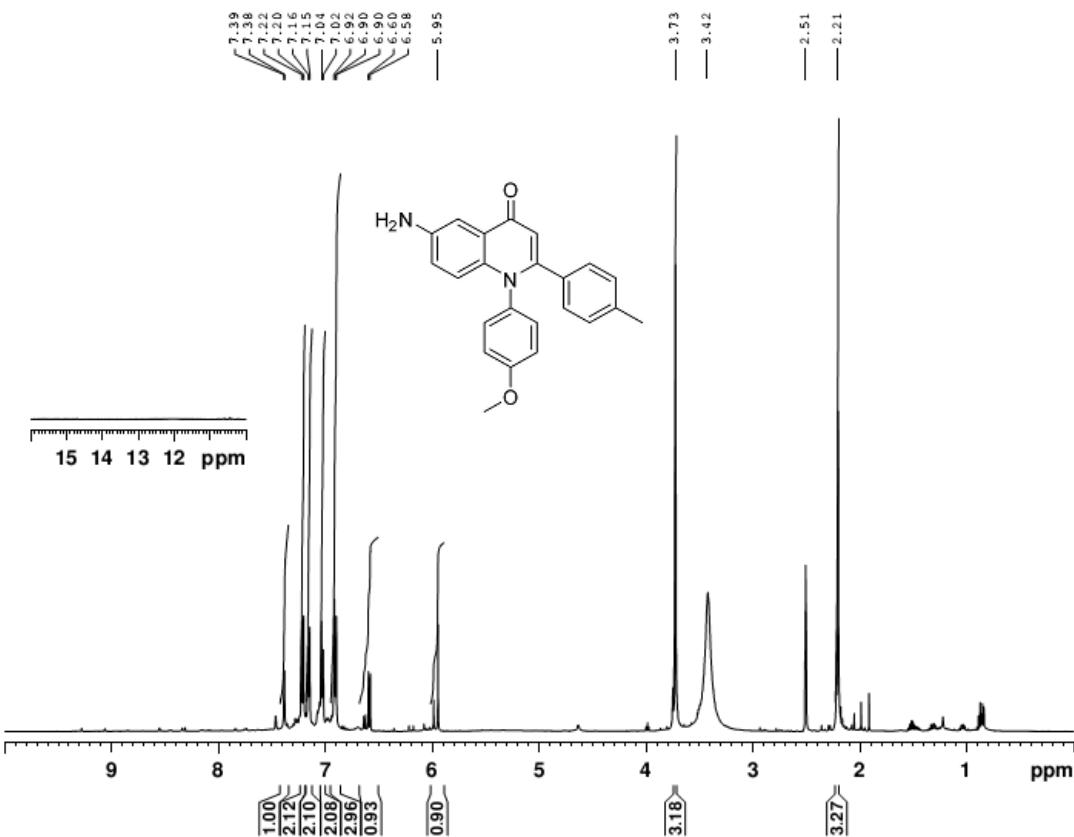


| **6-Amino-1-(2,3-dihydro-1*H*-inden-5-yl)-2-*p*-tolylquinolin-4(*1H*)-one (**8ann**).**



| 6-Amino-1-(4-methoxyphenyl)-2-p-tolylquinolin-4(1H)-one (**8apn**).

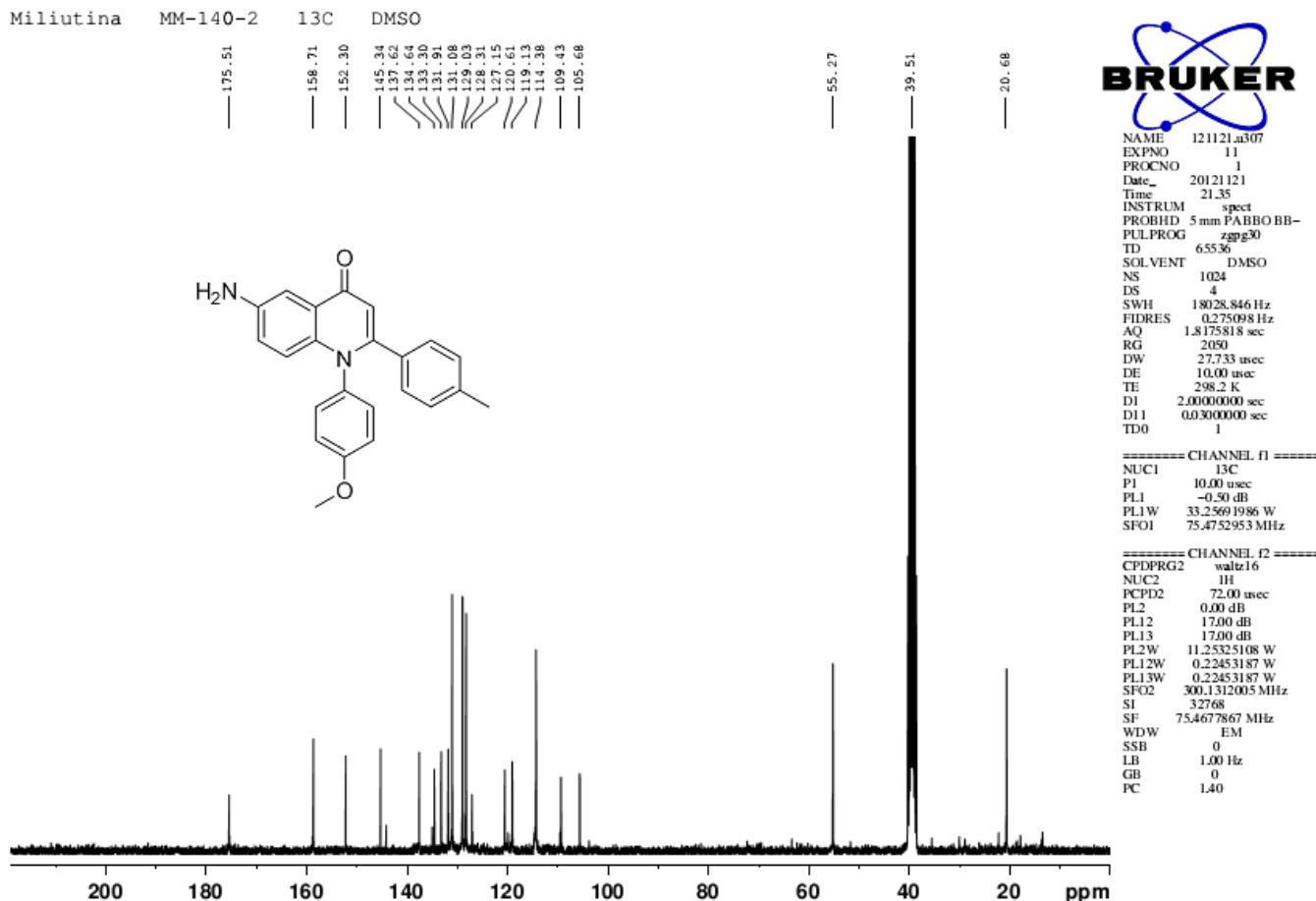
Mariia Miliutina, MM-140-2, 1H in DMSO



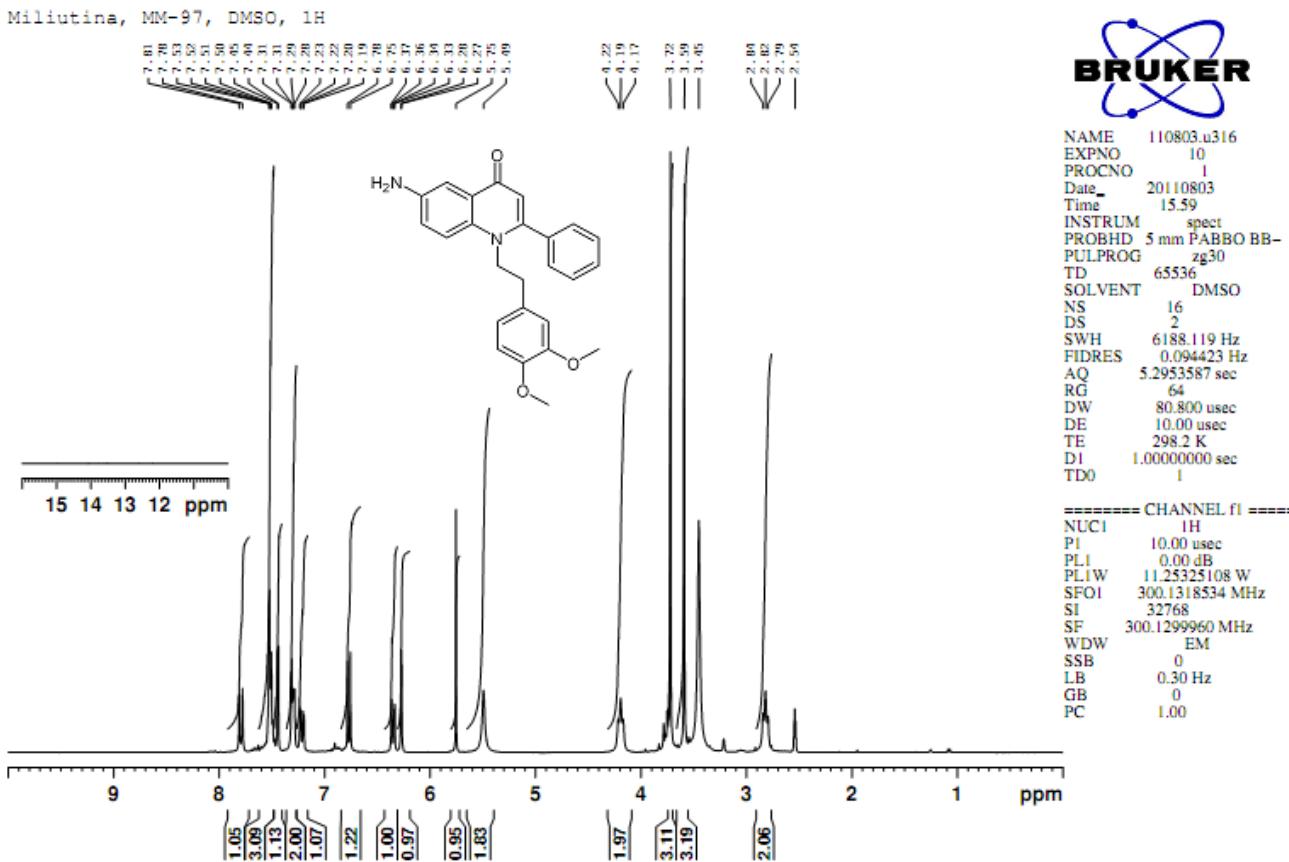
NAME 121128.511
EXPNO 10
PROCNO 1
Date 20121128
Time 16.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 45.3
DW 48.400 usec
DE 10.00 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.80 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

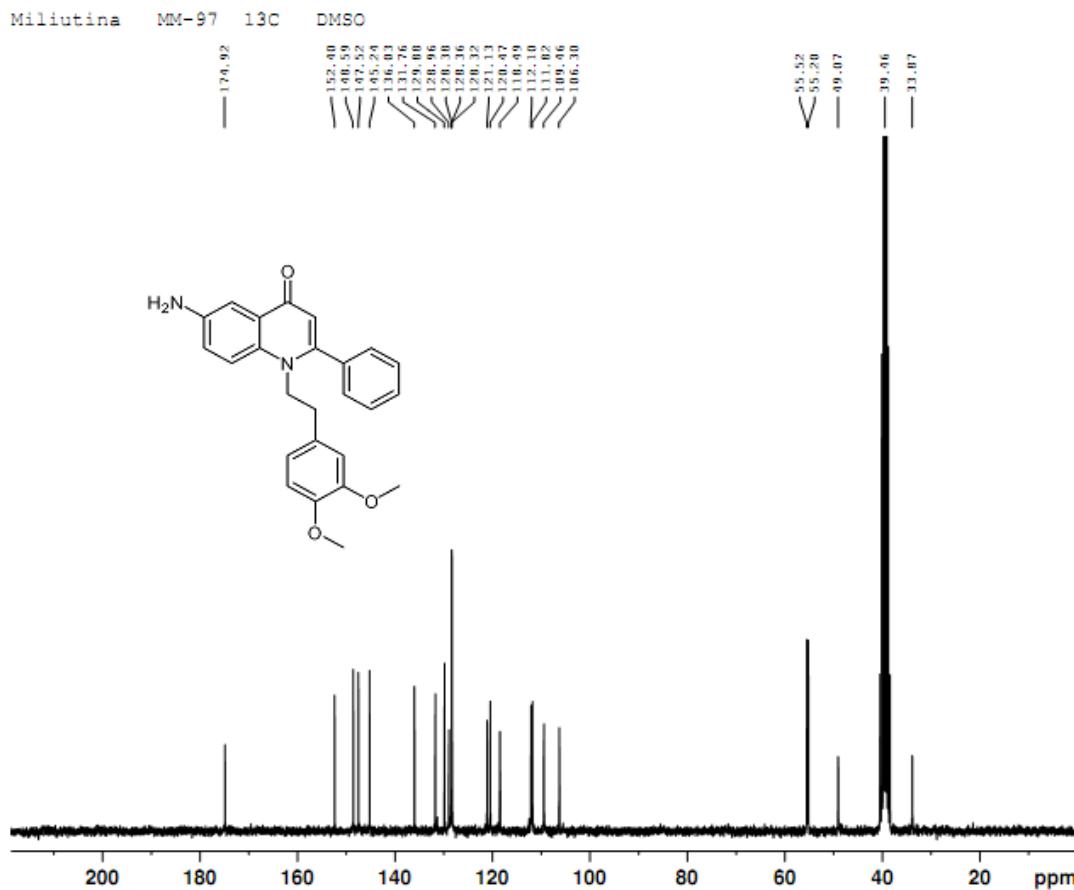
6-Amino-1-(4-methoxyphenyl)-2-*p*-tolylquinolin-4(1*H*)-one (8^{app}).



| **6-Amino-1-(3,4-dimethoxyphenethyl)-2-phenylquinolin-4(1H)-one (8bae).**



| **6-Amino-1-(3,4-dimethoxyphenethyl)-2-phenylquinolin-4(1H)-one (8bae).**

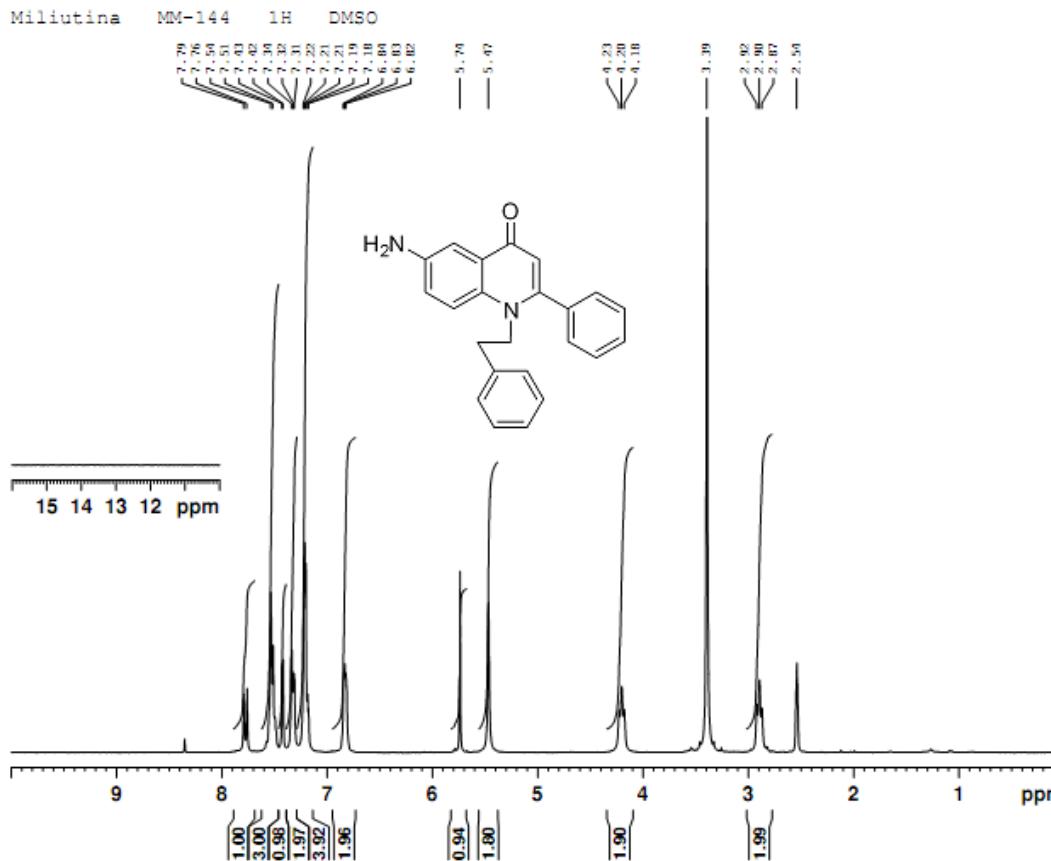


NAME 110802.205
 EXPNO 10
 PROCNO 1
 Date 20110802
 Time 19.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 299.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

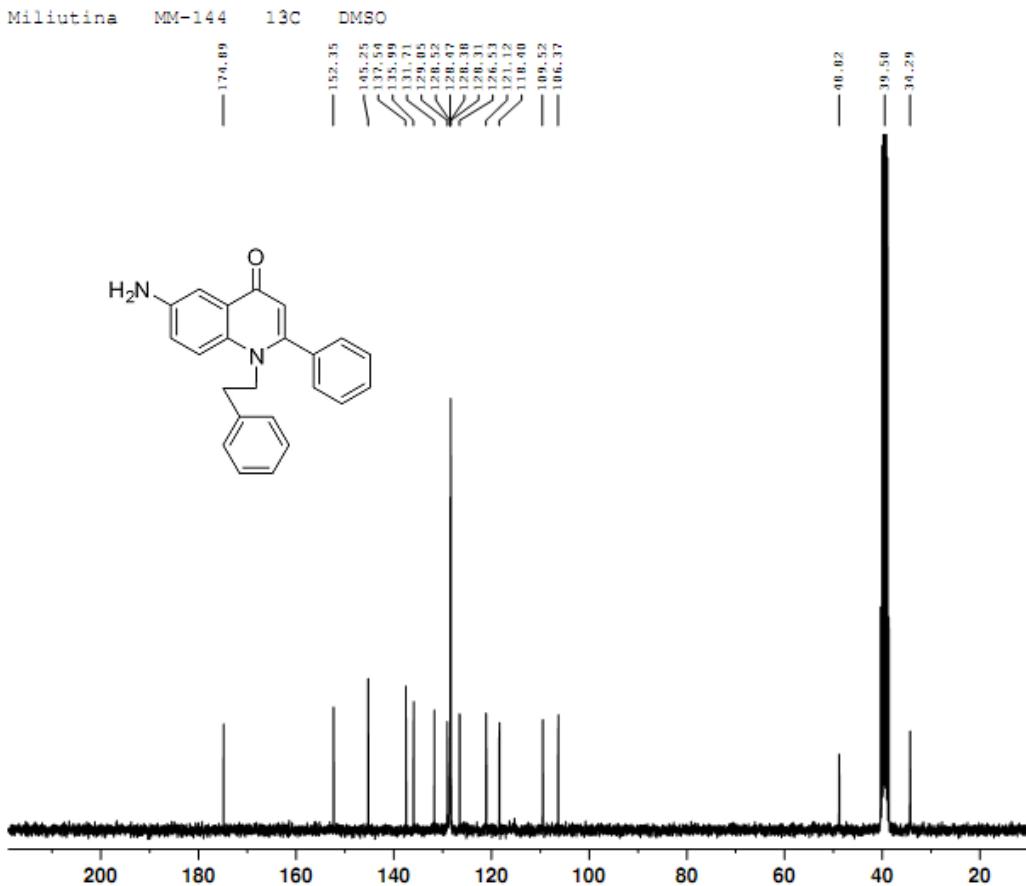
===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz
 SI 32768
 SF 62.8952704 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

| **6-Amino-1-phenethyl-2-phenylquinolin-4(1H)-one (8bcp).**



| **6-Amino-1-phenethyl-2-phenylquinolin-4(1H)-one (8bcp).**



NAME 120302.u308
 EXPNO 11
 PROCNO 1
 Date 20120304
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.735 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1

