

## Supplementary Material

### Synthesis, X-ray crystal structure and antimycobacterial activity of enantiomerically pure 1-ethyl-2,3-dicyano-5-(het)aryl-6-hetaryl-1,6-dihydropyrazines

Egor V. Verbitskiy,<sup>a,b\*</sup> Maria S. Toporova,<sup>a</sup> Mikhail I. Kodess,<sup>a</sup> Marina A. Ezhikova,<sup>a</sup> Maksim L. Isenov,<sup>a</sup> Marina G. Pervova,<sup>a</sup> Marionella A. Kravchenko,<sup>c</sup> Igor D. Medvinskiy,<sup>c</sup> Sergey N. Skorniyakov,<sup>c</sup> Gennady L. Rusinov,<sup>a,b</sup> and Valery N. Charushin<sup>a,b</sup>

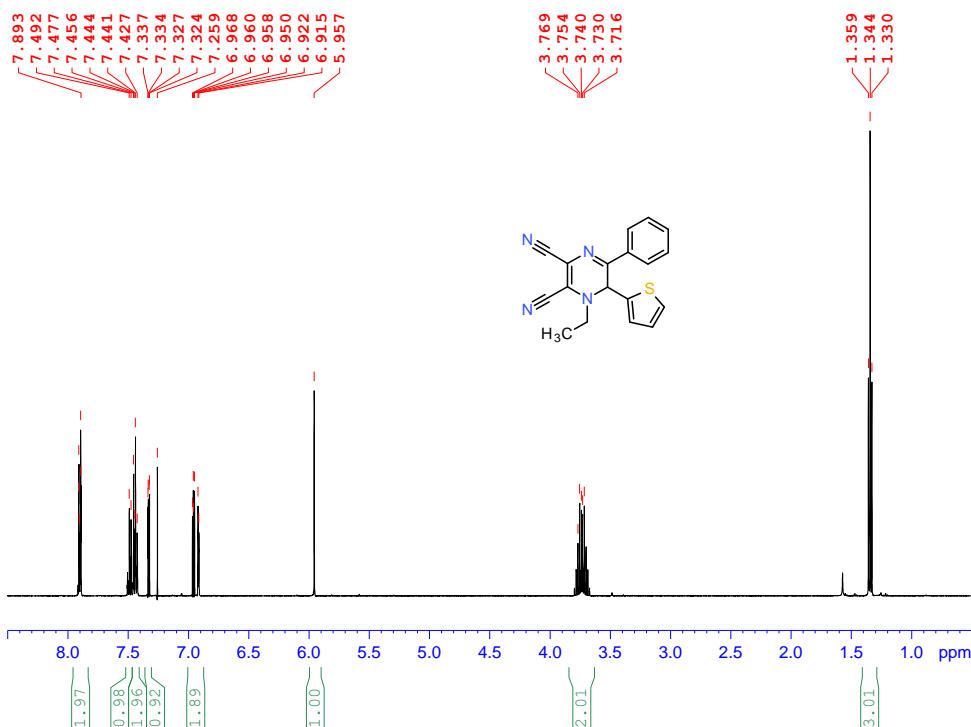
<sup>a</sup>*I. Postovsky Institute of Organic Synthesis, Ural Branch of the Russian Academy of Sciences, S. Kovalevskoy Str., 22, Ekaterinburg, 620990, Russia*

<sup>b</sup>*Ural Federal University, Mira St. 19, Ekaterinburg, 620002, Russia*

<sup>c</sup>*Ural Research Institute for Phthisiopulmonology, 22 Parts'ezda, 50, Ekaterinburg, 620039, Russia*