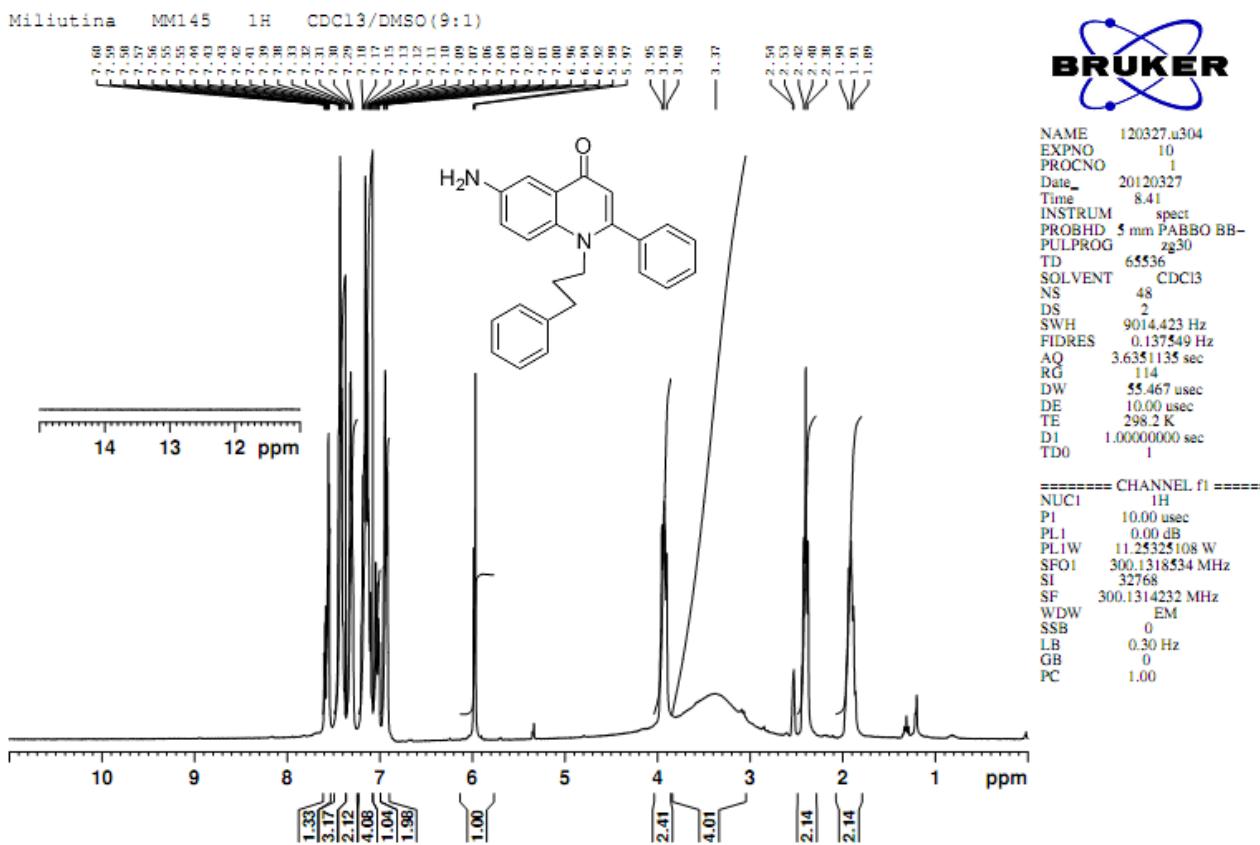
===== CHANNEL f1 =====

NUC1	¹³ C
P1	10.00 usec
PL1	-0.50 dB
PL1W	33.25691986 W
SFO1	75.4752953 MHz

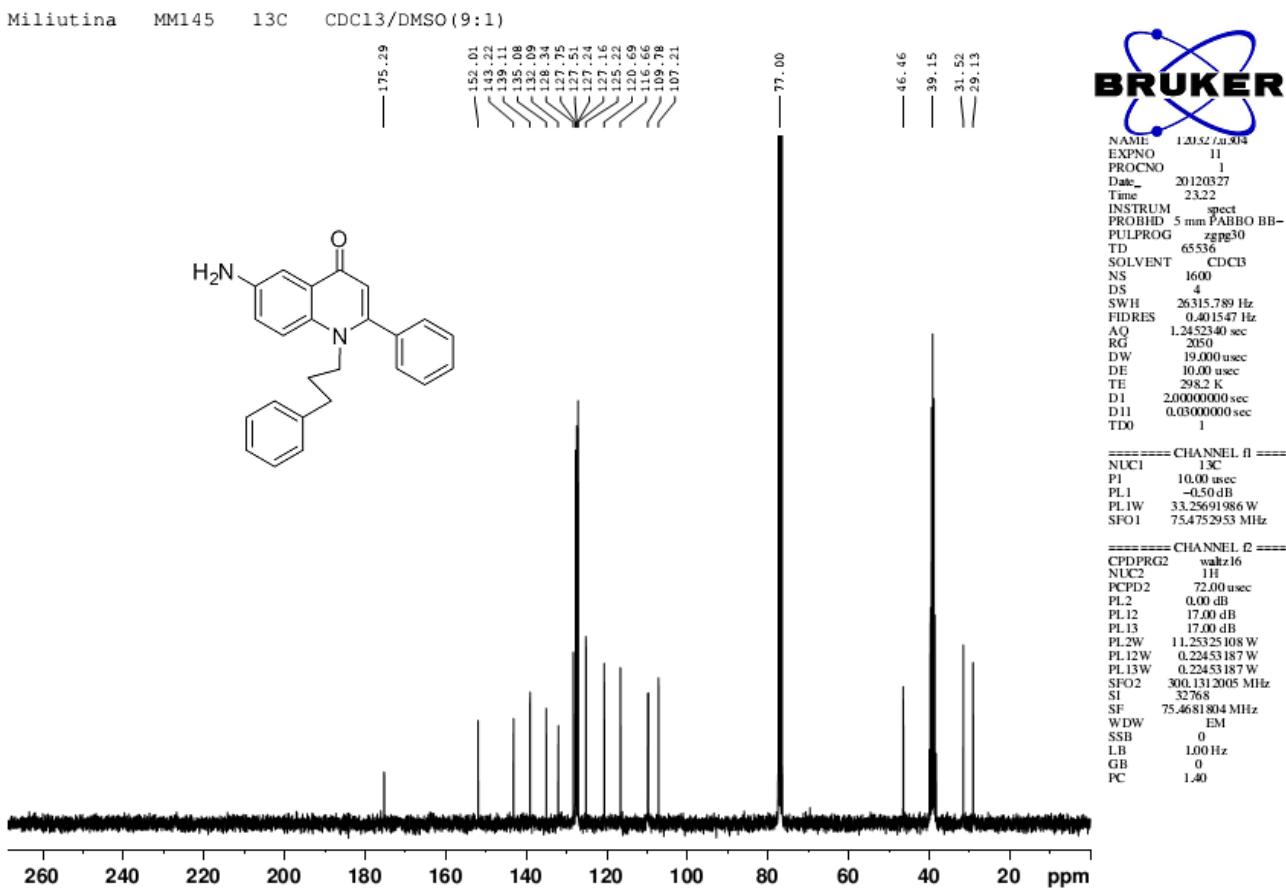
===== CHANNEL f2 =====

CPDPG2	waltz16
NUC2	¹ H
PCPD2	72.00 usec
PL2	0.00 dB
PL12	17.00 dB
PL13	17.00 dB
PL2W	11.25525108 W
PL12W	0.22453187 W
PL13W	0.22453187 W
SFO2	300.1312005 MHz
SI	32768
SF	75.46777867 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

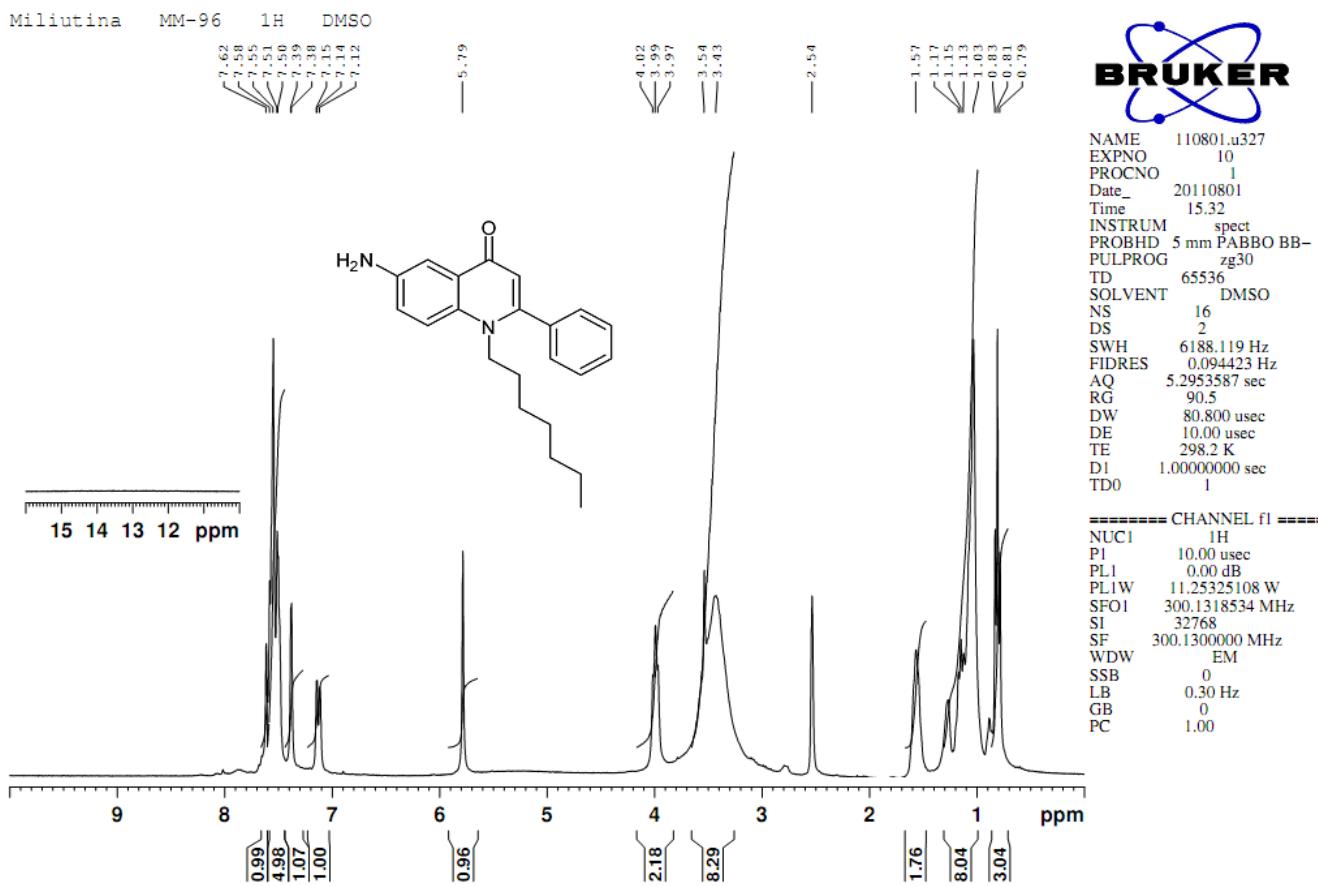
6-Amino-1-phenethyl-2-phenylquinolin-4(1*H*)-one (8bdq).



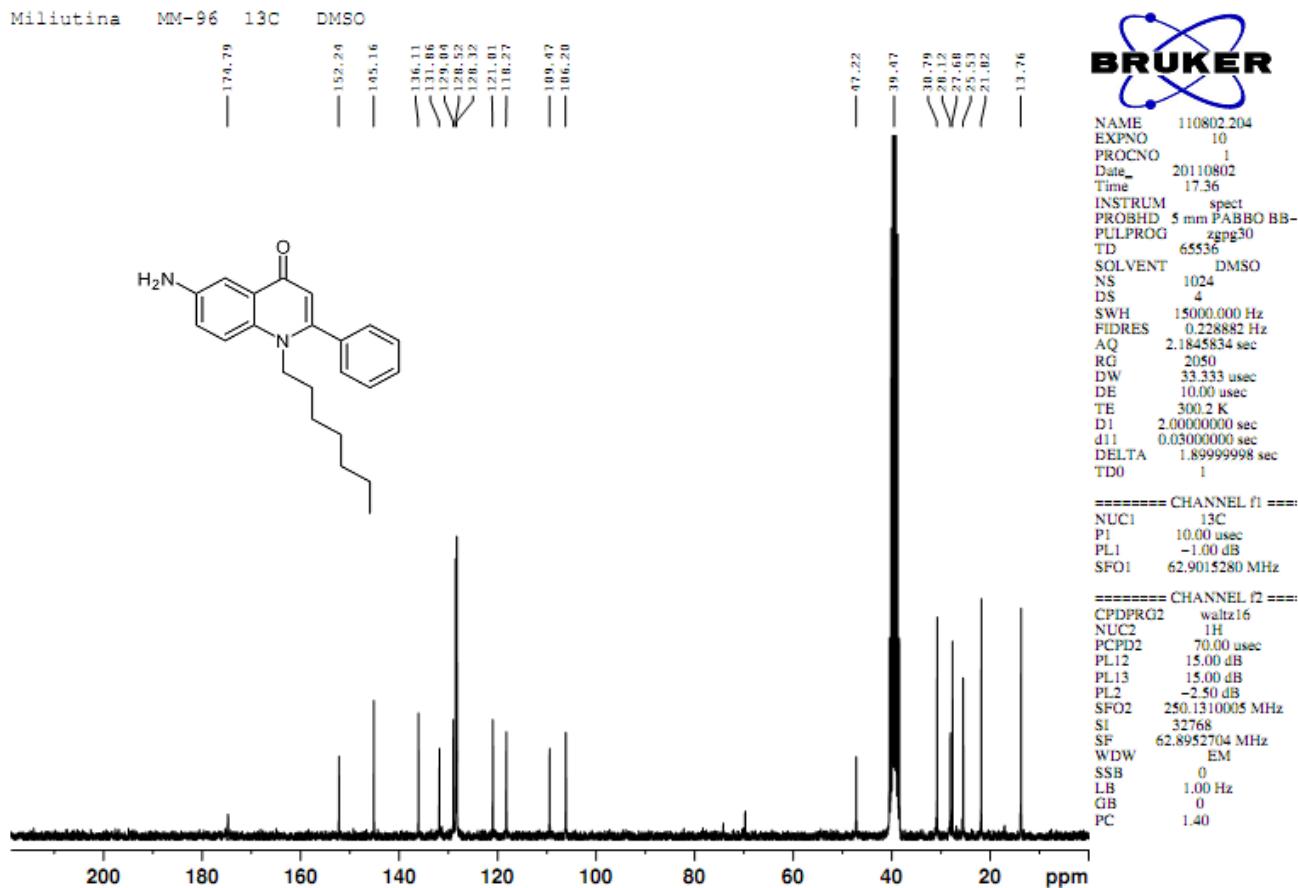
6-Amino-1-phenethyl-2-phenylquinolin-4(1*H*)-one (8**bdq**).



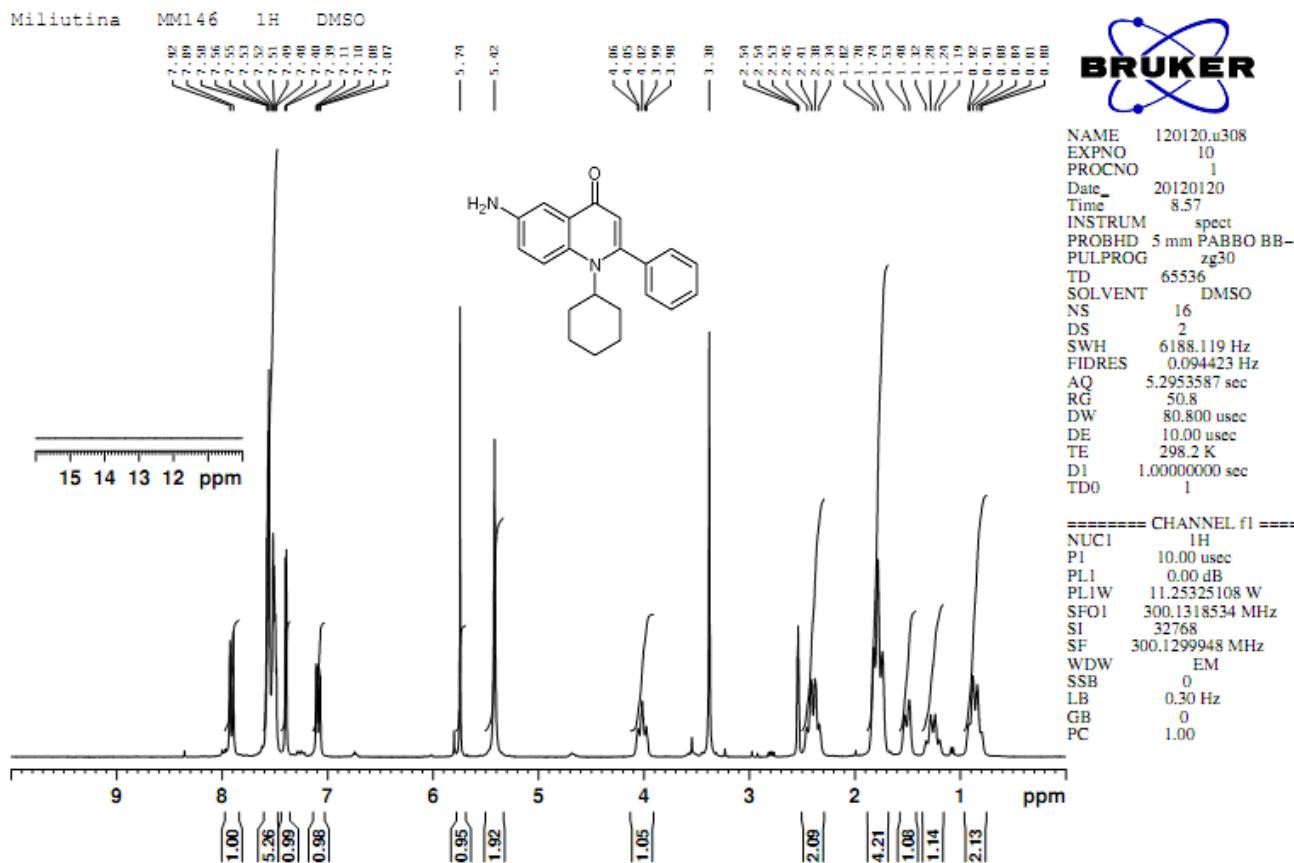
| **6-Amino-1-heptyl-2-phenylquinolin-4(1H)-one (8_{ber}).**



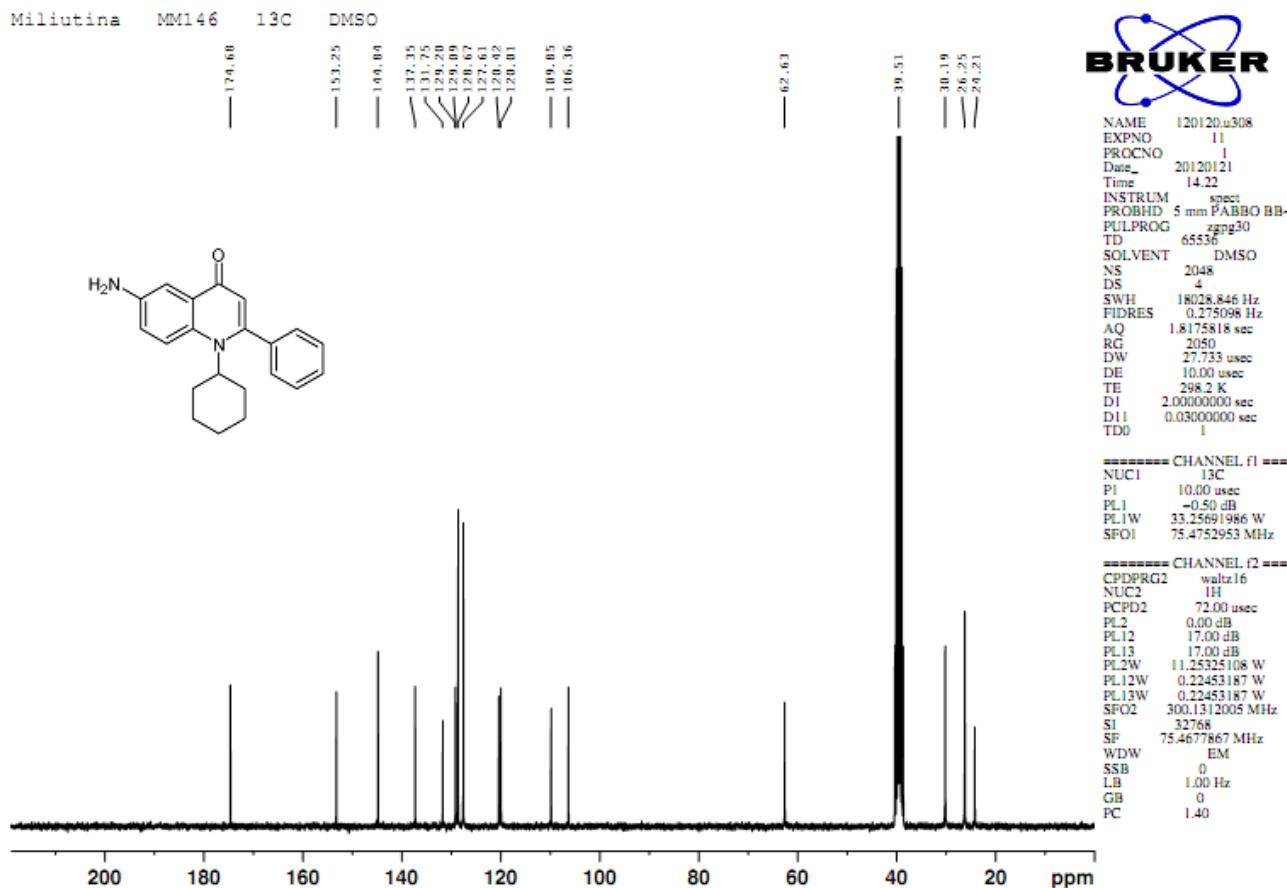
| 6-Amino-1-heptyl-2-phenylquinolin-4(1H)-one (**8ber**).



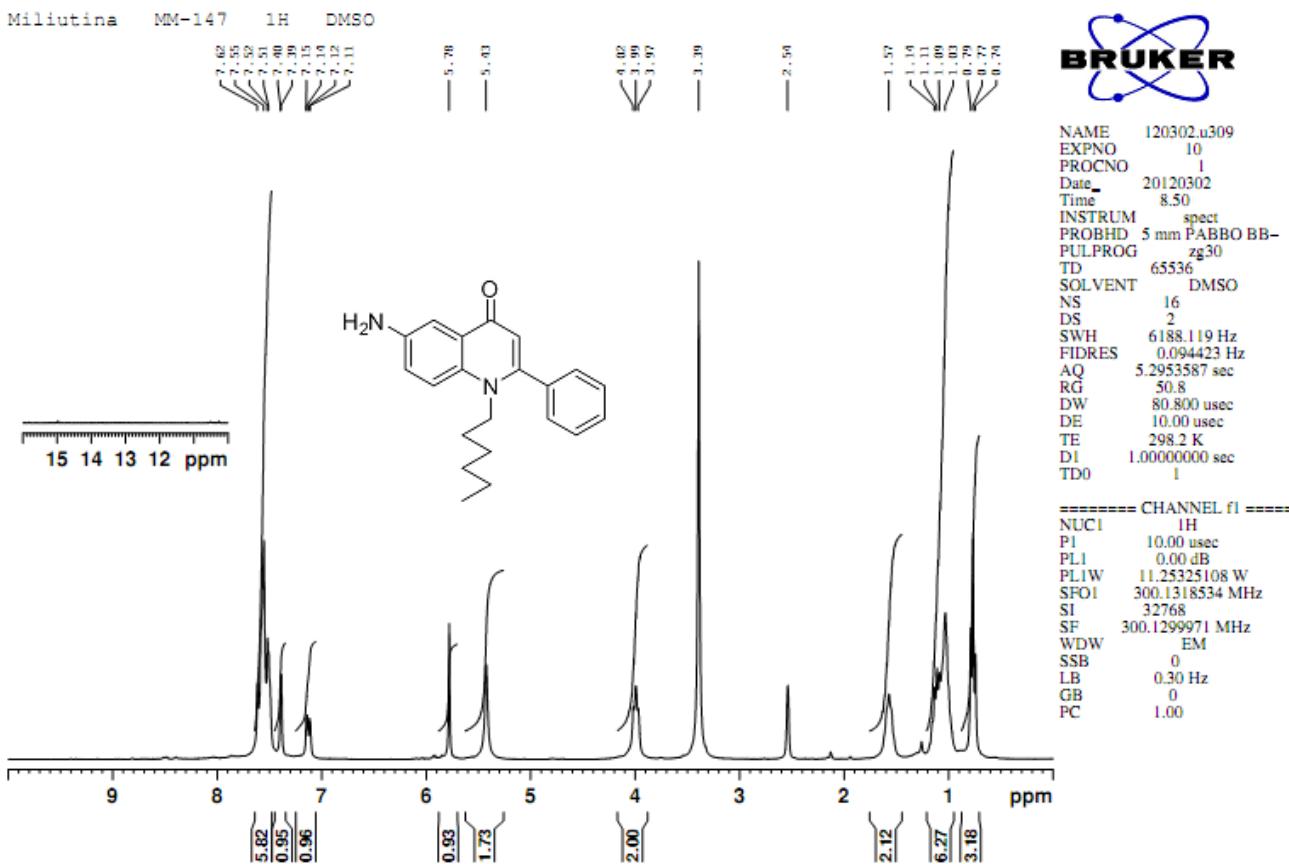
6-Amino-1-cyclohexyl-2-phenylquinolin-4(1*H*)-one (**8bfs**).



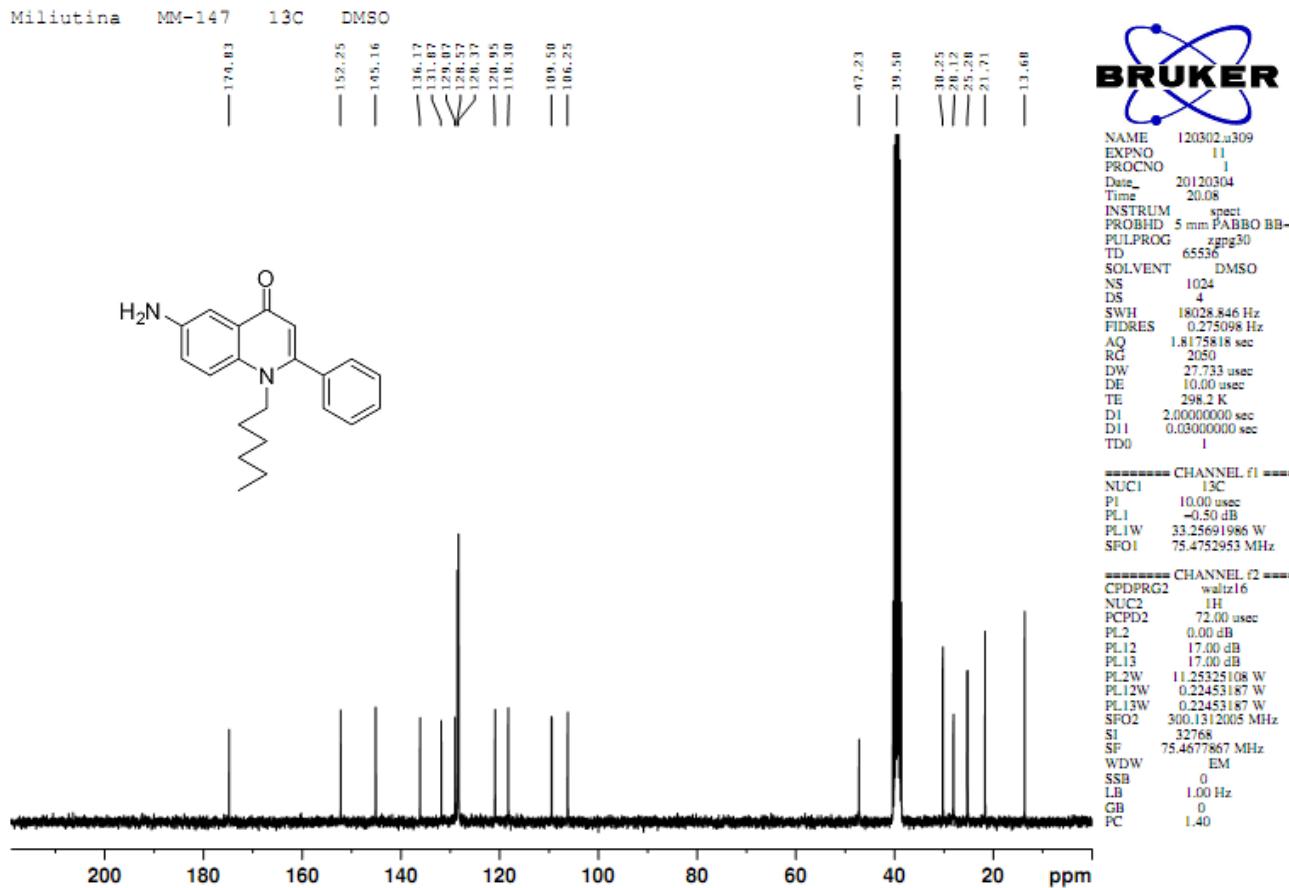
| **6-Amino-1-cyclohexyl-2-phenylquinolin-4(1H)-one (8bfs).**



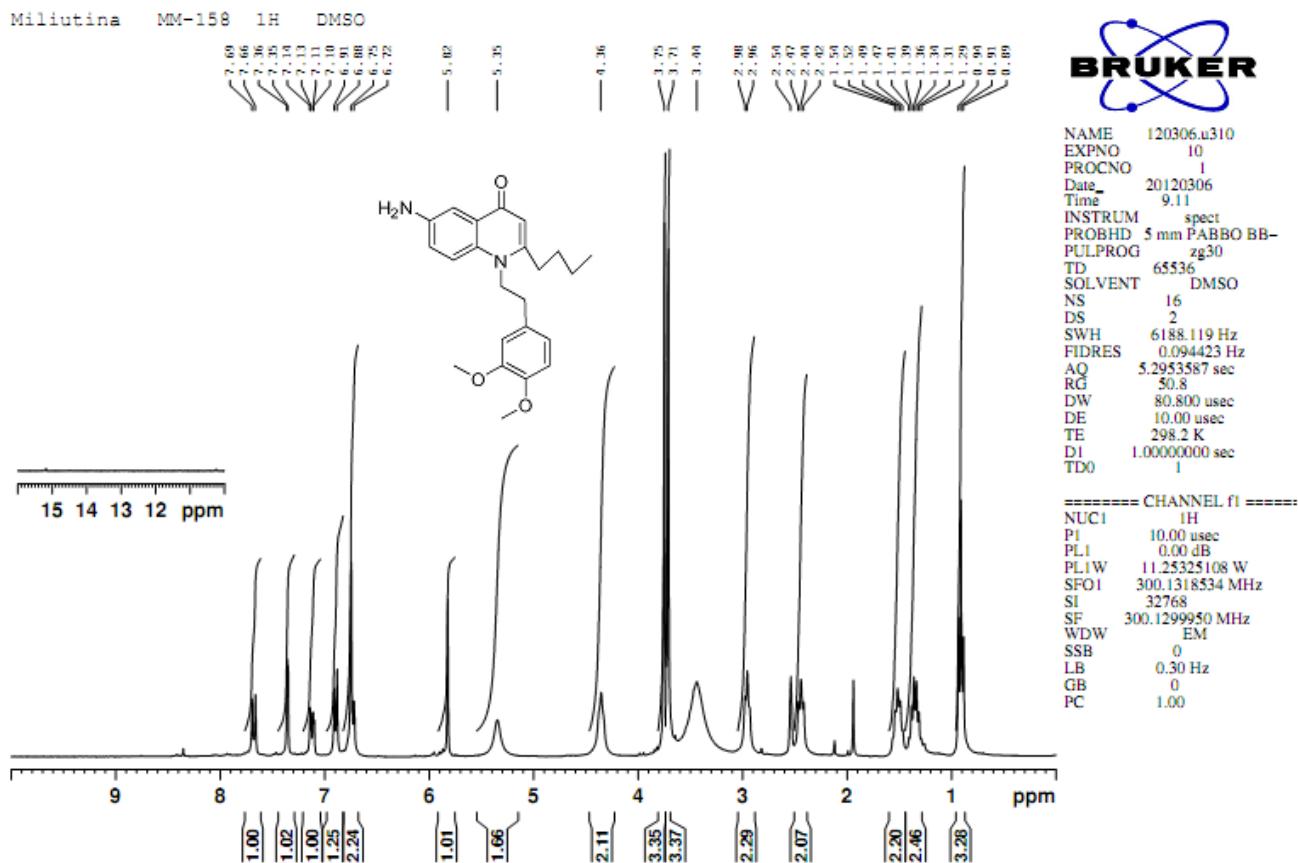
6-Amino-1-hexyl-2-phenylquinolin-4(1*H*)-one (8bgt).



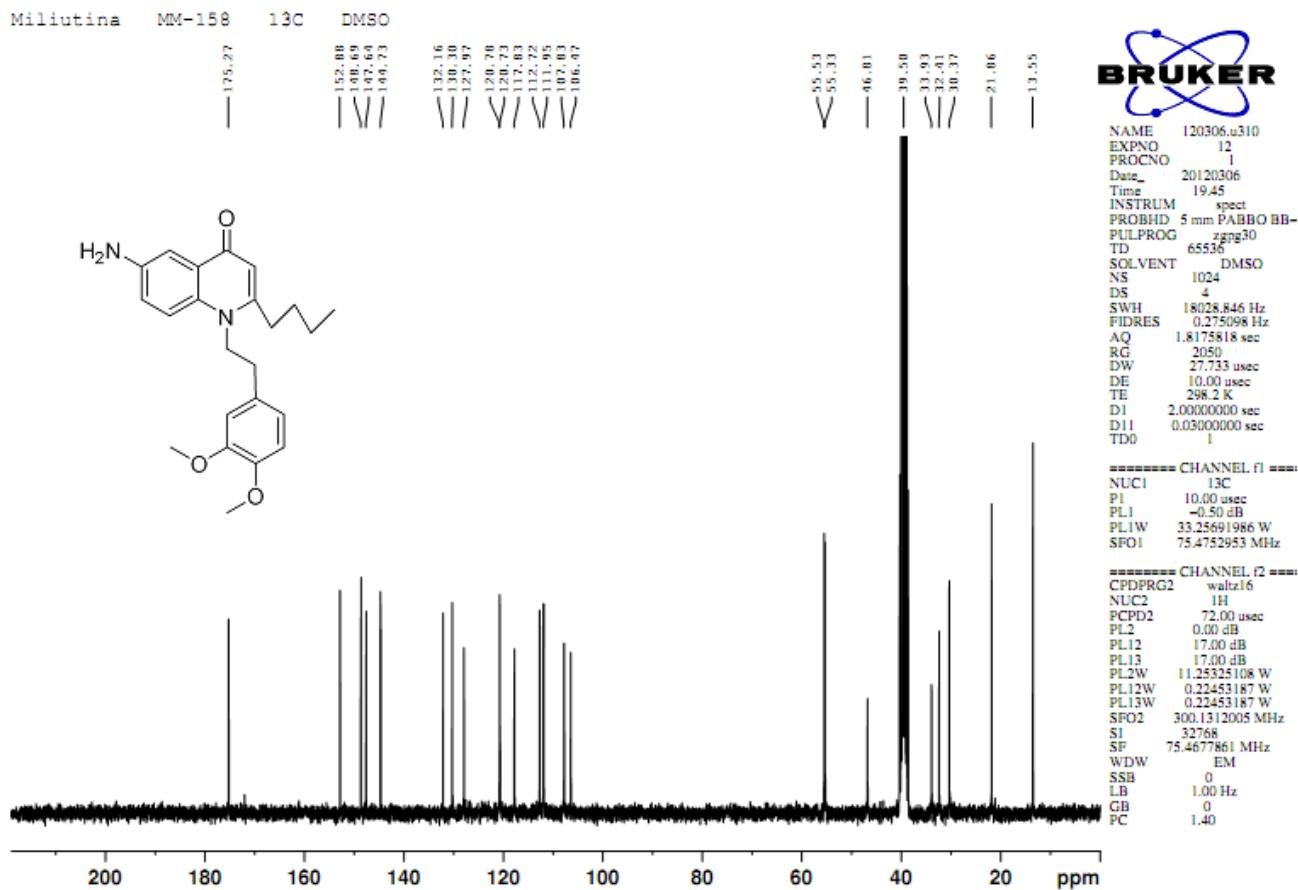
| **6-Amino-1-hexyl-2-phenylquinolin-4(1H)-one (8bgt).**



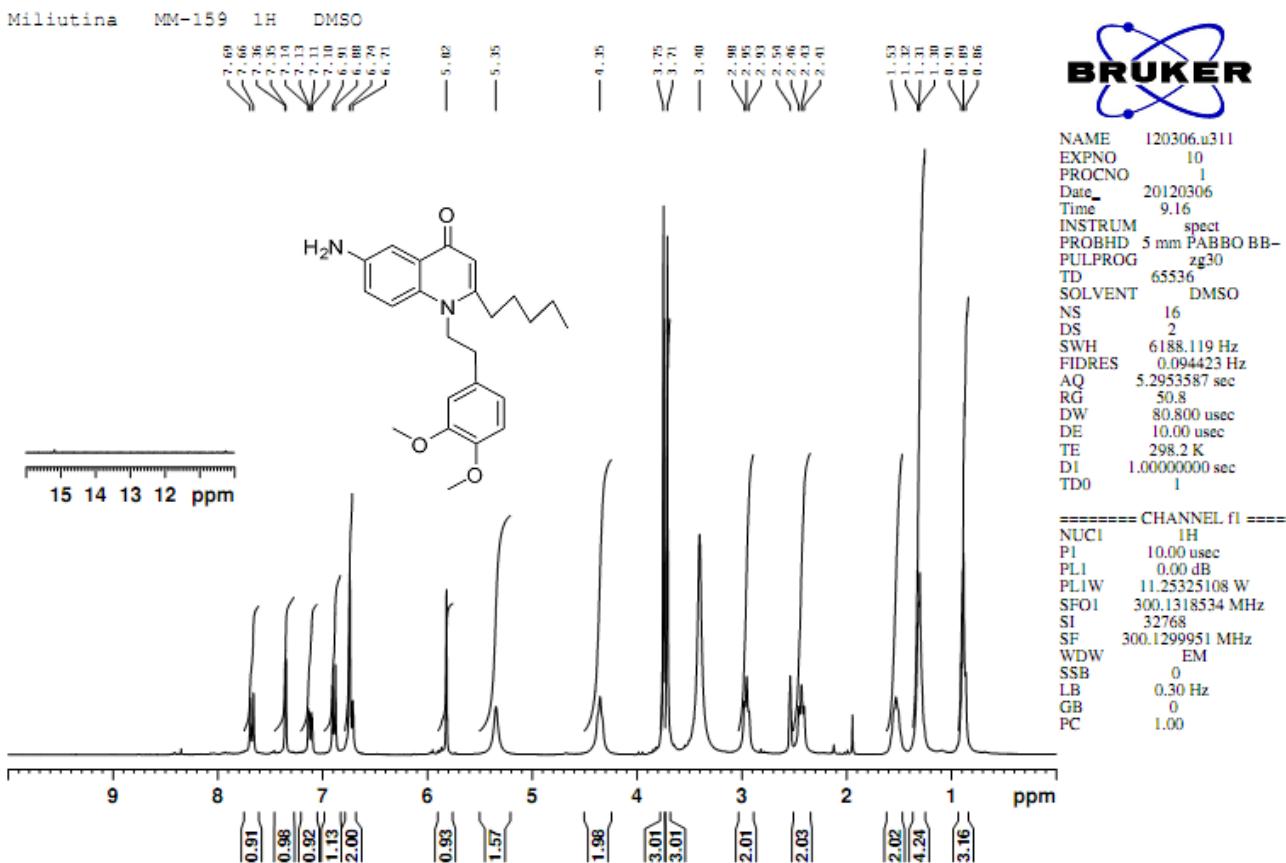
6-Amino-2-butyl-1-(3,4-dimethoxyphenethyl)quinolin-4(1*H*)-one (8ca).



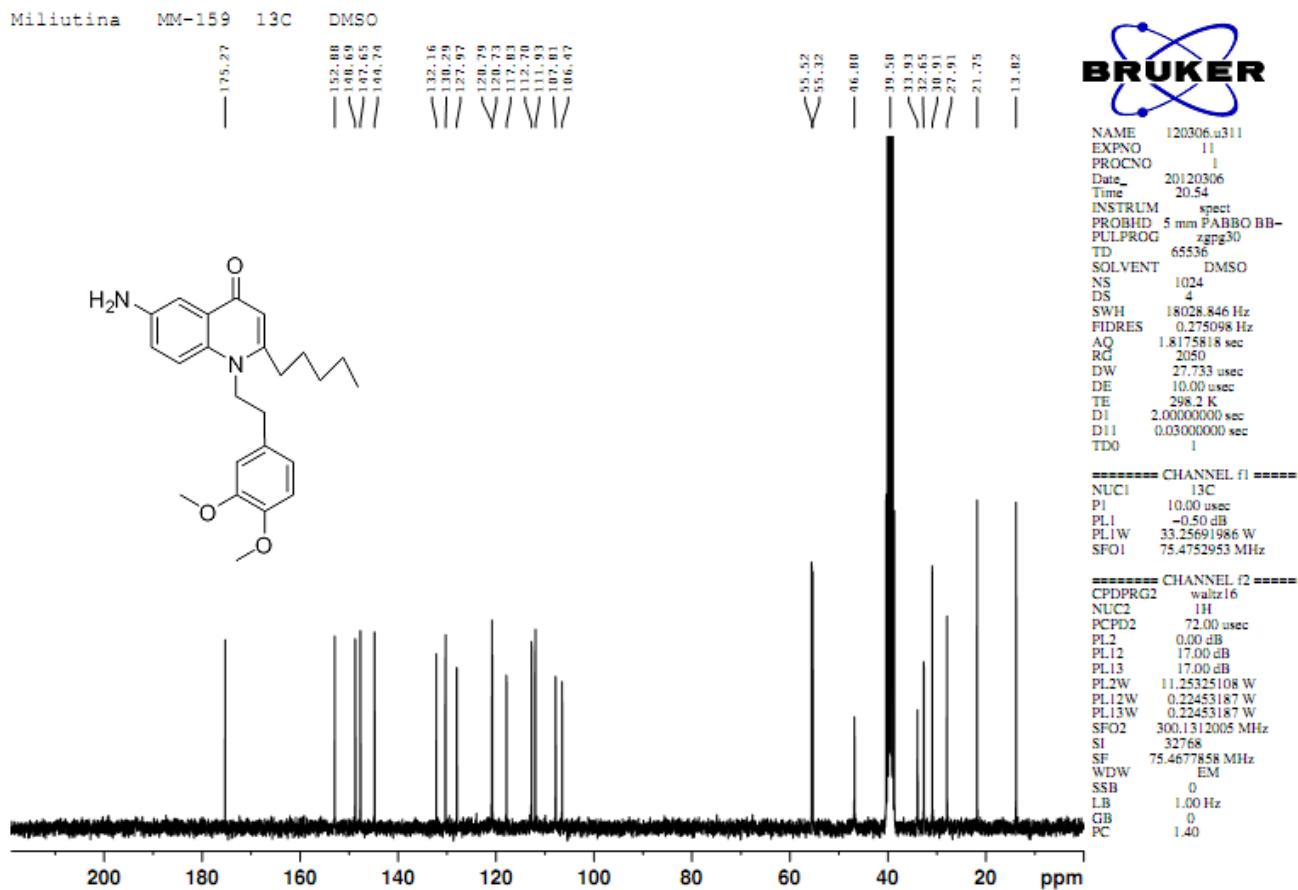
| **6-Amino-2-butyl-1-(3,4-dimethoxyphenethyl)quinolin-4(1*H*)-one (8cau).**



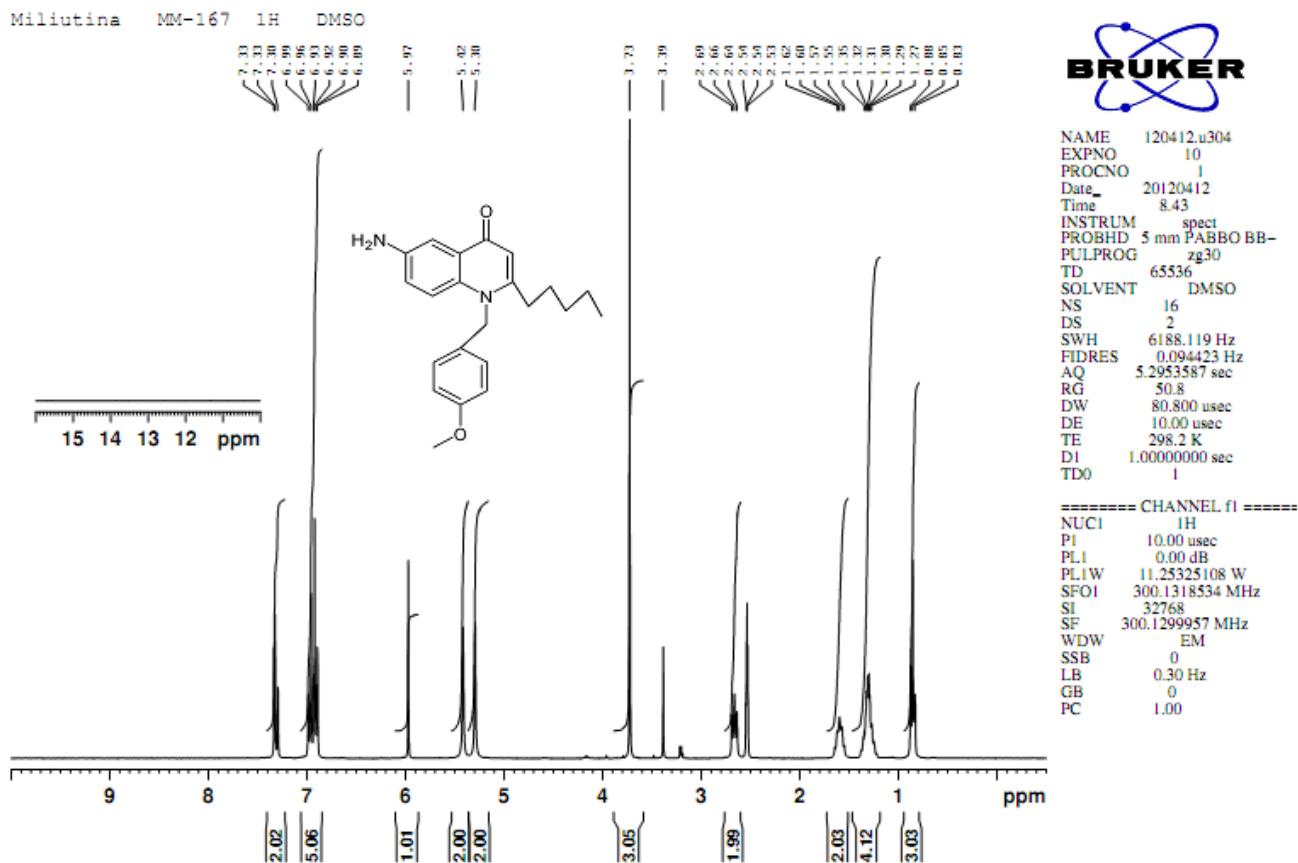
| 6-Amino-1-(3,4-dimethoxyphenethyl)-2-pentylquinolin-4(1H)-one (**8dav**).