*E-mail: [Verbitsky@ios.uran.ru](mailto:Verbitsky@ios.uran.ru)*

**Dedicated to Professor Oleg N. Chupakhin on the occasion of his 80th anniversary**



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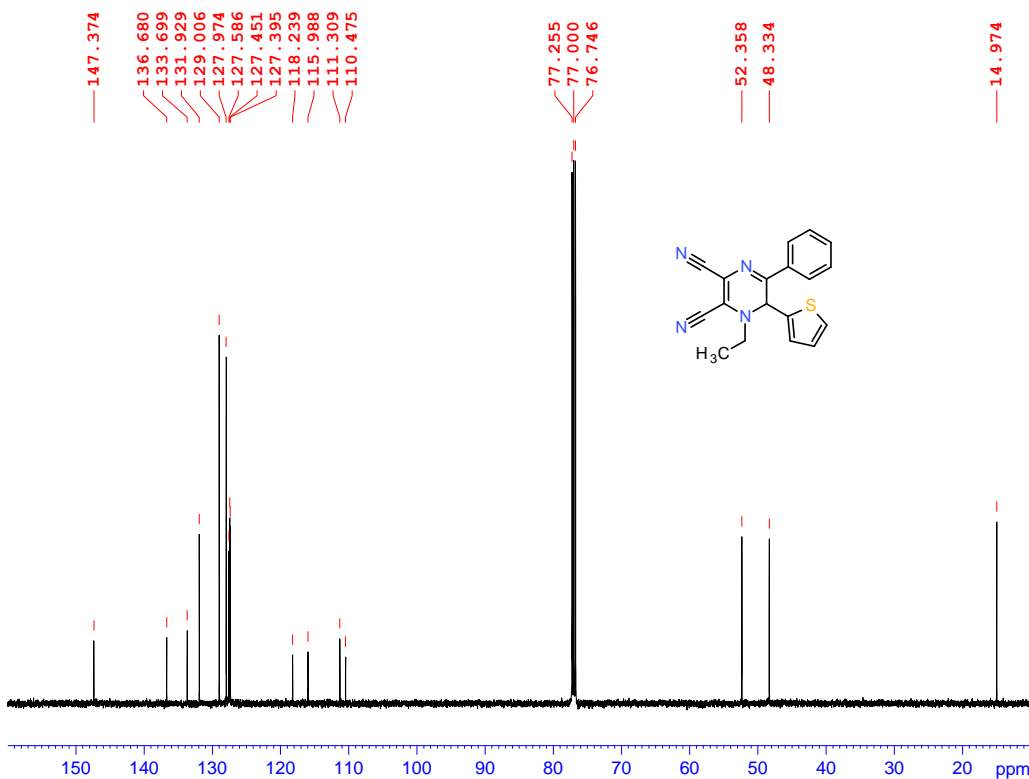
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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INSTRUM  AV500
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PULPROG  zg30
SOLVENT  CDCl3
TD        32768
SW        12.0160 ppm
O1P       5.000 ppm
FIDRES    0.183399 Hz
NS         8
DS         2
AQ        2.7263477 sec
RG         101
TE        297.0 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        12.00 usec
PL1       1.00 dB
PL1W      16.10176659 W
SF01      500.1325007 MHz

F2 - Processing parameters
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SF         500.1300146 MHz
WDW        GM
SSB        0
LB         -1.00 Hz
GB         0.3
PC         4.00
  
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ema: A\*01737

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **11a**.

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Current Data Parameters
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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PULPROG  zgpg30
SOLVENT  CDCl3
TD        32768
SW        180.7063 ppm
O1P       90.000 ppm
FIDRES    0.693581 Hz
NS         512
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AQ        0.7209460 sec
RG         203
TE        298.1 K
D1        0.80000001 sec
D11       0.03000000 sec
TD0       1