6-Amino-1-(3,4-dimethoxyphenethyl)-2-pentylquinolin-4(1*H*)-one (8dav).

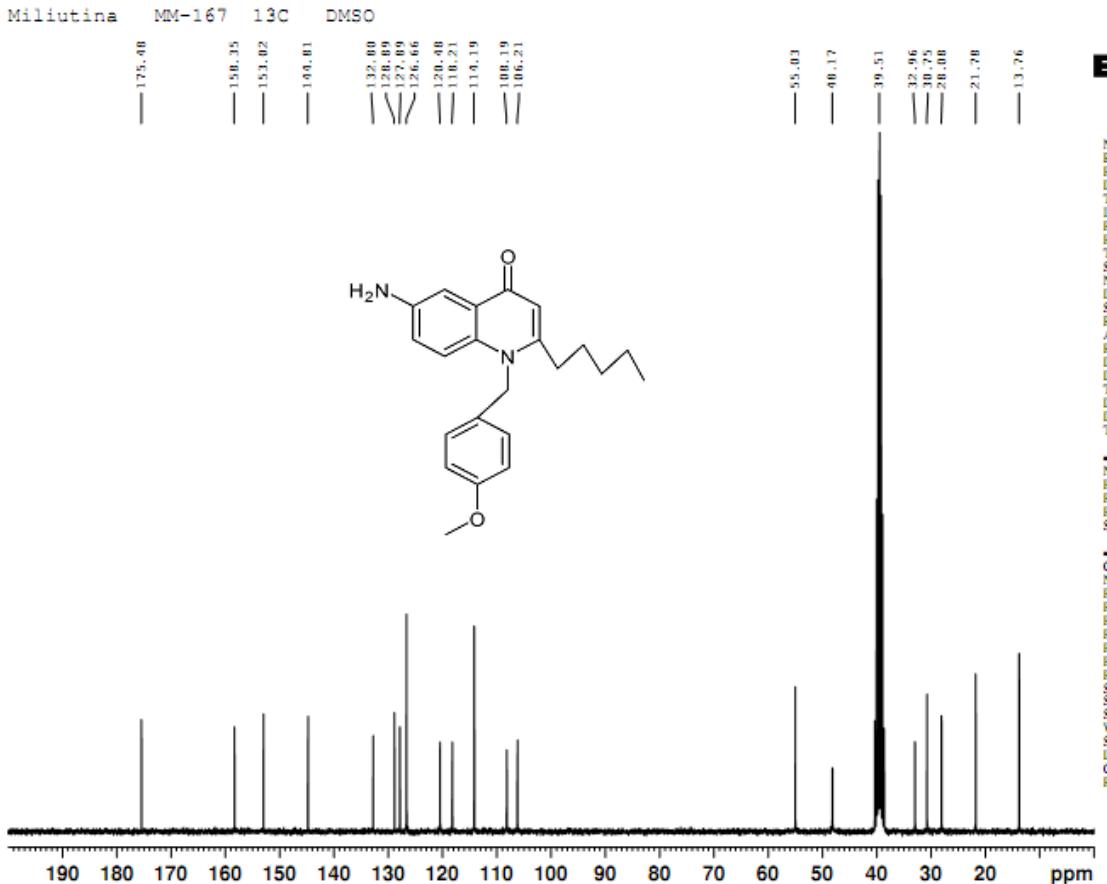


6-Amino-1-(4-methoxybenzyl)-2-pentylquinolin-4(1*H*)-one (8w^{db}).



6-Amino-1-(4-methoxybenzyl)-2-pentylquinolin-4(1H)-one (8^{www}db).

Formatiert: Englisch (USA)



```

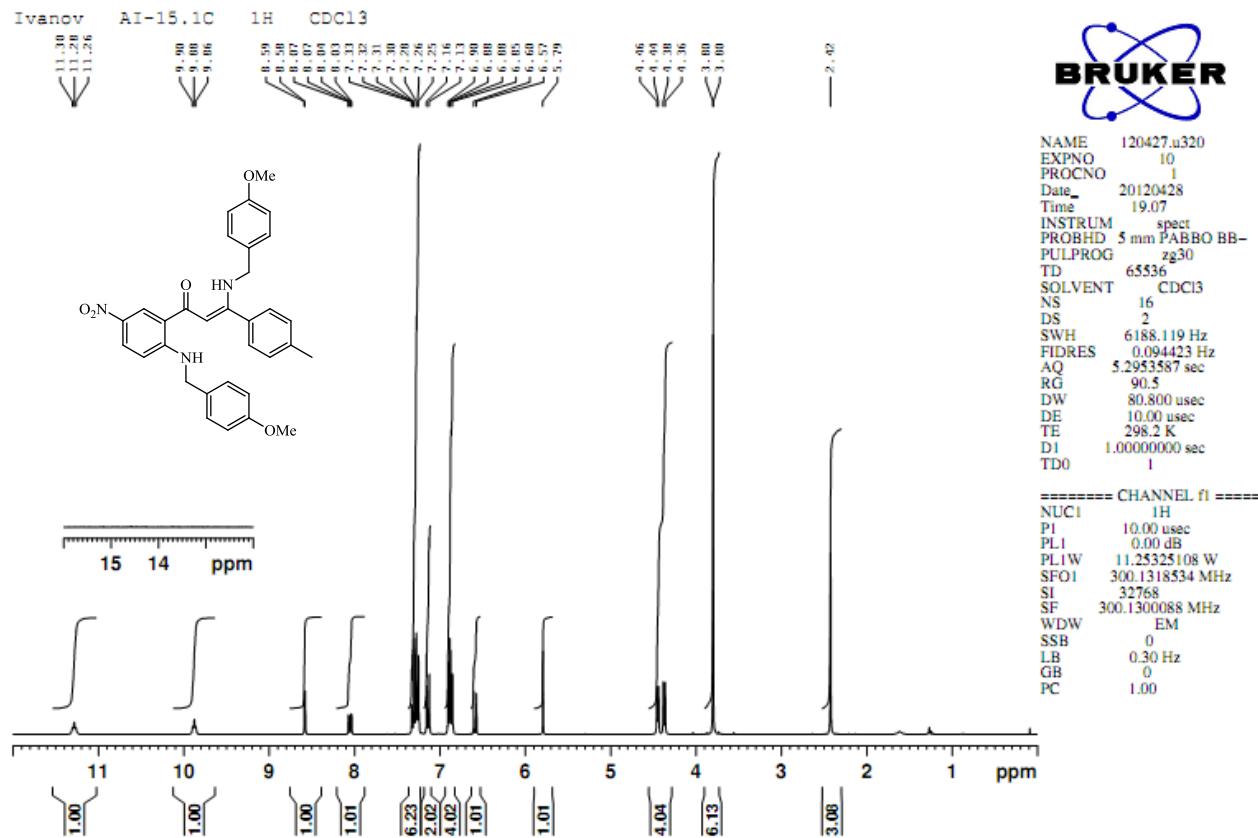
NAME 120412_004
EXPNO 12
PROCNO 1
Date 20120412
Time 12:23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.723 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

```

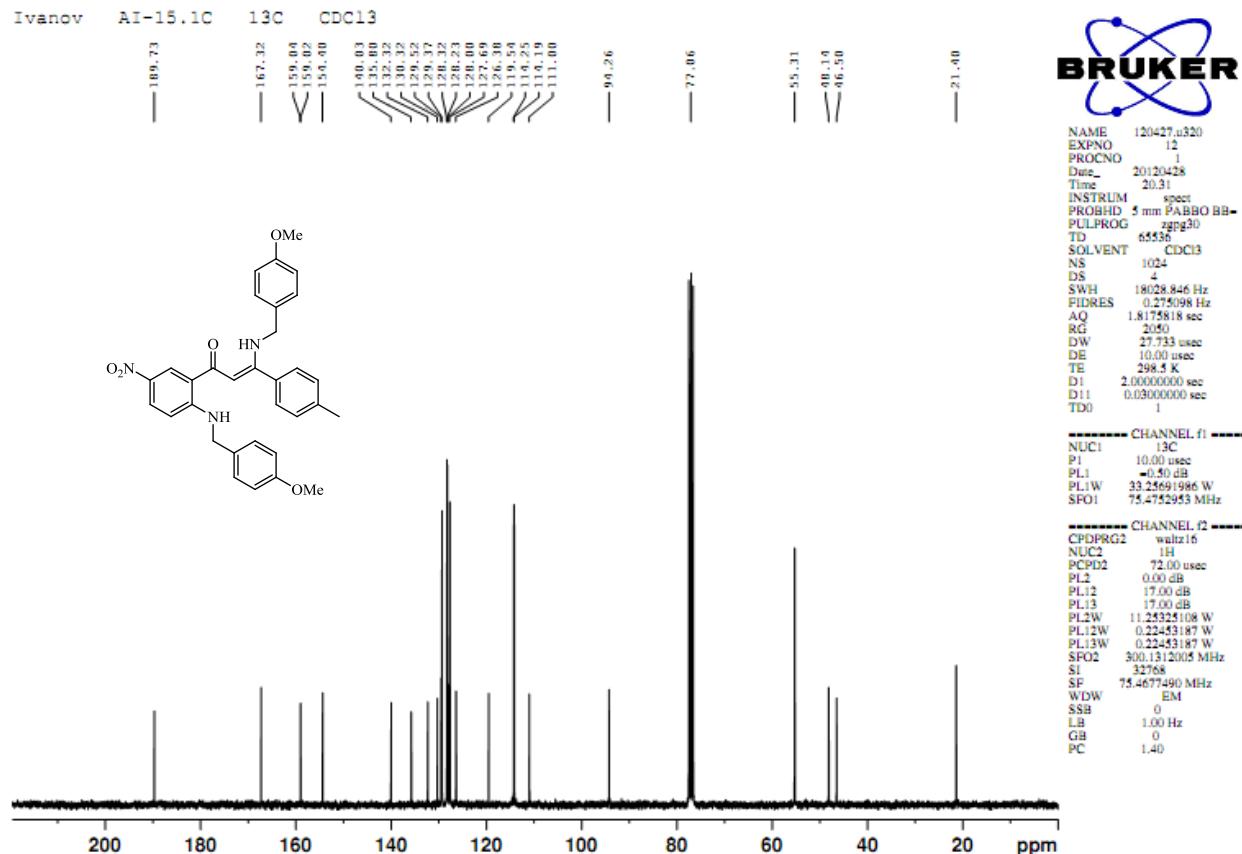
----- CHANNEL f1 -----
NUC1 ¹³C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

----- CHANNEL f2 -----
CPDPG2 waltz16
NUC2 ¹H
PCPD2 72.00 usec
PL1 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SF02 300.131205 MHz
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

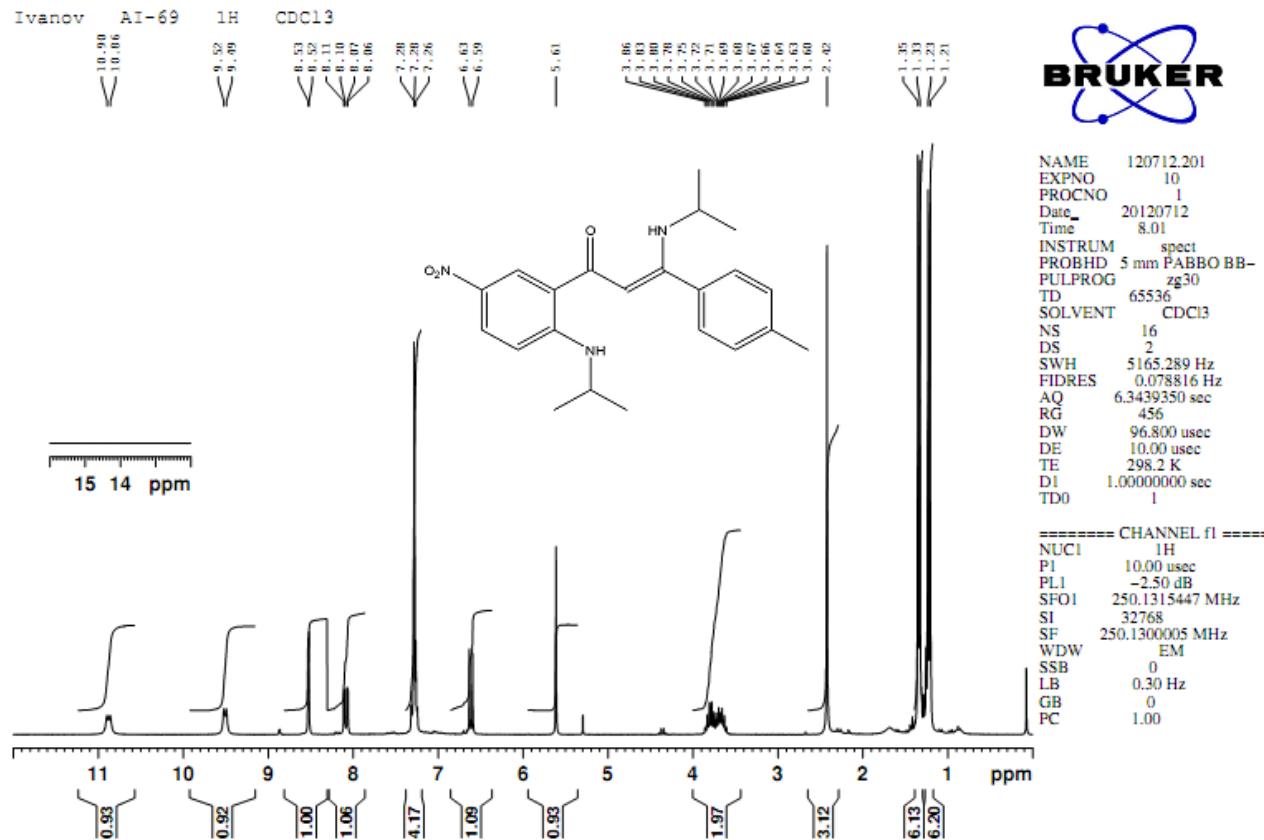
(Z)-3-(4-Methoxybenzylamino)-1-(2-(4-methoxybenzylamino)-5-nitrophenyl)-3-*p*-tolylprop-2-en-1-one (9a).



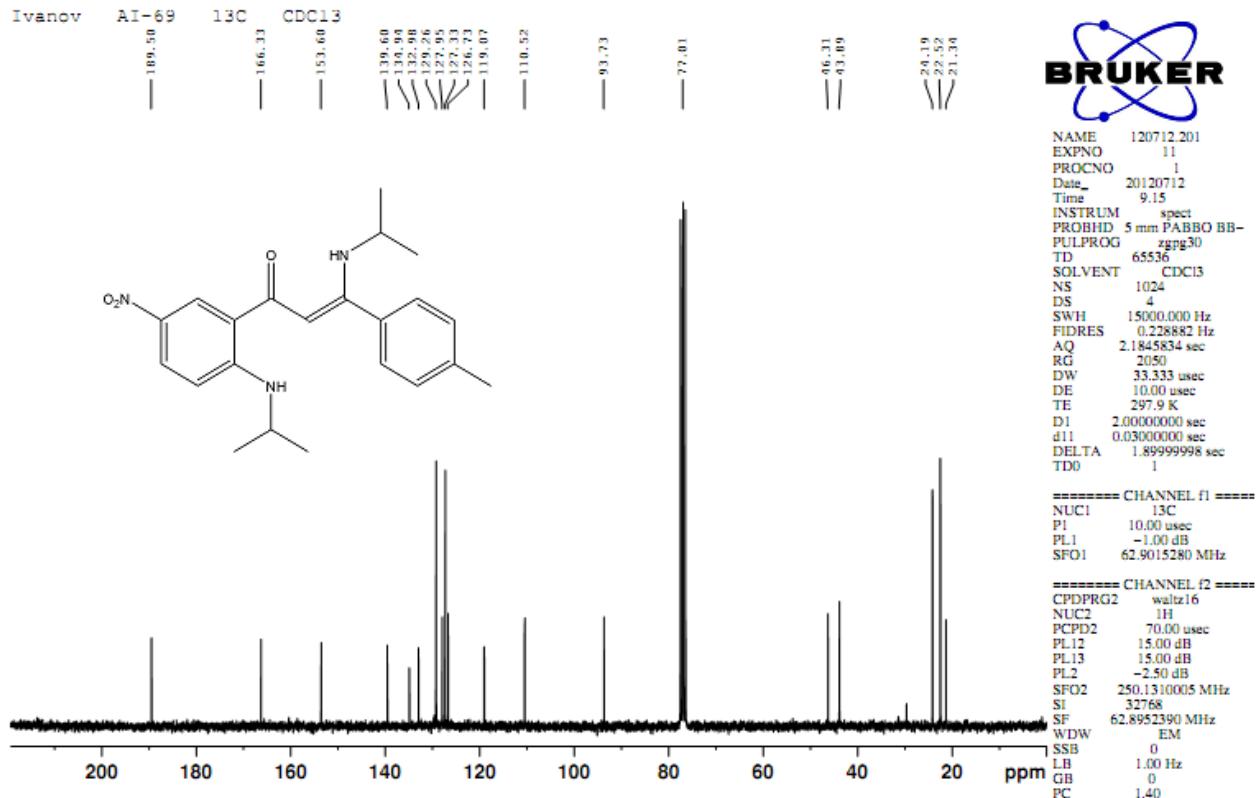
(Z)-3-(4-Methoxybenzylamino)-1-(2-(4-methoxybenzylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9a).



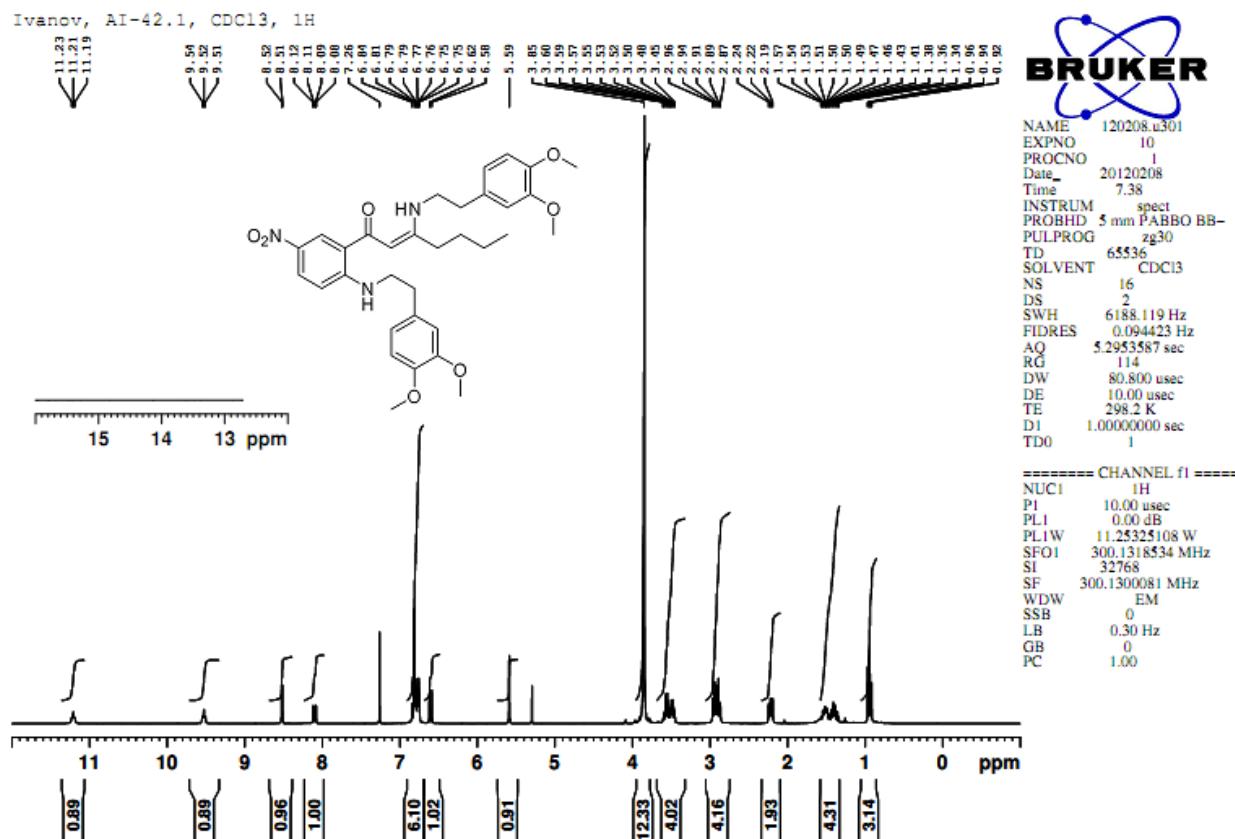
(Z)-3-(Isopropylamino)-1-(2-(isopropylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9b).



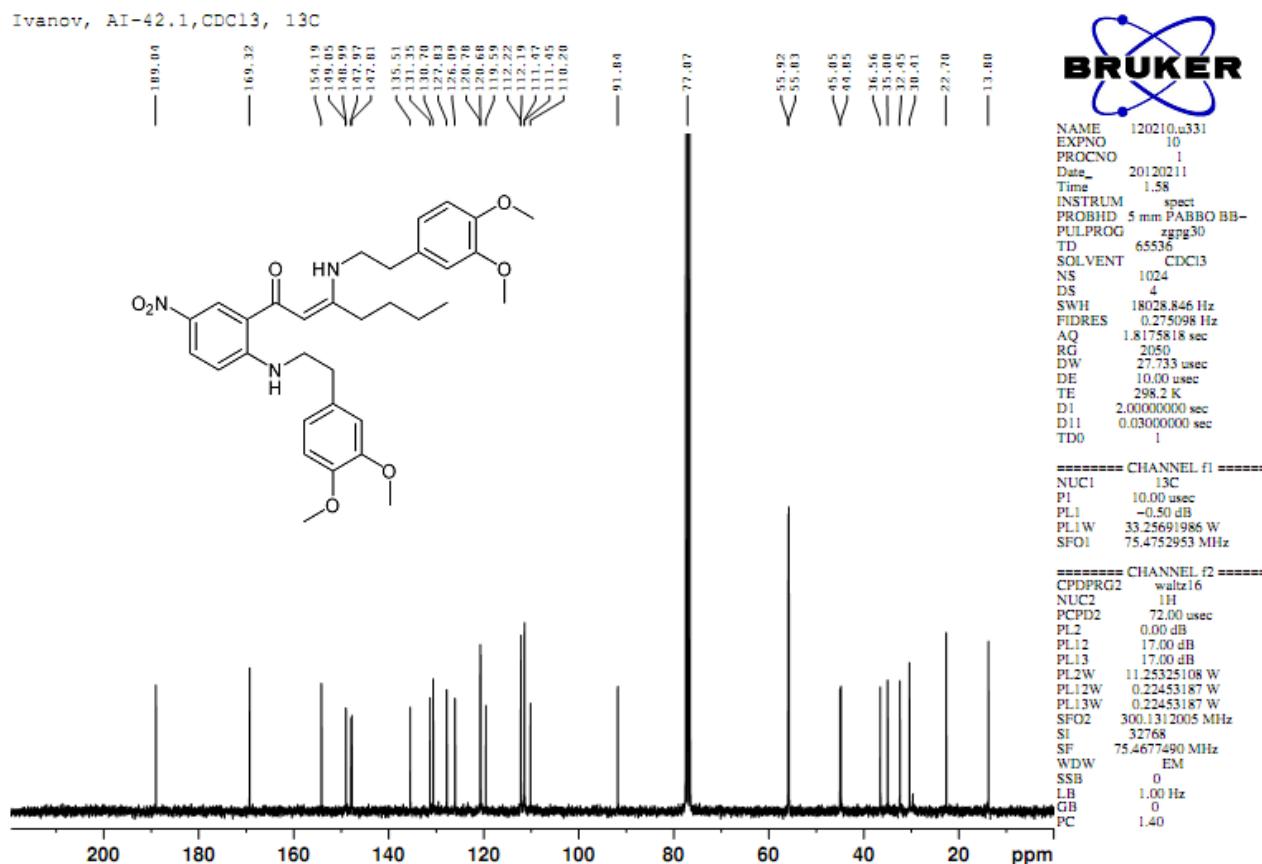
(Z)-3-(Isopropylamino)-1-(2-(isopropylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9b).



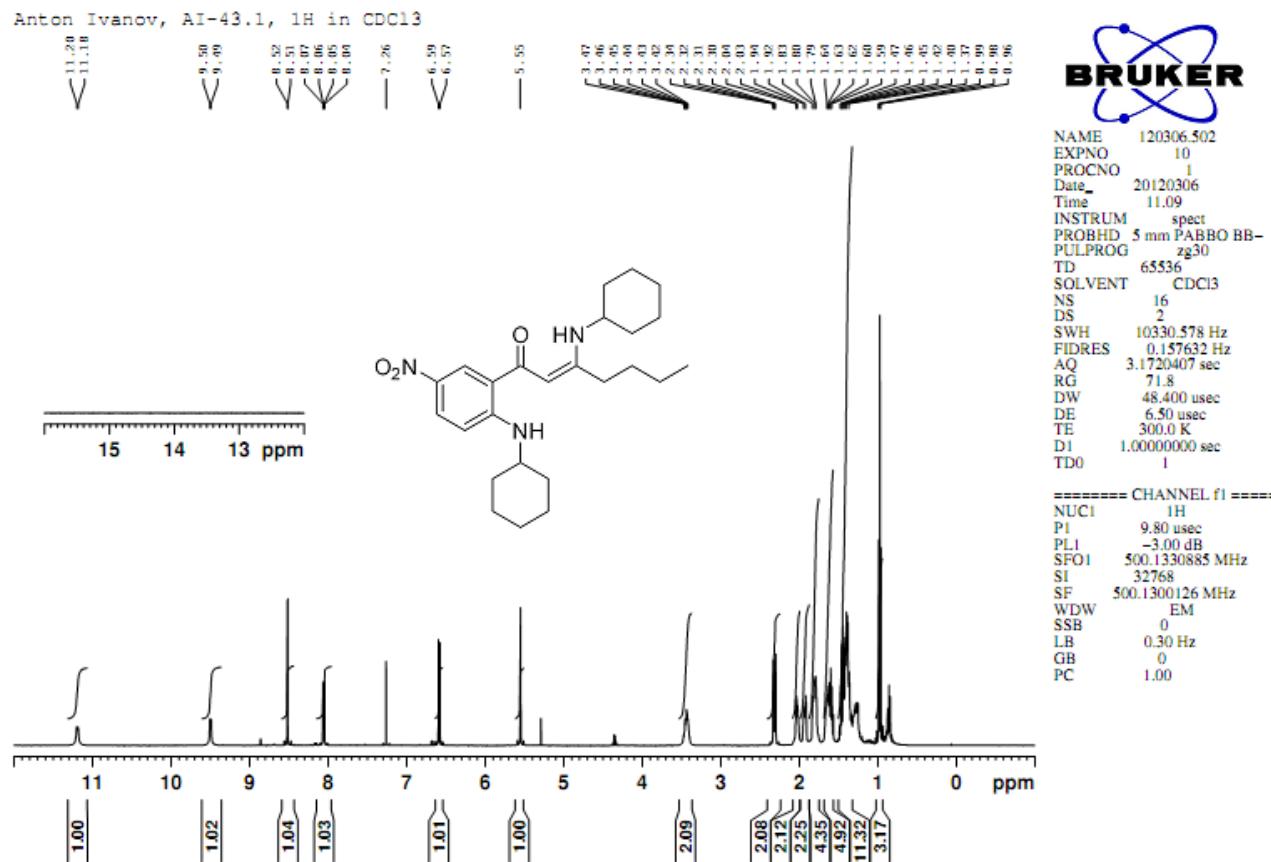
(Z)-3-(3,4-Dimethoxyphenethylamino)-1-(2-(3,4-dimethoxyphenethylamino)-5-nitrophenyl)hept-2-en-1-one (**9c**).



(Z)-3-(3,4-Dimethoxyphenethylamino)-1-(2-(3,4-dimethoxyphenethylamino)-5-nitrophenyl)hept-2-en-1-one (9c).

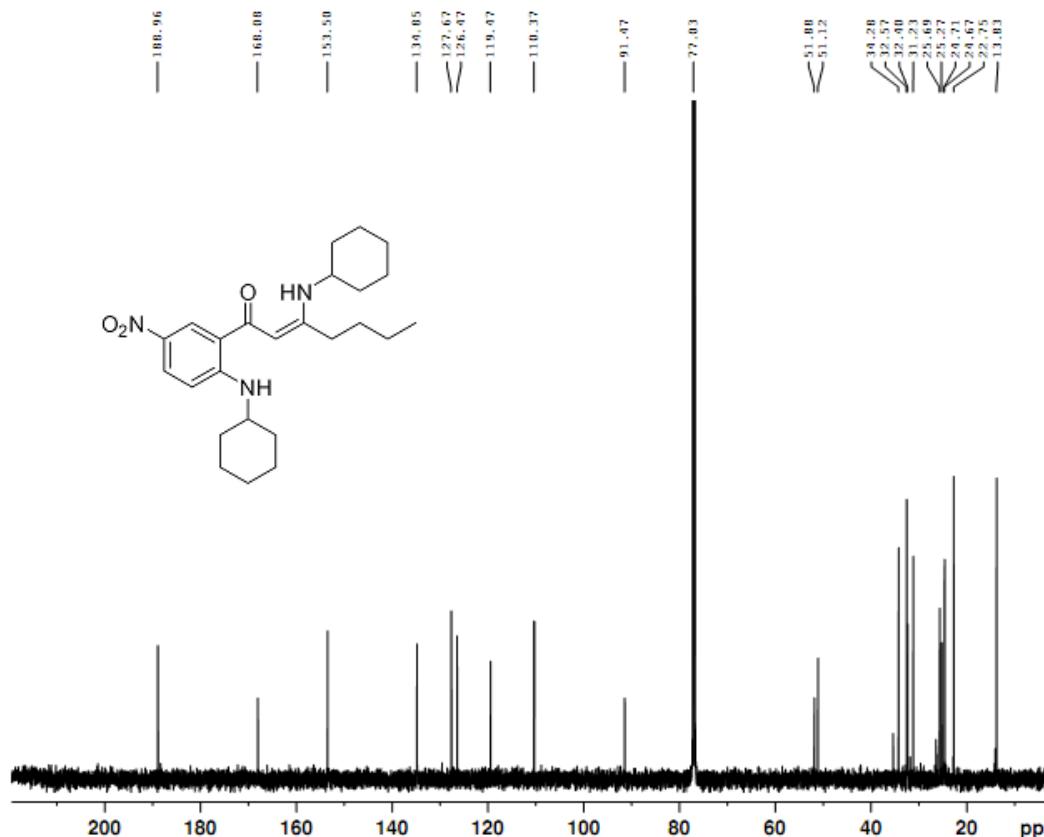


(Z)-3-(Cyclohexylamino)-1-(2-(cyclohexylamino)-5-nitrophenyl)hept-2-en-1-one (9d).



(Z)-3-(Cyclohexylamino)-1-(2-(cyclohexylamino)-5-nitrophenyl)hept-2-en-1-one (9d).

Anton Ivanov, AI-43.1, ^{13}C in CDCl_3



```

NAME 120306.502
EXPNO 13
PROCNO 1
Date_ 20120306
Time 12.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 2896.3
DW 16.650 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.50 dB
SFO1 125.7703643 MHz

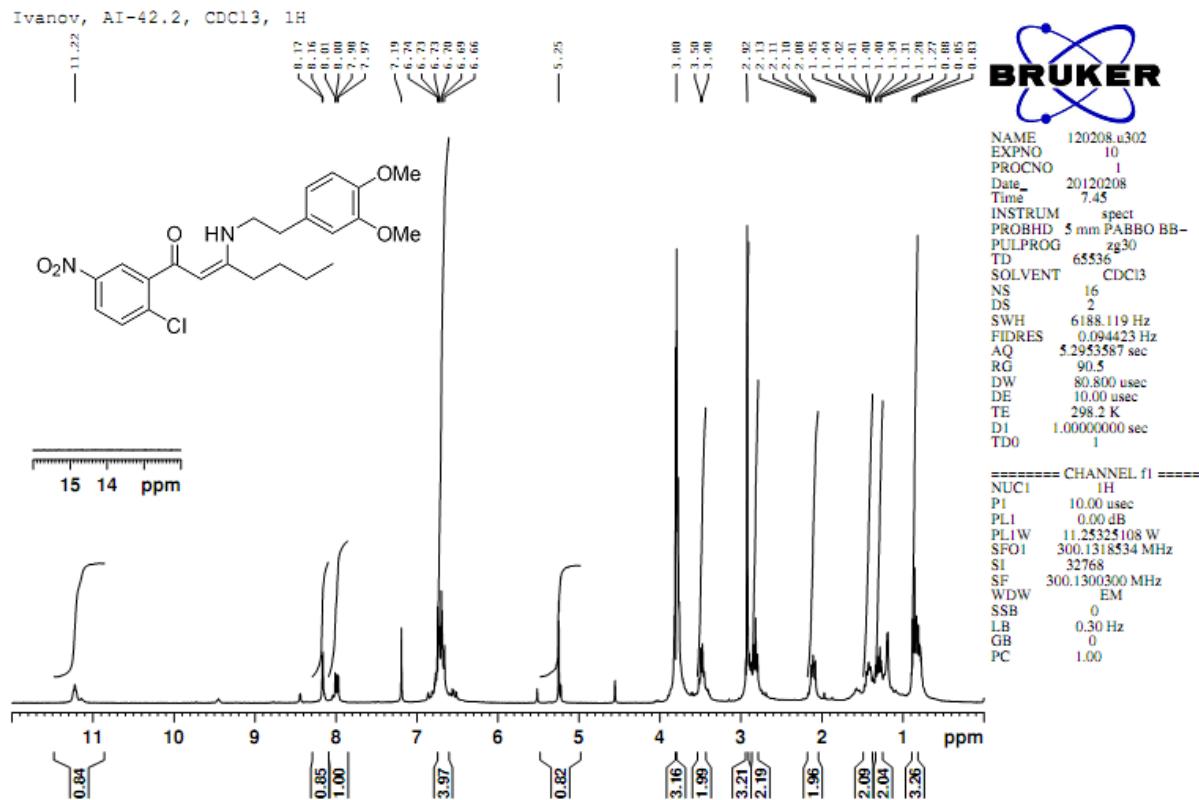
```

```

===== CHANNEL f2 =====
CPDPG02 waltz16
NUC2 1H
PCPDPG2 70.00 usec
PL2 -3.00 dB
PL12 14.08 dB
PL13 120.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

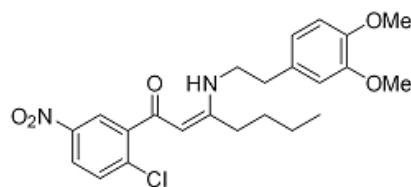
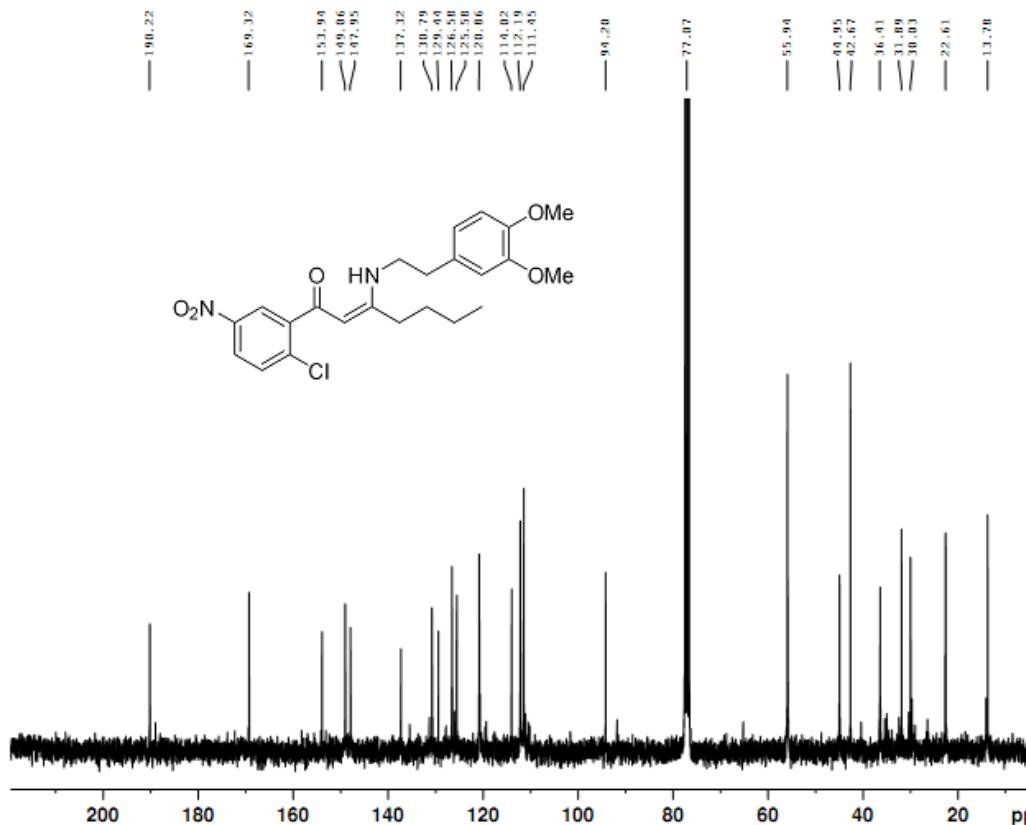
```

(Z)-1-(2-Chloro-5-nitrophenyl)-3-(3,4-dimethoxyphenethylamino)hept-2-en-1-one (10a).



(Z)-1-(2-Chloro-5-nitrophenyl)-3-(3,4-dimethoxyphenethylamino)hept-2-en-1-one (**10a**).

Ivanov, AI-42.2, CDC13, 13C



BRUKER

```

NAME      120210.n329
EXPNO          10
PROCNO         1
Date_        20120210
Time         18.18
INSTRUM     spect
PROBHD  5 mm PABBO BB
TD       65536
SOLVENT      CDCl3
NS          1024
DS           4
SWH      18028.846 Hz
FIDRES    0.257098 Hz
AQ      1.8175818 sec
RG        2050
DW       27.733 usec
DE        10.0 deg
TE       291.2 K
D1   2.0000000 sec
D11      0.03000000 sec
TD0             1.

```

----- CHANNEL f1 -----
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFQ1 75.4332943 MHz

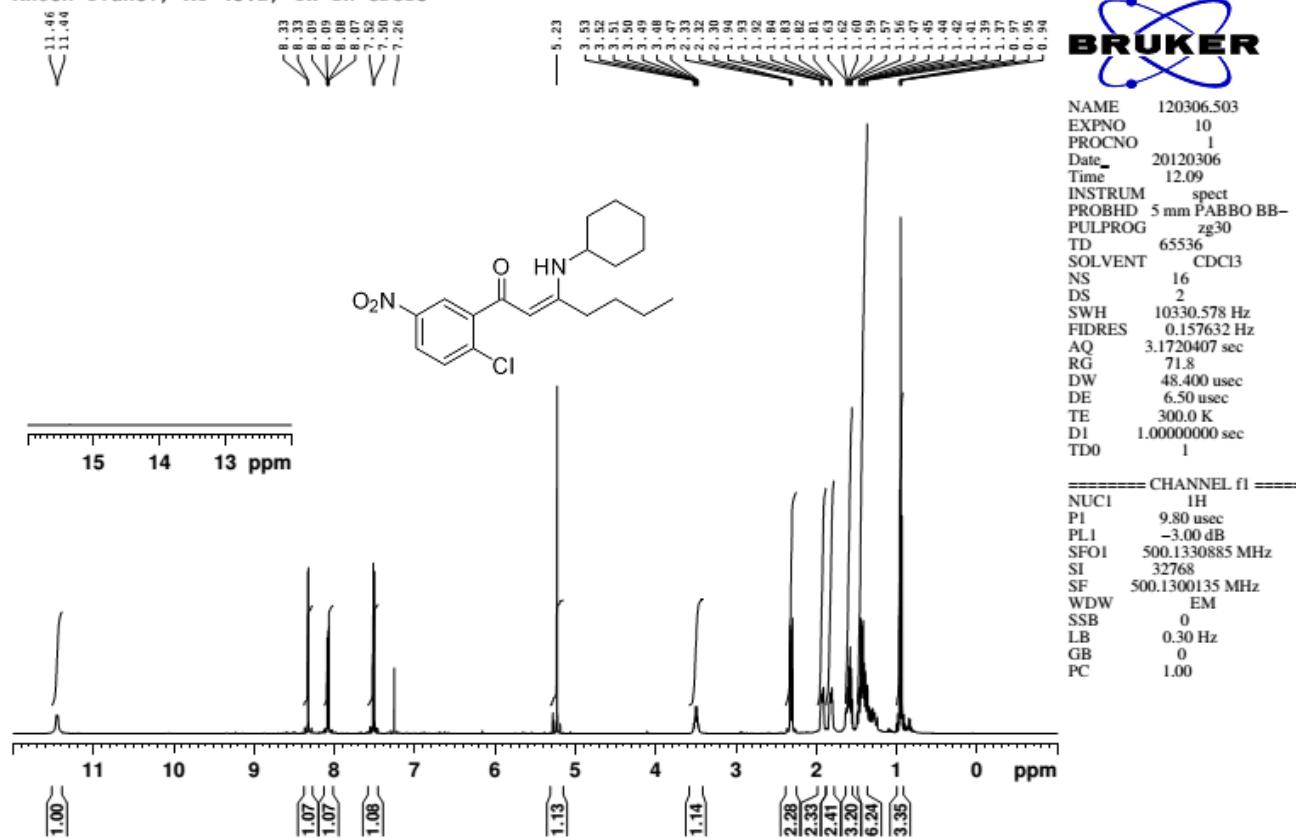
```

CHANNEL 12
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 used
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.235210W
PL12W 0.2243187W
PL13W 0.2243187W
SF02 300.1312005 MHz
SF1 32768
SF2 75.4677490 MHz
WDW 2M
SSB 0
LB 1.00 Hz
GB 0
BS 1.40

```

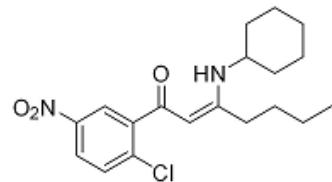
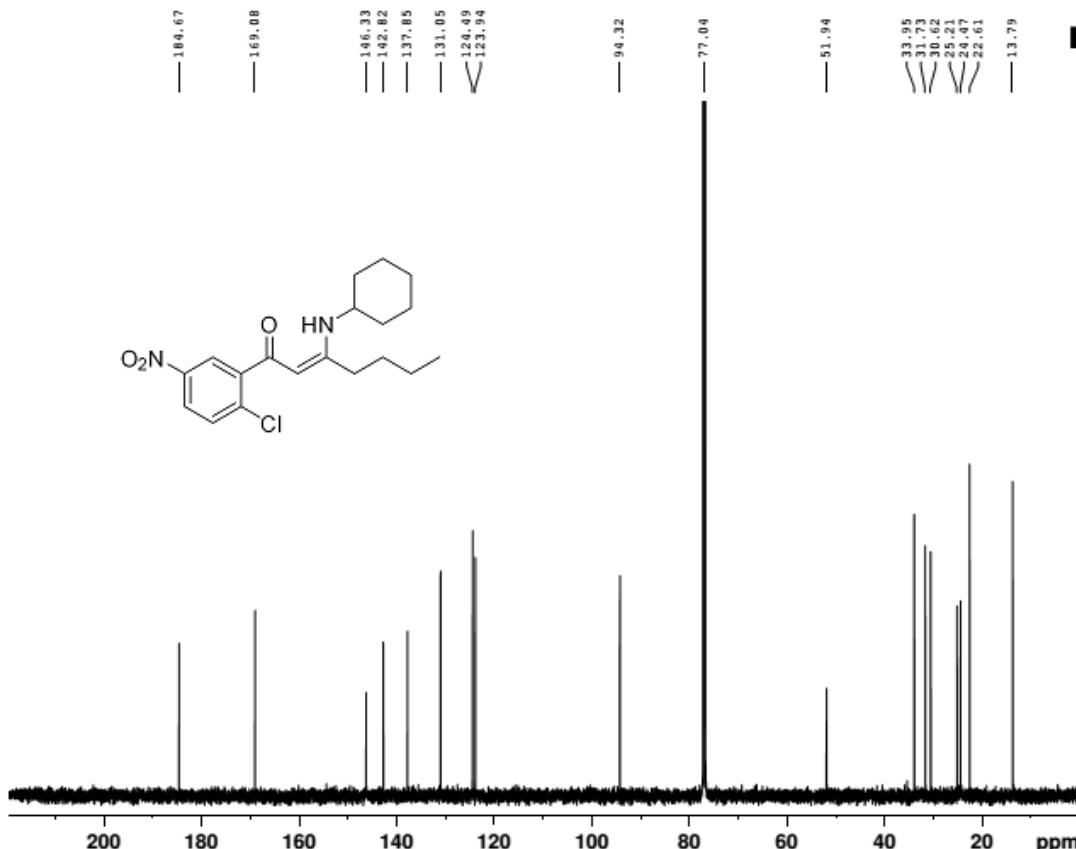
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(cyclohexylamino) hept-2-en-1-one (10b).