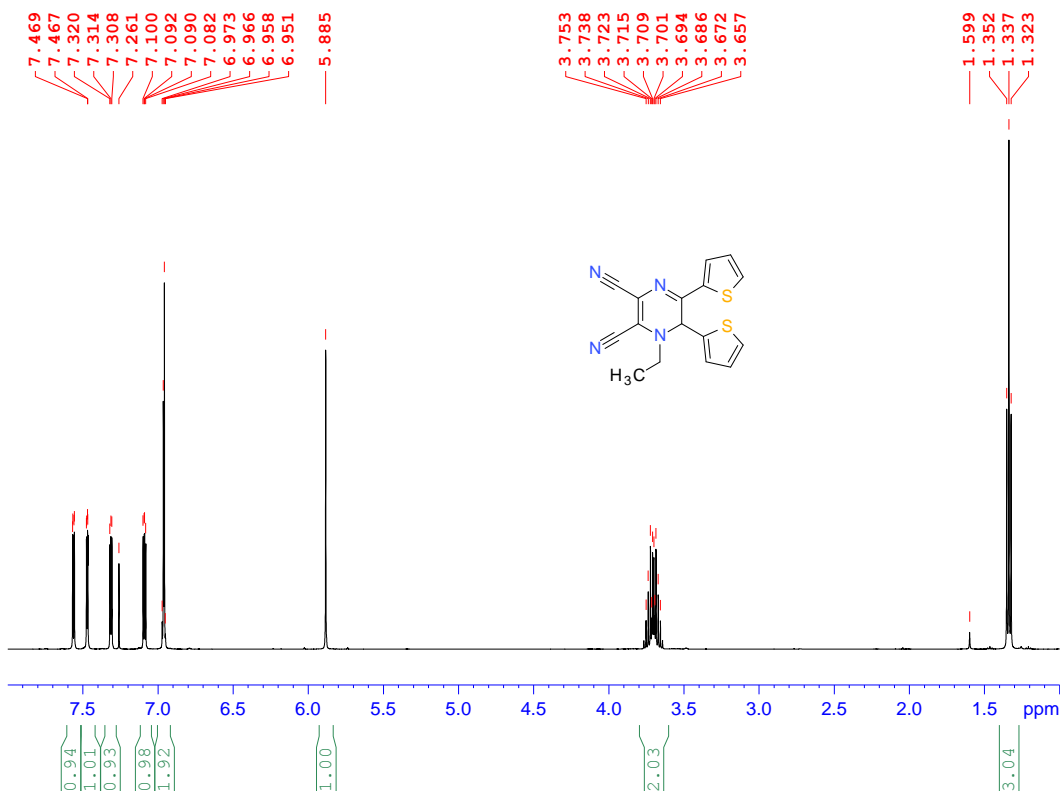
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NUC1      13C
P1        9.00 usec
PL1       0 dB
PL1W      115.29558563 W
SF01      125.7691072 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    75.00 usec
PL2       120.00 dB
PL12     17.00 dB
PL13     20.00 dB
PL2W     0 W
PL12W    0.40445811 W
PL13W    0.20270923 W
SF02     500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         125.7577945 MHz
WDW        EM
SSB        0
LB         1.00 Hz
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ema: A\*01738

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **11a**



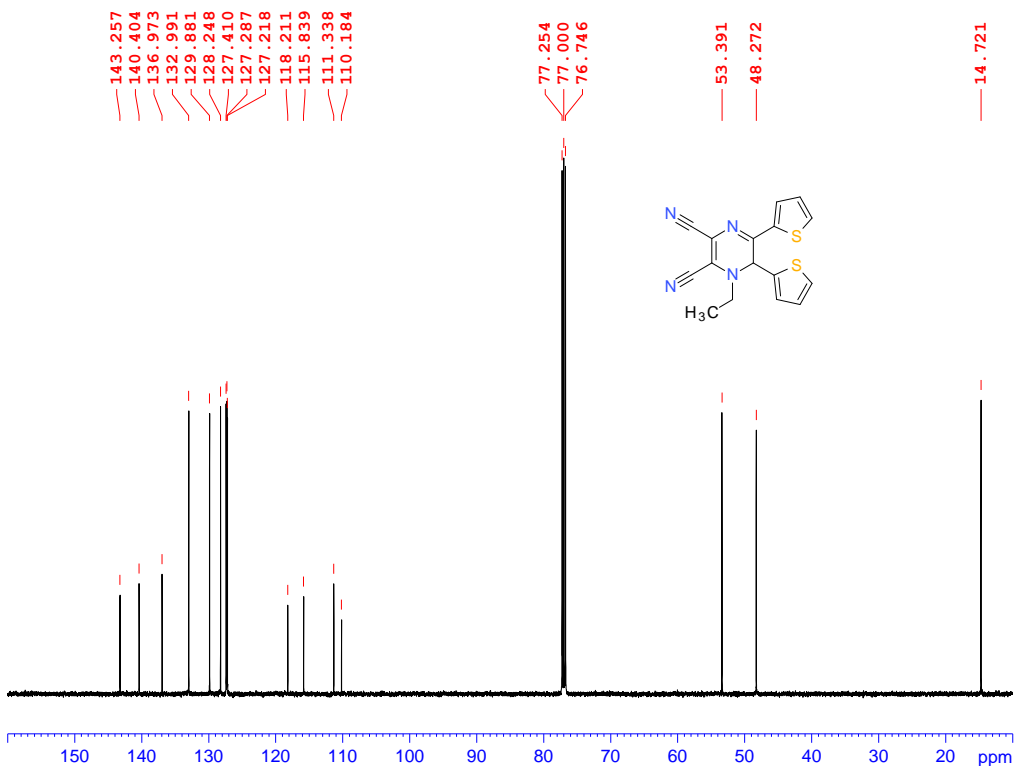
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 PROCNO 1