Anton Ivanov, AI-43.2, 1H in CDCl₃



(Z)-1-(2-Chloro-5-nitrophenyl)-3-(cyclohexylamino) hept-2-en-1-one (10b).

Anton Ivanov, AI-43.2, ¹³C in CDCl₃



```

NAME 120306.503
EXPNO 13
PROCNO 1
Date_ 20120306
Time 13.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpp30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 3251
DW 16.650 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.50 dB
SFO1 125.7703643 MHz

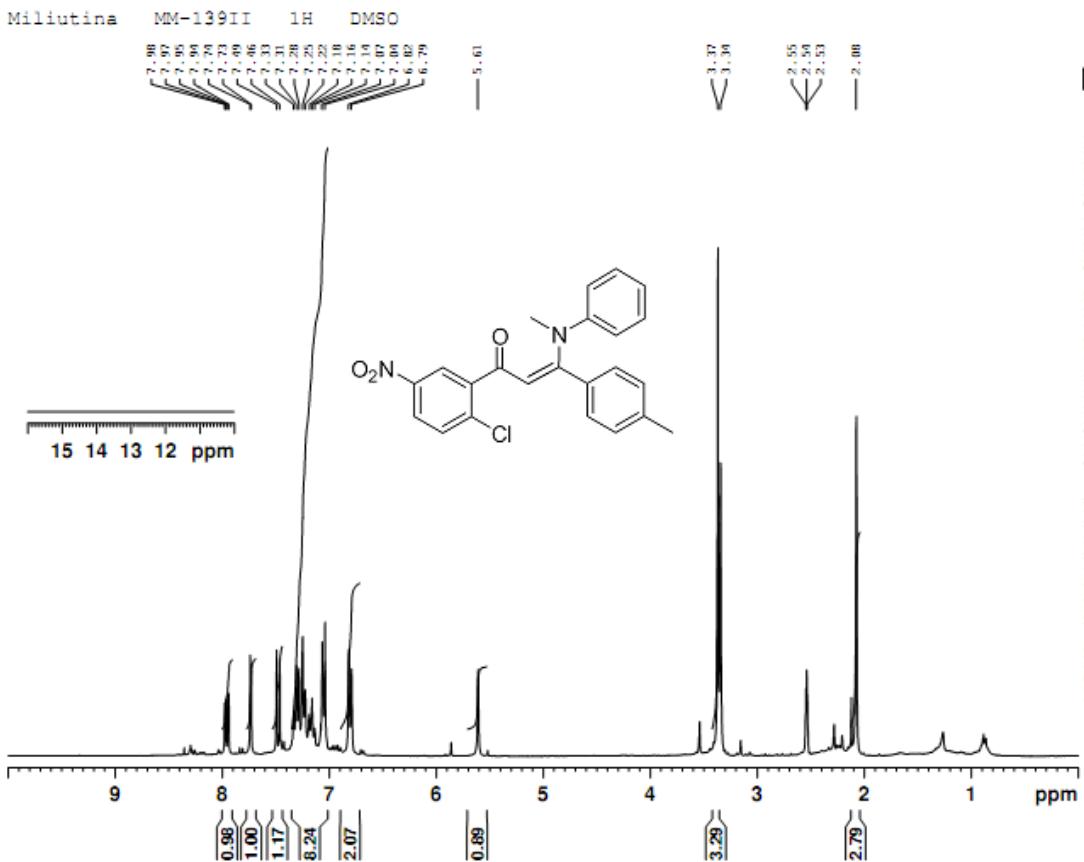
```

```

===== CHANNEL f2 =====
CPDPGR2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 14.08 dB
PL13 120.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

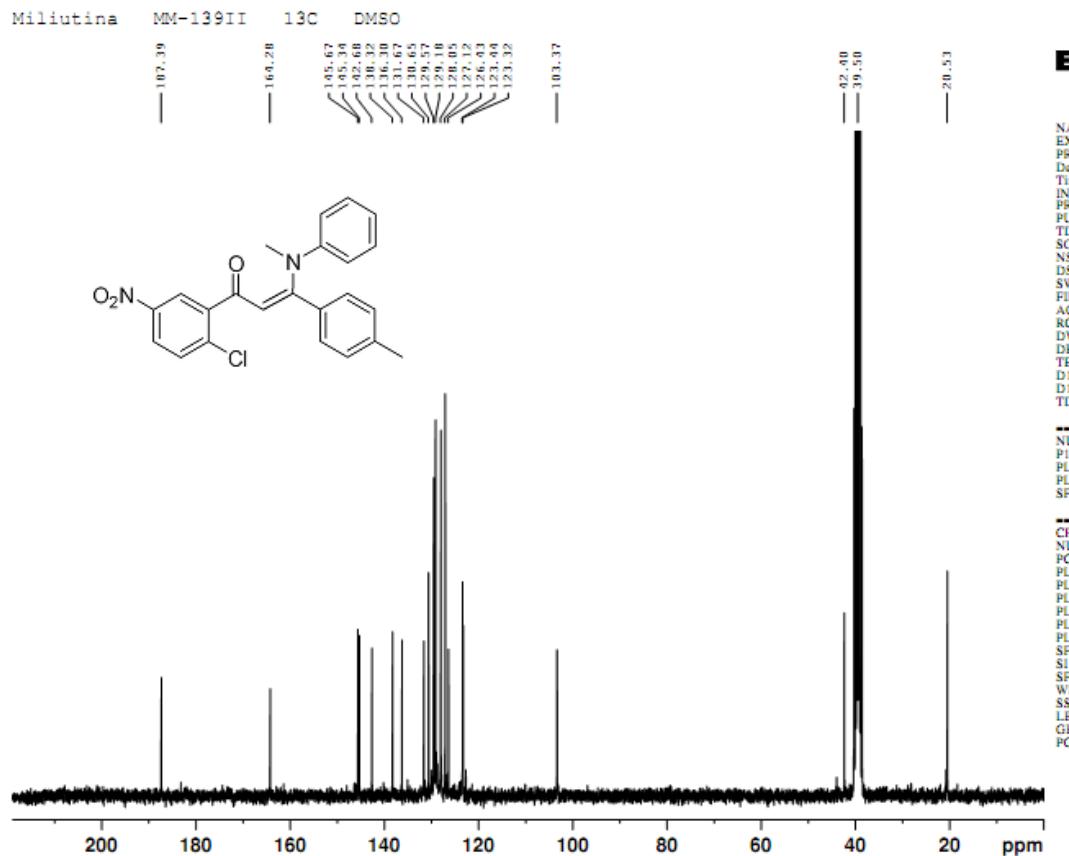
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(methyl(phenyl)amino)-3-p-tolylprop-2-en-1-one (11).



NAME 111209.u331
EXPNO 10
PROCNO 1
Date 20111210
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 297.5 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
PI 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299946 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

(Z)-1-(2-Chloro-5-nitrophenyl)-3-(methyl(phenyl)amino)-3-p-tolylprop-2-en-1-one (11).



BRUKER

```

NAME 111209u331
EXPNO 11
PROCNO 1
Date_ 20111210
Time 18.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 297.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

```

```

----- CHANNEL f1 -----
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.47525953 MHz

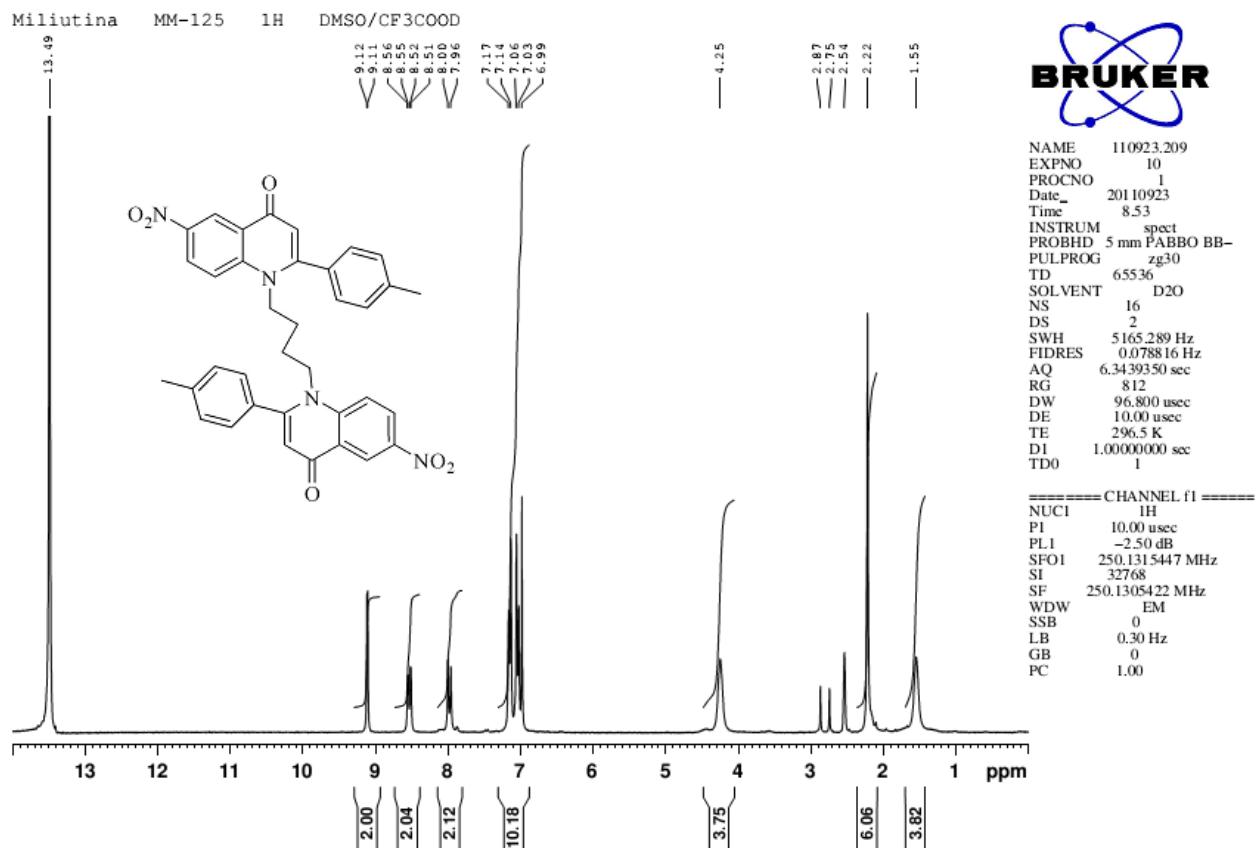
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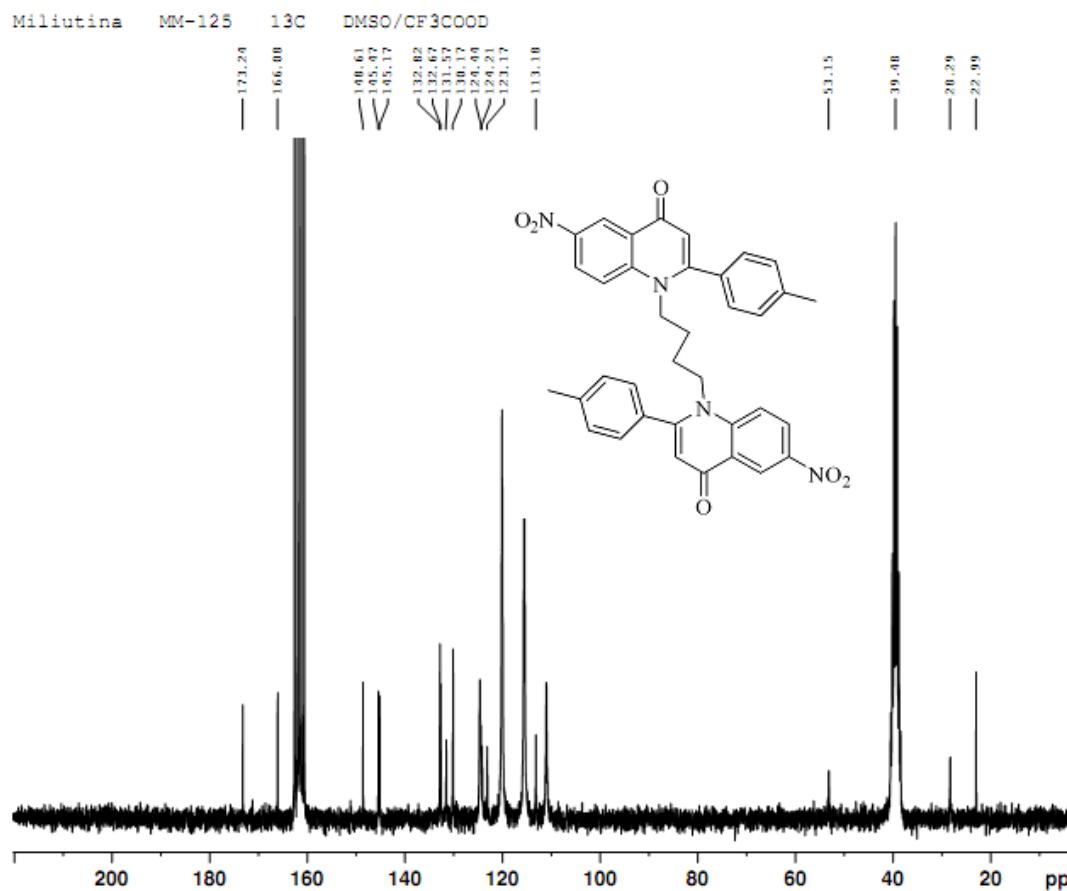
----- CHANNEL f2 -----
CPDPKG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.24325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677875 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

1,1'-(Butane-1,4-diyl)bis(6-nitro-2-p-tolylquinolin-4(1*H*)-one) (12a).



1,1'-(Butane-1,4-diyl)bis(6-nitro-2-p-tolylquinolin-4(1H)-one) (12a).



```

NAME      110923.209
EXPNO     11
PROCNO    1
Date_     20110923
Time     15.15
INSTRUM   spec
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT   D2O
NS        1024
DS         4
SWH      15000.000 Hz
FIDRES   0.228882 Hz
AQ        2.1845834 sec
RG        2050
DW        33.333 usec
DE        10.00 usec
TE        298.9 K
DI        2.0000000 sec
d11      0.03000000 sec
DELTA    1.8999998 sec
TD0       1

```

```

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1      -1.00 dB
SFO1     62.9015280 MHz

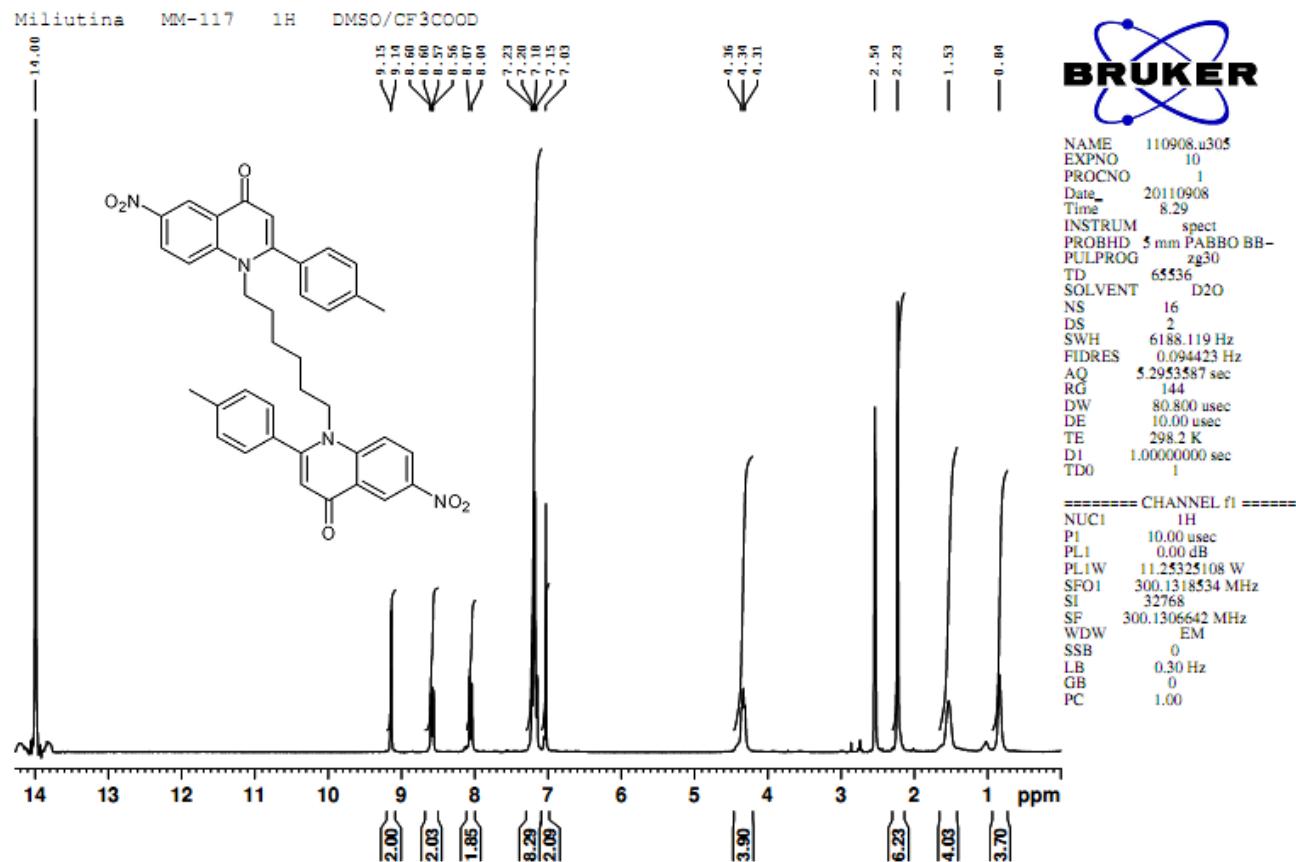
```

```

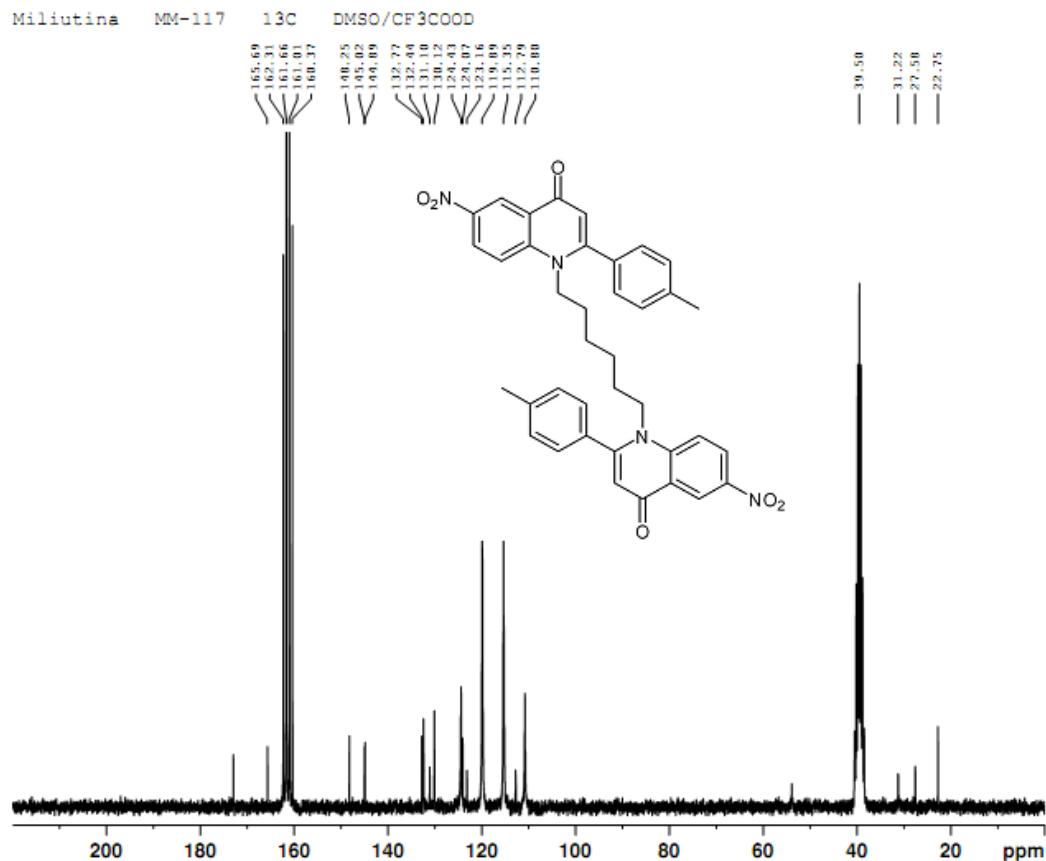
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     70.00 usec
PL12     15.00 dB
PL13     15.00 dB
PL2      -2.50 dB
SFO2     250.1310005 MHz
SI        32768
SF       62.8951757 MHz
WDW       EM
SSB        0
LB        1.00 Hz
GB        0
PC        1.40

```

1,1'-(Hexane-1,6-diyl)bis(6-nitro-2-p-tolylquinolin-4(1H)-one) (12b).



1,1'-(Hexane-1,6-diyl)bis(6-nitro-2-p-tolylquinolin-4(1H)-one) (12b).

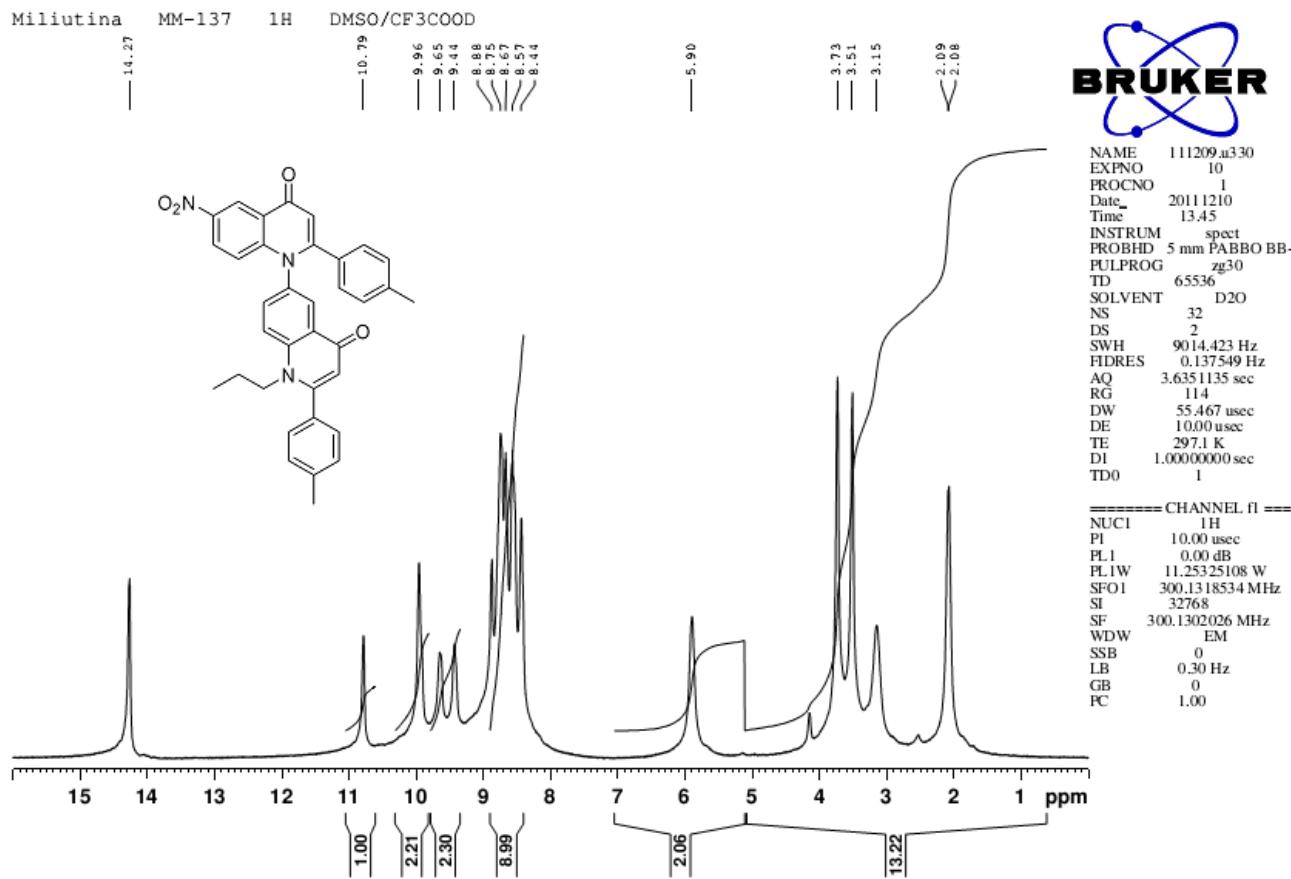


NAME 110914.209
 EXPNO 10
 PROCNO 1
 Date 20110914
 Time 16.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.1 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 T00 1

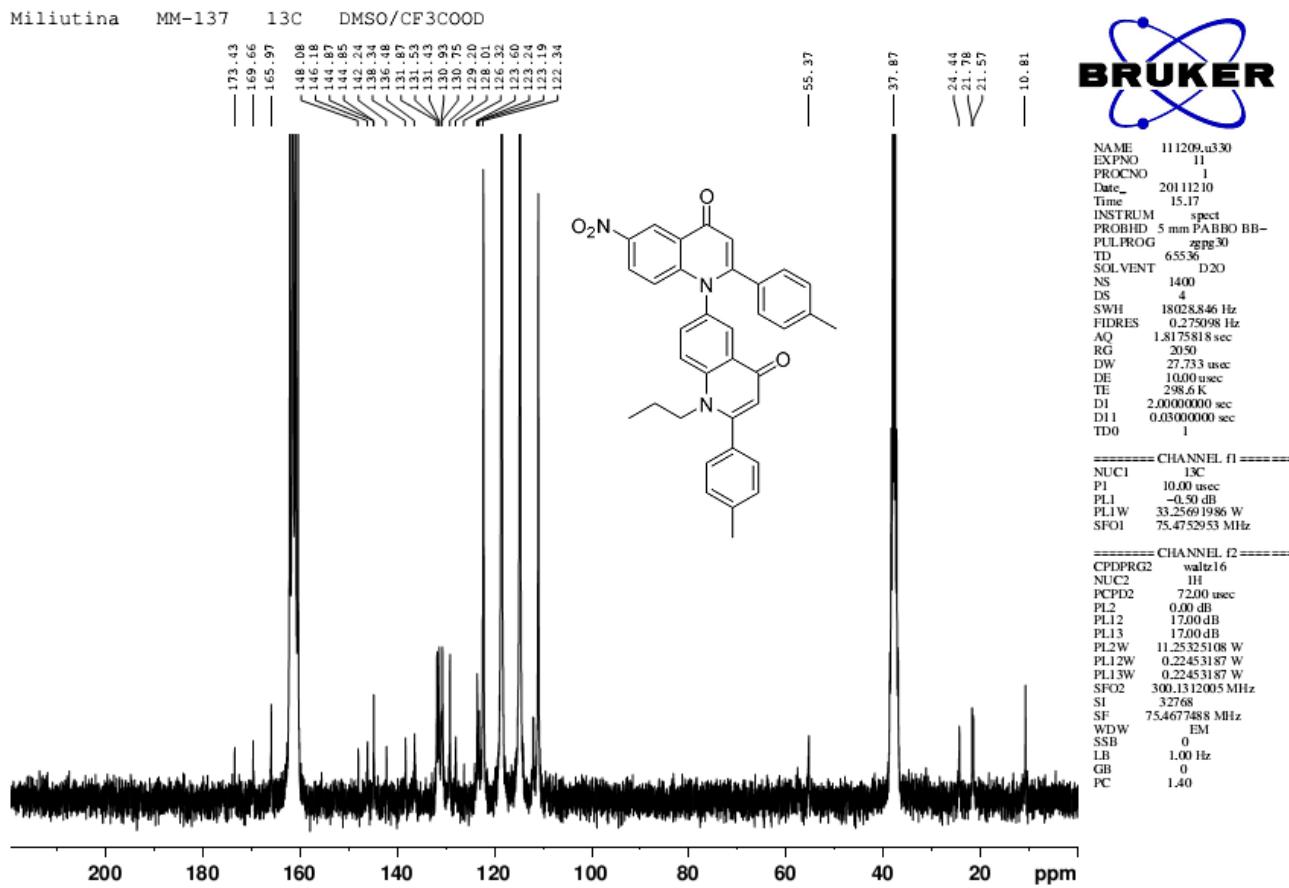
===== CHANNEL f1 =====
 NUC1 ^{13}C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^1H
 PCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz
 SI 32768
 SF 62.8951970 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

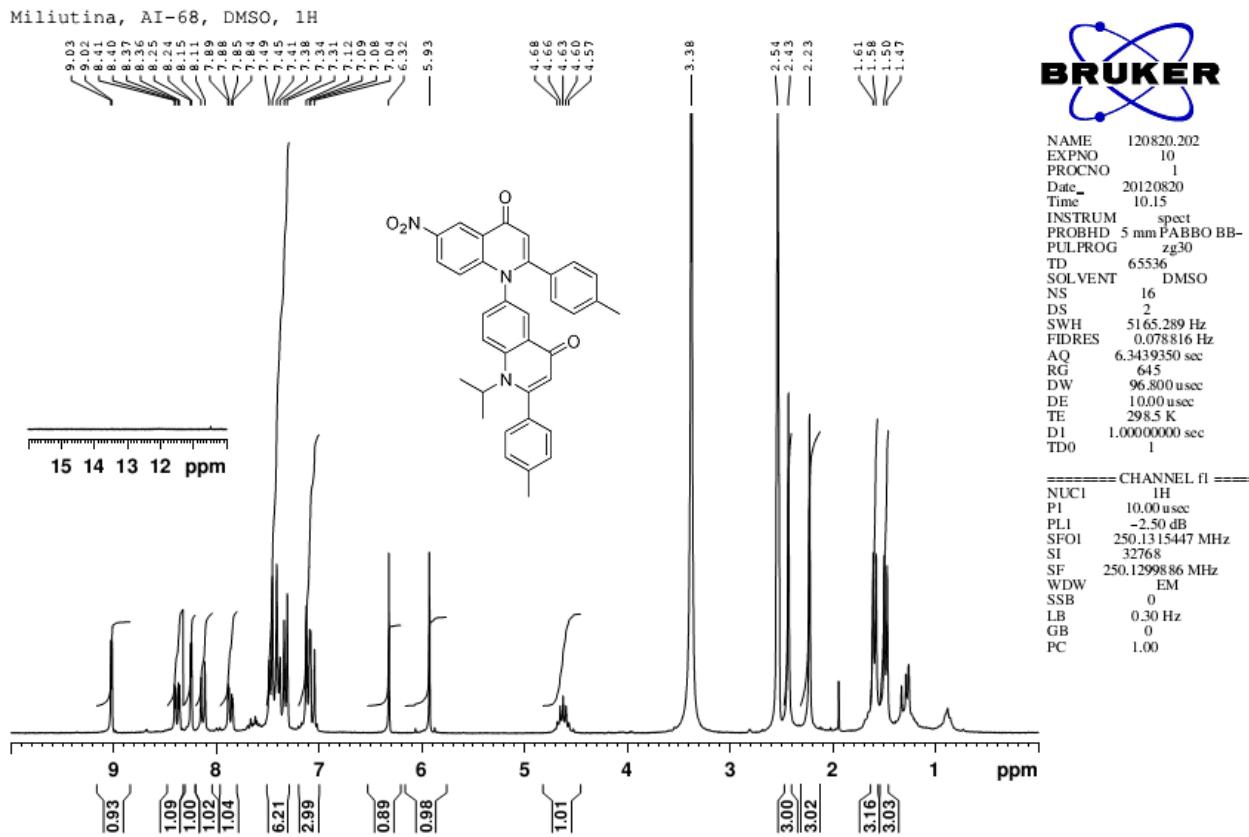
6-Nitro-1'-propyl-2,2'-dip-tolyl-4H-1,6'-biquinoline-4,4'(1'H)-dione (13a).



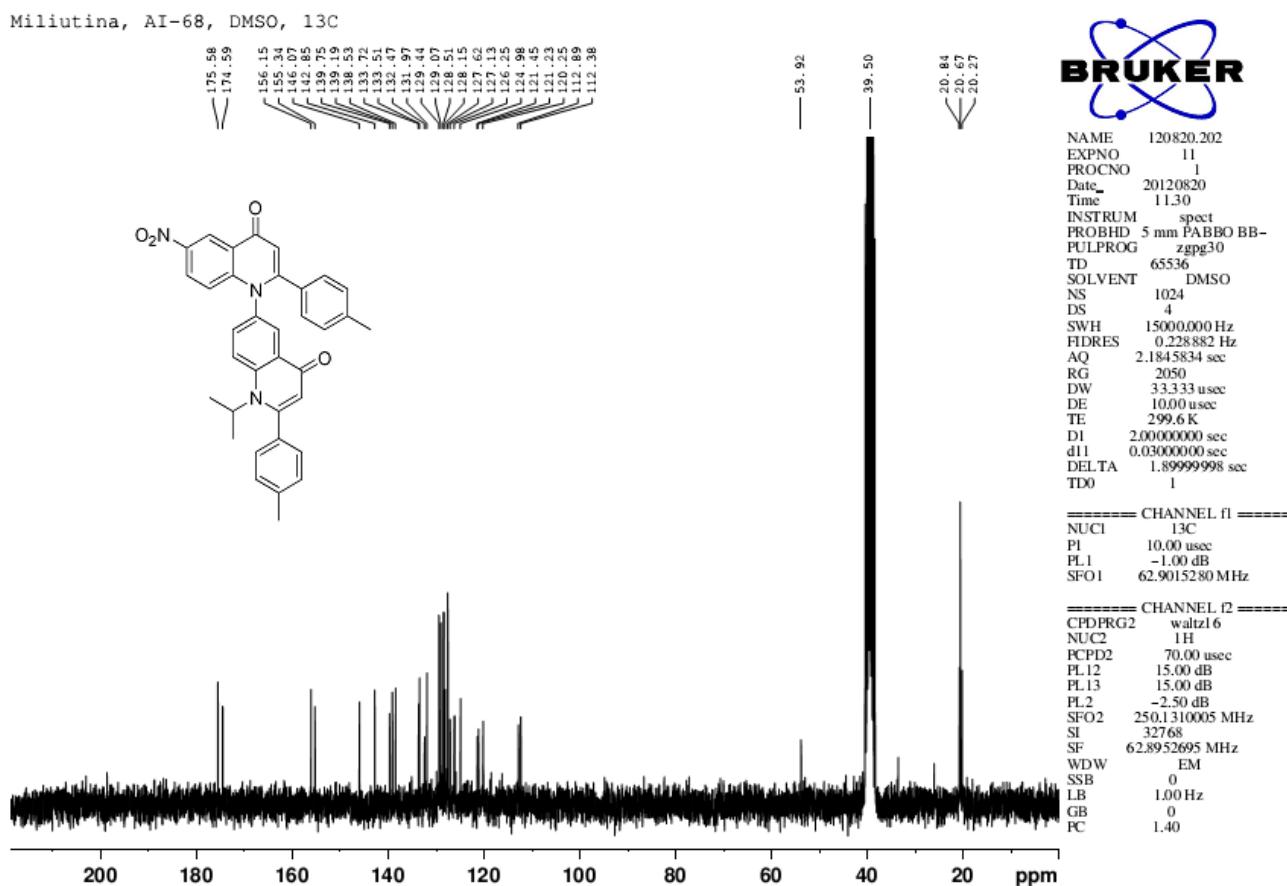
6-Nitro-1'-propyl-2,2'-dip-tolyl-4H-1,6'-biquinoline-4,4'(1'H)-dione (13a).



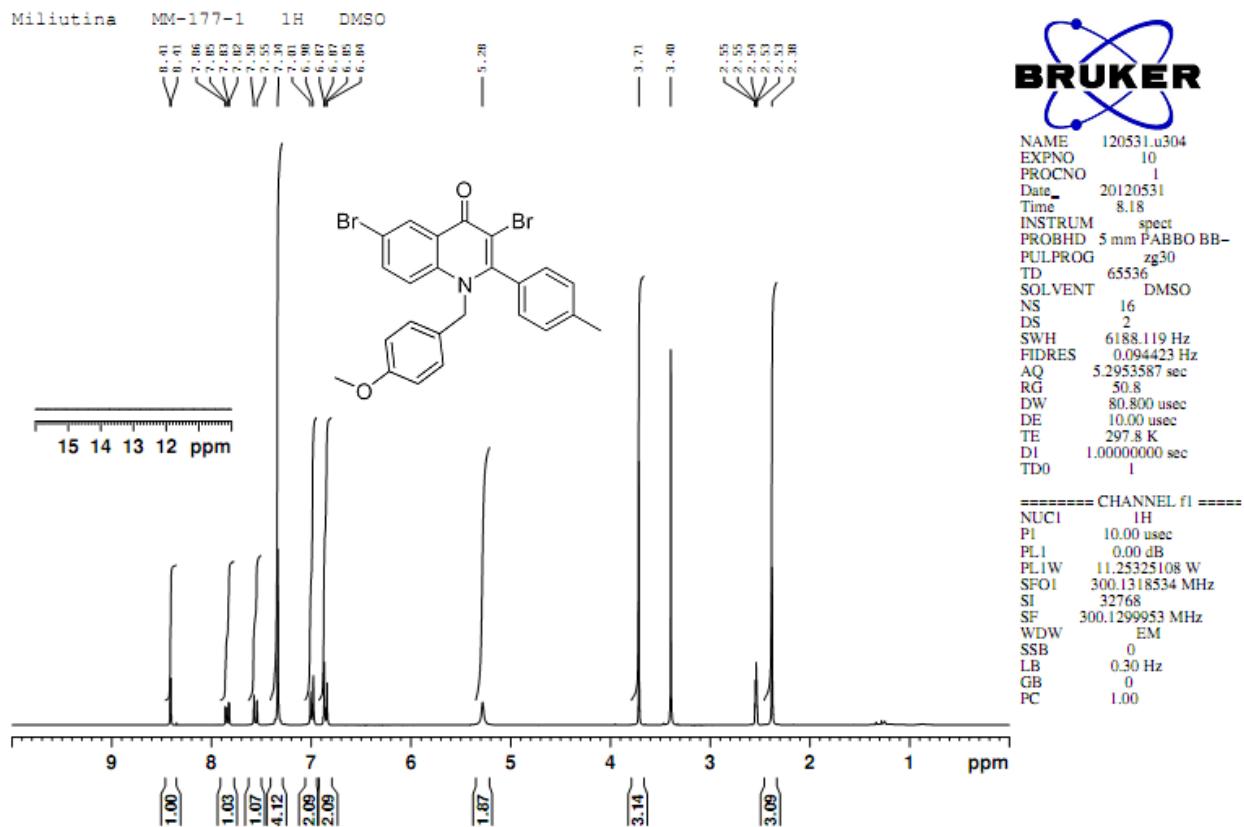
1'-Isopropyl-6-nitro-2,2'-dip-tolyl-4H-1,6'-biquinoline-4,4'(1'H)-dione (13b).



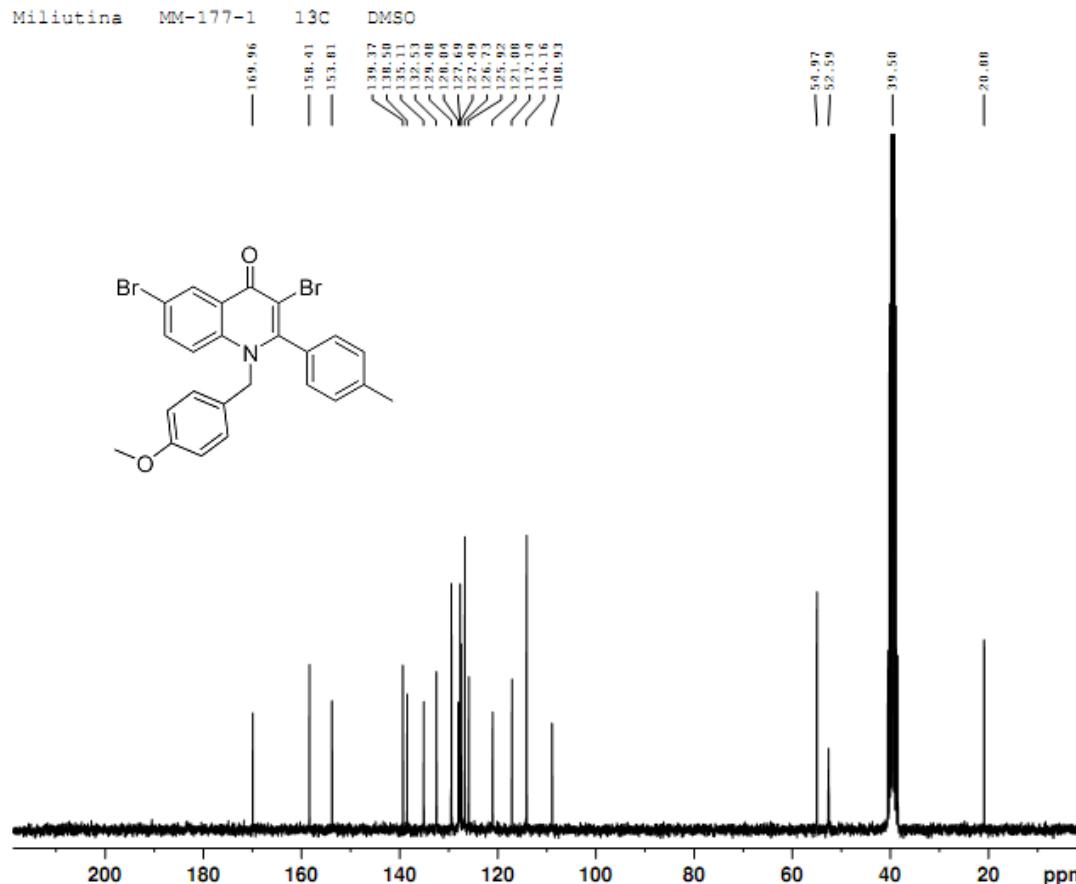
1'-Isopropyl-6-nitro-2,2'-dip-tolyl-4H-1,6'-biquinoline-4,4'(1'H)-dione (13b).