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 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 16  
 DS 2  
 AQ 2.7263477 sec  
 RG 101  
 TE 296.5 K  
 D1 1.0000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300134 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

ema: A\*01690

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **11b**.

Current Data Parameters  
 NAME VEV912b  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20111227  
 Time 17.02  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 1024  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 298.0 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TD0 1

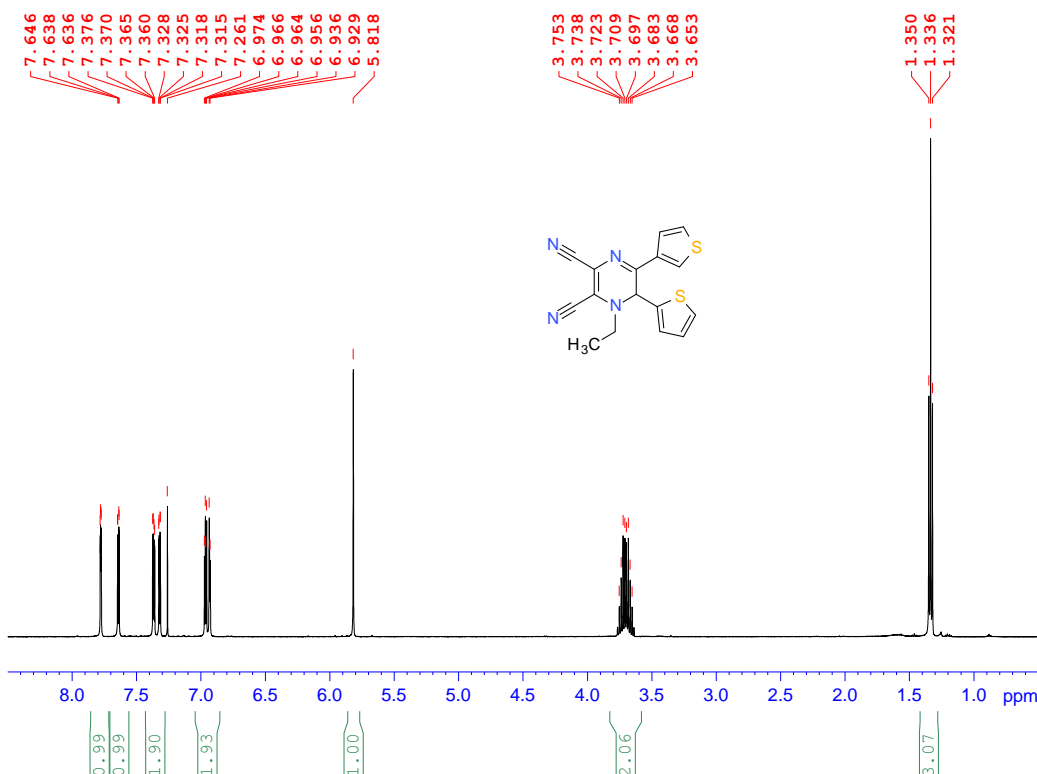
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 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 FCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577970 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.80

ema: A\*01691

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **11b**.



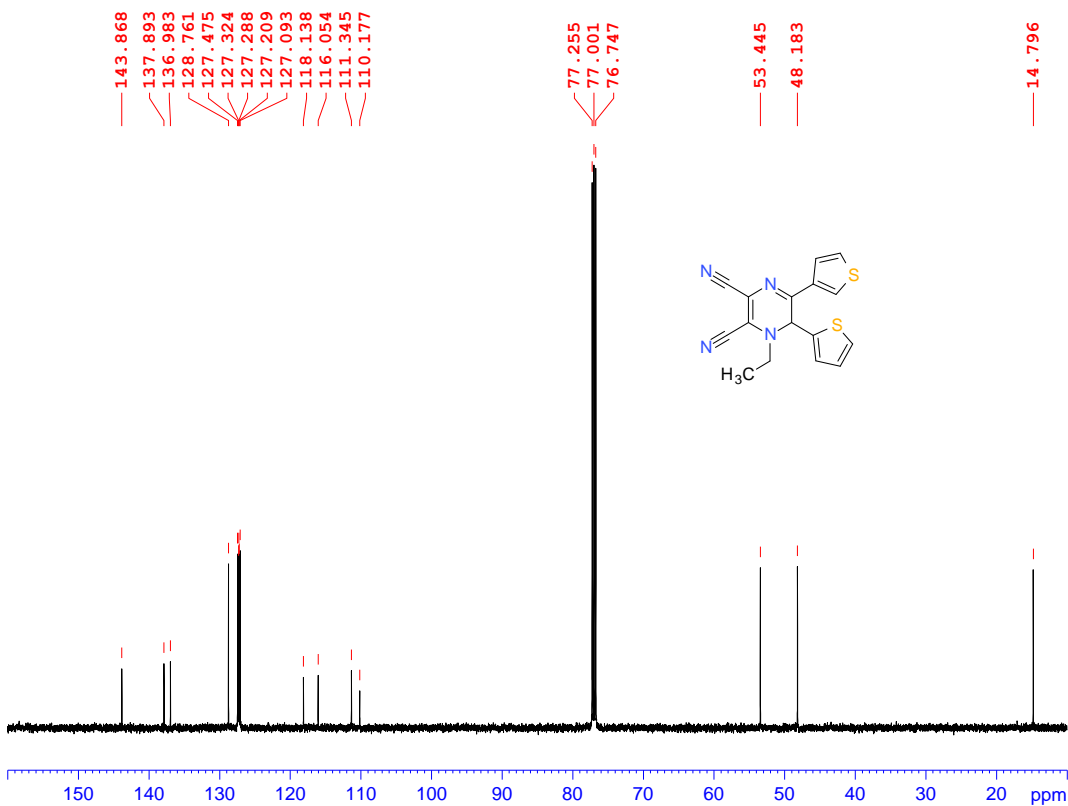
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 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 16  
 DS 2  
 AQ 2.7263477 sec  
 RG 101  
 TE 296.5 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
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 SF 500.1300136 MHz  
 WDW GM  
 SSB 0  
 LB -1.00 Hz  
 GB 0.3  
 PC 2.00

ema: A\*01709

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **11c**.

Current Data Parameters  
 NAME VEV892b  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120113  
 Time 12.33  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 512  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.3 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TDO 1