3,6-Dibromo-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (14).



3,6-Dibromo-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (14).



```

NAME 120531.204
EXPNO 10
PROCNO 1
Date_ 20120531
Time 12.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.3 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

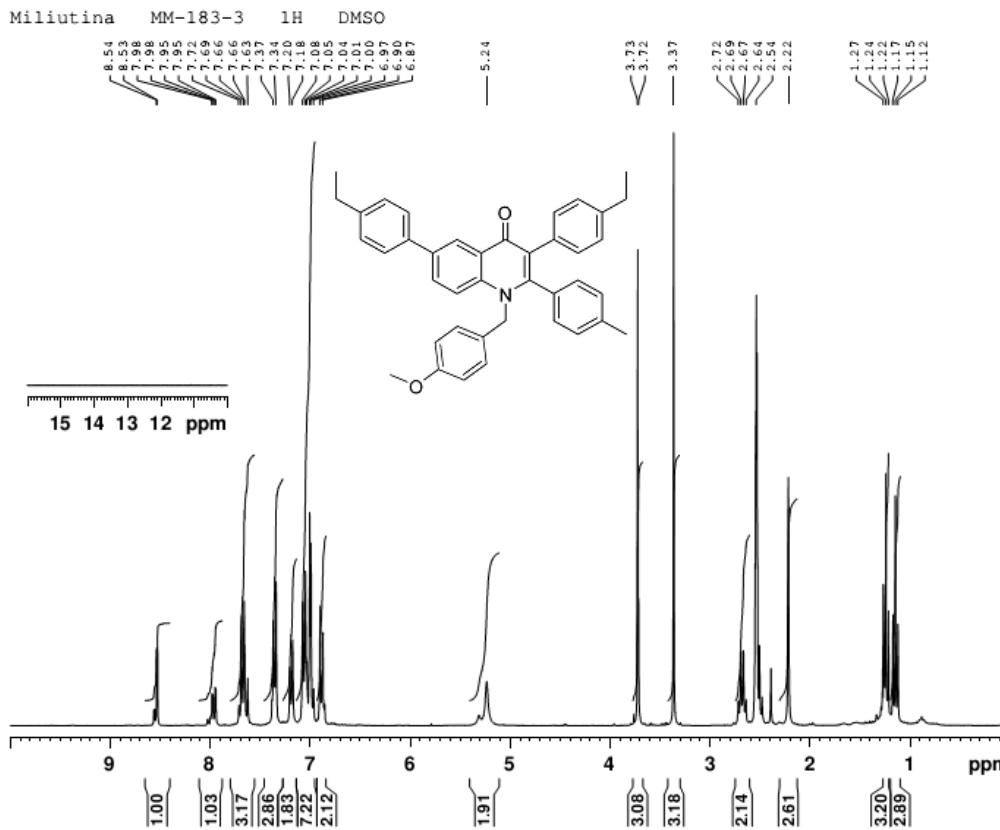
```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.131/0005 MHz
SI 32768
SF 62.8952699 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

3,6-Bis(4-ethylphenyl)-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (15).



```

NAME 120716.u314
EXPNO 10
PROCNO 1
Date_ 20120716
Time 11.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 90.5
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
DI 1.0000000 sec
TD0 1

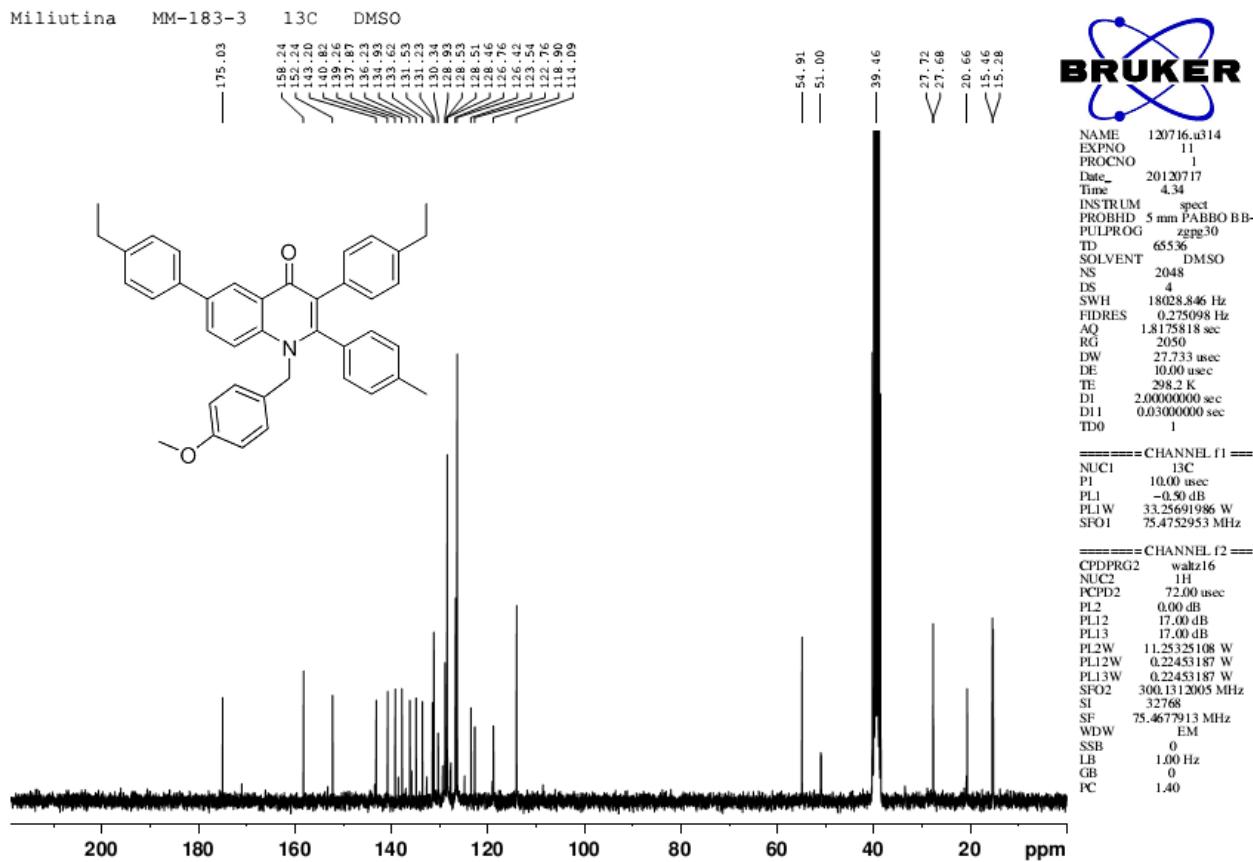
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```

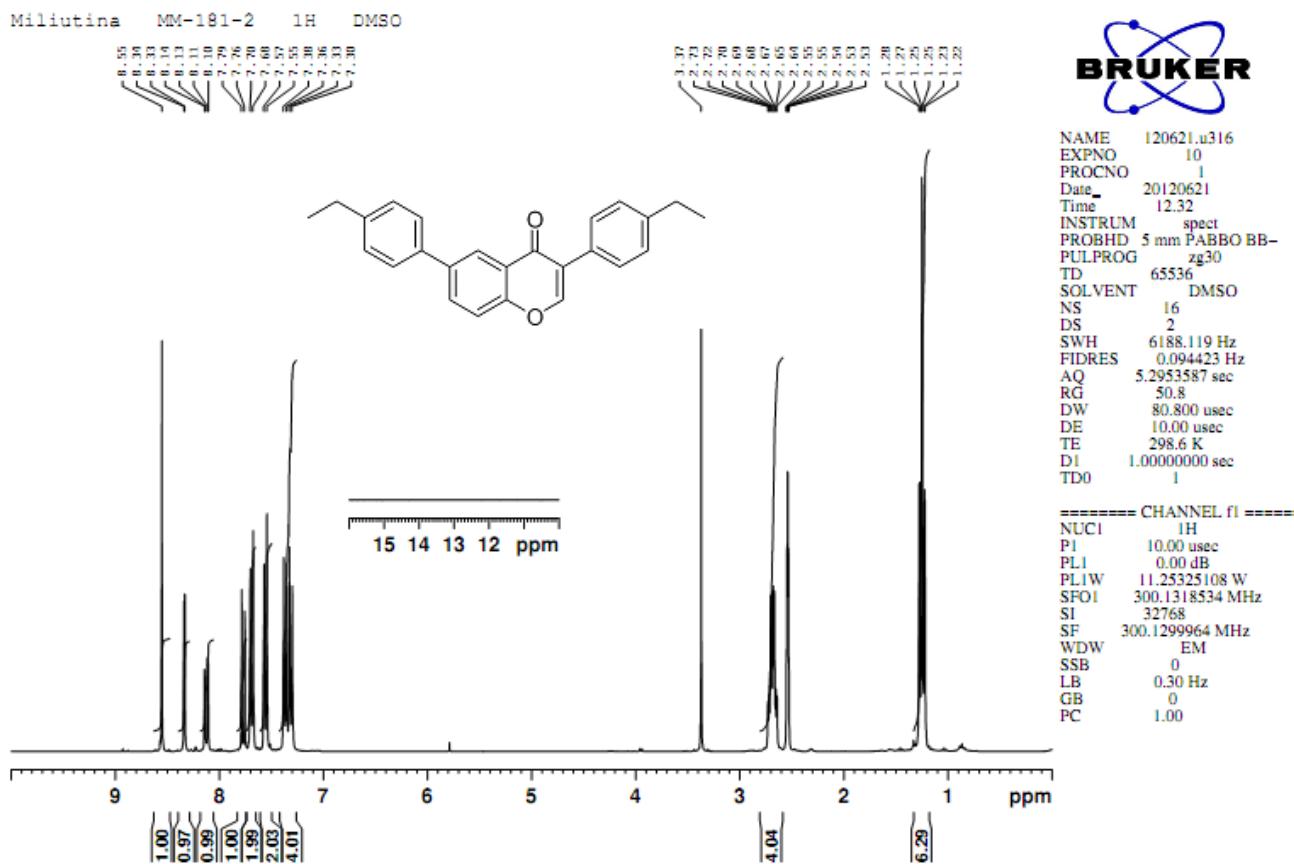
===== CHANNEL f1 =====
NUCI 1H
PI 10.00 usec
PLI 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299965 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

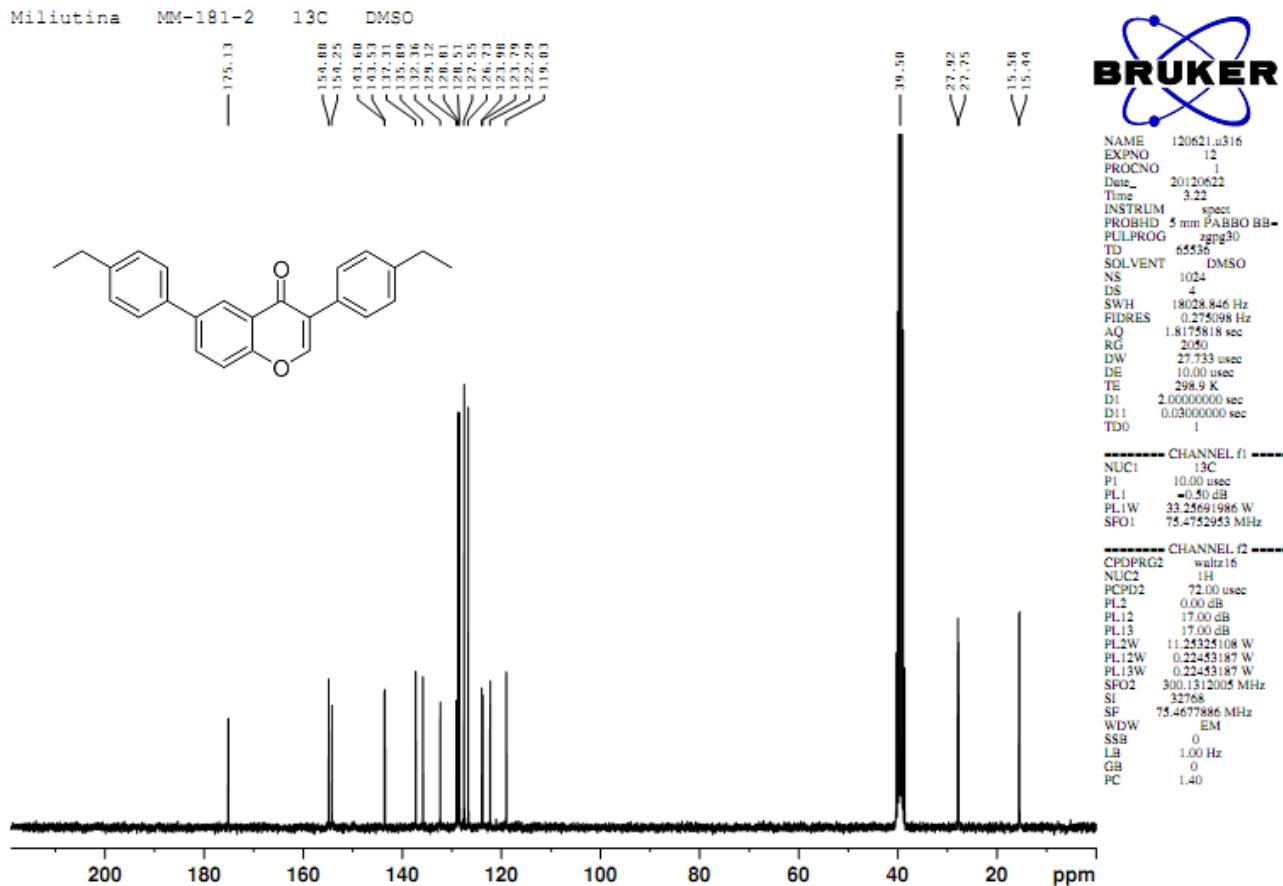
3,6-Bis(4-ethylphenyl)-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (15).



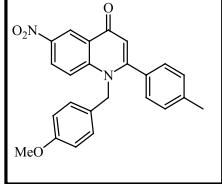
3,6-Bis(4-ethylphenyl)-4*H*-chromen-4-one (16).



3,6-Bis(4-ethylphenyl)-4H-chromen-4-one (16).

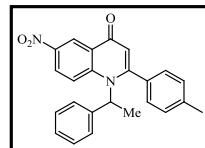


X-Ray structure of compound 7ab

Identification code	is_mm127	
Empirical formula	C24 H20 N2 O4	
Formula weight	400.42	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group (H.-M.)	<i>P</i> 2 ₁ /c	
Space group (Hall)	-P 2ybc	
Unit cell dimensions	a = 10.4745(6) Å b = 10.6976(6) Å c = 17.8031(11) Å	α = 90.00° β = 91.384(3)° γ = 90.00°
Volume	1994.3(2) Å ³	
Z	4	
Calculated density	1.334 mg/m ³	
Absorption coefficient	0.092 mm ⁻¹	
F(000)	840	
Crystal size	0.37 x 0.13 x 0.07 mm ³	
Θ range for data collection	1.94 to 28.00°	
Index ranges	-13 ≤ h ≤ 13, -9 ≤ k ≤ 14, -23 ≤ l ≤ 22	
Reflections collected	19220	
Independent reflections	4810 [R(int) = 0.0664]	
Completeness to Θ = 28.00°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9936 and 0.9668	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2565 / 0 / 273	
Goodness-of-fit on F ²	1.000	
Final R indices [I>2σ (I)]	R1 = 0.0505, wR2 = 0.1045	
R indices (all data)	R1 = 0.1164, wR2 = 0.1328	
Largest diff. peak and hole	0.167 and -0.270 e.Å ⁻³	

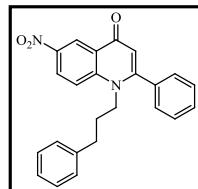
X-Ray structure of compound 7ac

Identification code	is_mm115_118
Empirical formula	C24 H20 N2 O3
Formula weight	384.42
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group (H.-M.)	P 2 ₁ 2 ₁ 2 ₁
Space group (Hall)	P 2ac 2ab
Unit cell dimensions	a = 9.9322(10) Å α = 90° b = 13.6154(10) Å β = 90° c = 14.4052(15) Å γ = 90°
Volume	1948.0(3) Å ³
Z	4
Calculated density	1.311 mg/m ³
Absorption coefficient	0.087 mm ⁻¹
F(000)	808
Crystal size	0.430 x 0.170 x 0.140 mm ³
Θ range for data collection	3.628 to 28.999°
Index ranges	-13 ≤ h ≤ 13, -11 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	15463
Independent reflections	5004 [R(int) = 0.0466]
Completeness to Θ = 28.00°	96.9%
Absorption correction	Multi-scan
Max. and min. transmission	0.7460 and 0.6977
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3347 / 0 / 265
Goodness-of-fit on F ²	1.074
Final R indices [I>2σ (I)]	R1 = 0.0414, wR2 = 0.0724
R indices (all data)	R1 = 0.0851, wR2 = 0.0959
Largest diff. peak and hole	0.191 and -0.178 e.Å ⁻³



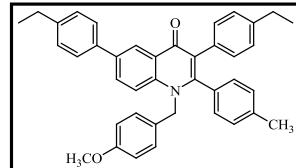
X-Ray structure of compound 7bd

Identification code	av_mm89
Empirical formula	C24 H20 N2 O3
Formula weight	384.42
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group (H.-M.)	P b c a
Space group (Hall)	-P 2ac 2ab
Unit cell dimensions	a = 10.4213(5) Å α = 90.00° b = 15.0974(8) Å β = 90.00° c = 24.6279(14) Å γ = 90.00°
Volume	3874.8(4) Å ³
Z	8
Calculated density	1.318 mg/m ³
Absorption coefficient	0.088 mm ⁻¹
F(000)	1616
Crystal size	0.68 x 0.20 x 0.15 mm ³
Θ range for data collection	2.51 to 30.00°
Index ranges	-14 ≤ h ≤ 12, -19 ≤ k ≤ 21, -34 ≤ l ≤ 24
Reflections collected	22580
Independent reflections	5541 [R(int) = 0.0292]
Completeness to Θ = 28.00°	98.0%
Absorption correction	Multi-scan
Max. and min. transmission	0.9870 and 0.9427
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3855 / 0 / 262
Goodness-of-fit on F ²	1.049
Final R indices [I>2σ (I)]	R1 = 0.0493, wR2 = 0.1103
R indices (all data)	R1 = 0.0799, wR2 = 0.1234
Largest diff. peak and hole	0.208 and -0.245 e.Å ⁻³

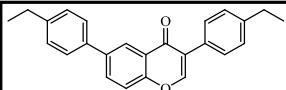


X-Ray structure of compound 15

Identification code	is_mm183	
Empirical formula	C39.74 H36.71 Br0.03 N O2	
Formula weight	562.69	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group (H.-M.)	P̄1	
Space group (Hall)	-P 1	
Unit cell dimensions	a = 10.5670(5) Å b = 12.7739(5) Å c = 12.9152(5) Å	$\alpha = 109.863(2)^\circ$ $\beta = 101.516(2)^\circ$ $\gamma = 105.361(2)^\circ$
Volume	1498.23(11) Å^3	
Z	2	
Calculated density	1.247 mg/m³	
Absorption coefficient	0.115 mm⁻¹	
F(000)	598	
Crystal size	0.24 x 0.22 x 0.05 mm³	
Θ range for data collection	2.80 to 30.00°	
Index ranges	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -18 ≤ l ≤ 18	
Reflections collected	39715	
Independent reflections	8694 [R(int) = 0.0471]	
Completeness to Θ = 28.00°	99.6%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9943 and 0.9728	
Refinement method	Full-matrix least-squares on F²	
Data / restraints / parameters	5050 / 0 / 396	
Goodness-of-fit on F²	1.013	
Final R indices [I>2σ (I)]	R1 = 0.0558, wR2 = 0.1135	
R indices (all data)	R1 = 0.1178, wR2 = 0.1406	
Largest diff. peak and hole	0.445 and -0.255 e.Å⁻³	



X-Ray structure of compound 16

Identification code	ch_mm181	
Empirical formula	C25 H22 O2	
Formula weight	354.43	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group (H.-M.)	<i>P</i> 2 ₁ / <i>n</i>	
Space group (Hall)	-P 2yn	
Unit cell dimensions	a = 5.8177(4) Å b = 10.2341(6) Å c = 31.4579(18) Å	α = 90.00° β = 94.982(2)° γ = 90.00°
Volume	1865.9(2) Å ³	
Z	4	
Calculated density	1.262 mg/m ³	
Absorption coefficient	0.079 mm ⁻¹	
F(000)	752	
Crystal size	0.57 x 0.16 x 0.15 mm ³	
Θ range for data collection	1.30 to 28.00°	
Index ranges	-7 ≤ h ≤ 7, -13 ≤ k ≤ 13, -41 ≤ l ≤ 41	
Reflections collected	24058	
Independent reflections	4514 [R(int) = 0.0339]	
Completeness to Θ = 28.00°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9883 and 0.9566	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3522 / 0 / 273	
Goodness-of-fit on F ²	1.017	
Final R indices [I>2σ (I)]	R1 = 0.0513, wR2 = 0.1247	
R indices (all data)	R1 = 0.0674, wR2 = 0.1374	
Largest diff. peak and hole	0.488 and -0.350 e.Å ⁻³	