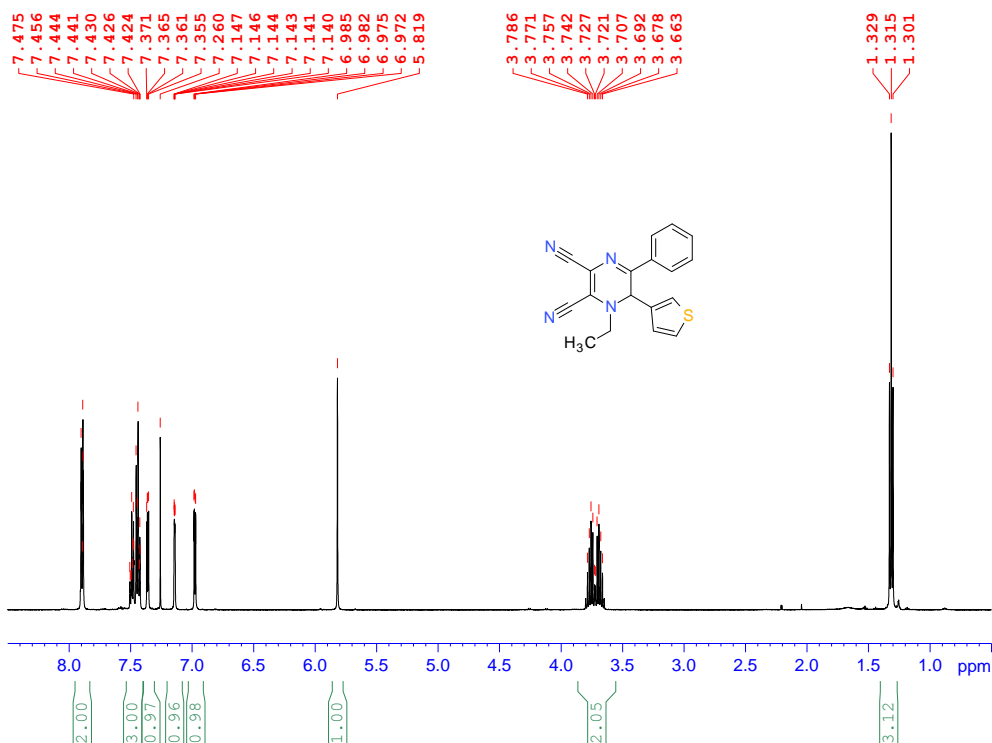
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SPOZ 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577943 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.80

ema: A\*01710

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **11c**.



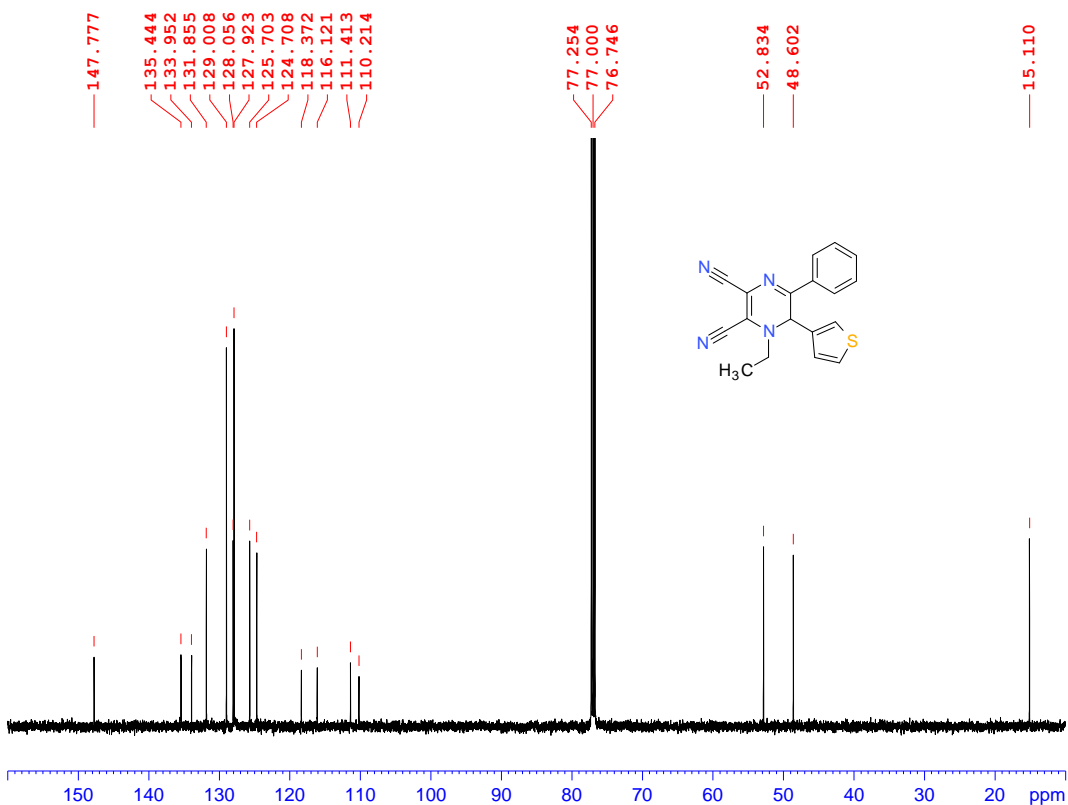
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 PROCNO 1

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 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 8  
 DS 2  
 AQ 2.7263477 sec  
 RG 181  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300139 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

ema: A\*01746

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 12a.

Current Data Parameters  
 NAME VEV918b  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120118  
 Time\_ 15.03  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 512  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.3 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TD0 1

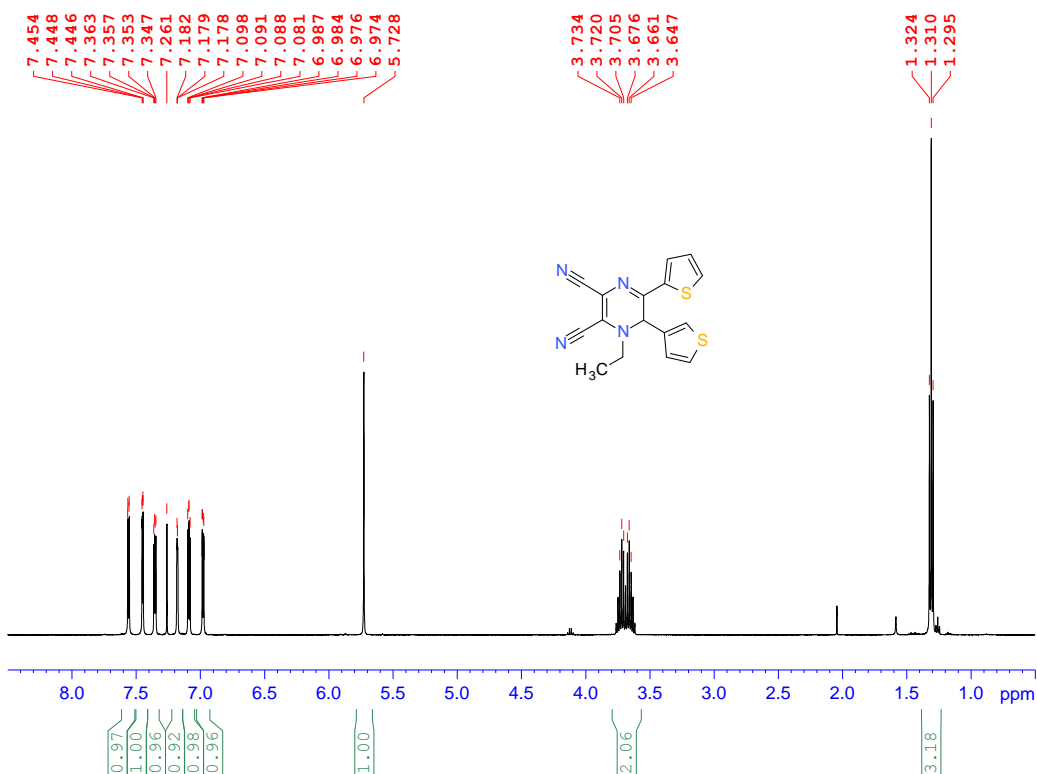
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 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577934 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.80

ema: A\*01747

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of 12a.



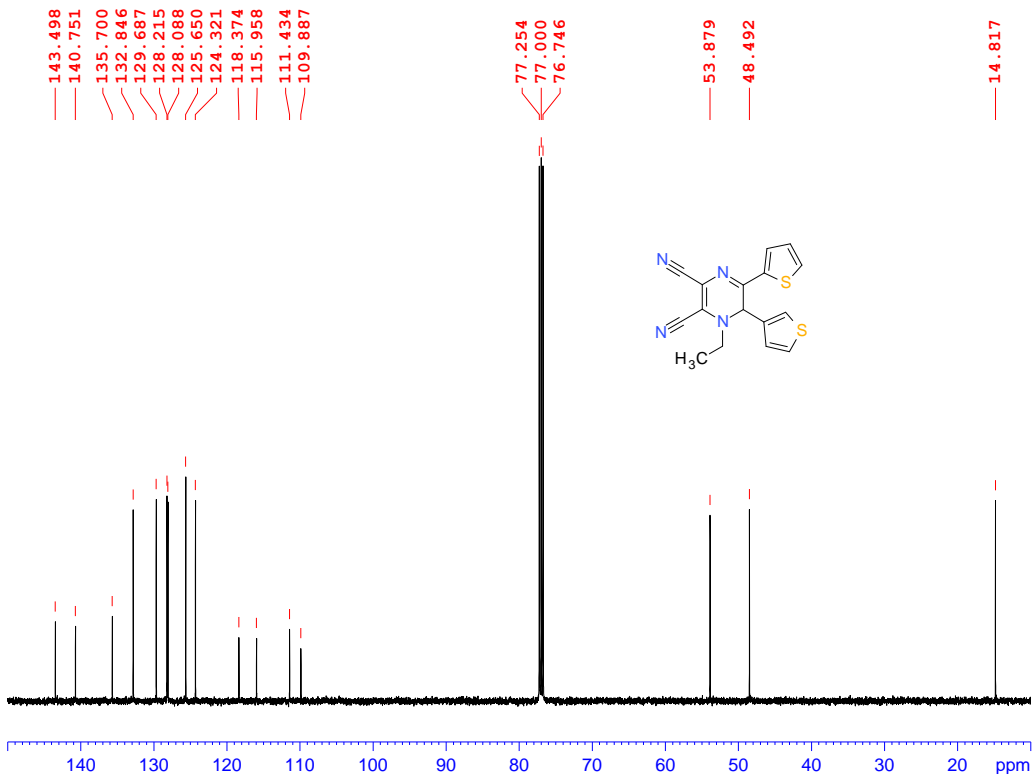
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 PROCNO 1

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 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 8  
 DS 2  
 AQ 2.7263477 sec  
 RG 101  
 TE 296.1 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300132 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 4.00

ema: A\*01714

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **12b**.

Current Data Parameters  
 NAME VEV919b  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120113  
 Time 16.20  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 512  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.2 K  
 D1 0.8000001 sec  
 D11 0.0300000 sec  
 TD0 1

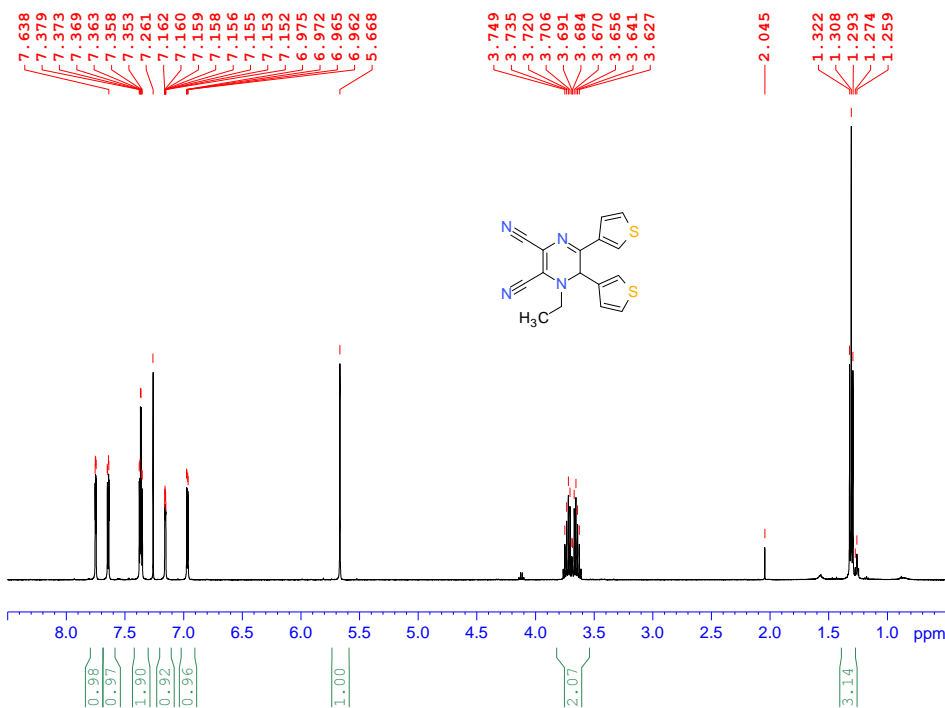
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 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 FCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577957 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 0.80

ema: A\*01715

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **12b**.



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 12c.



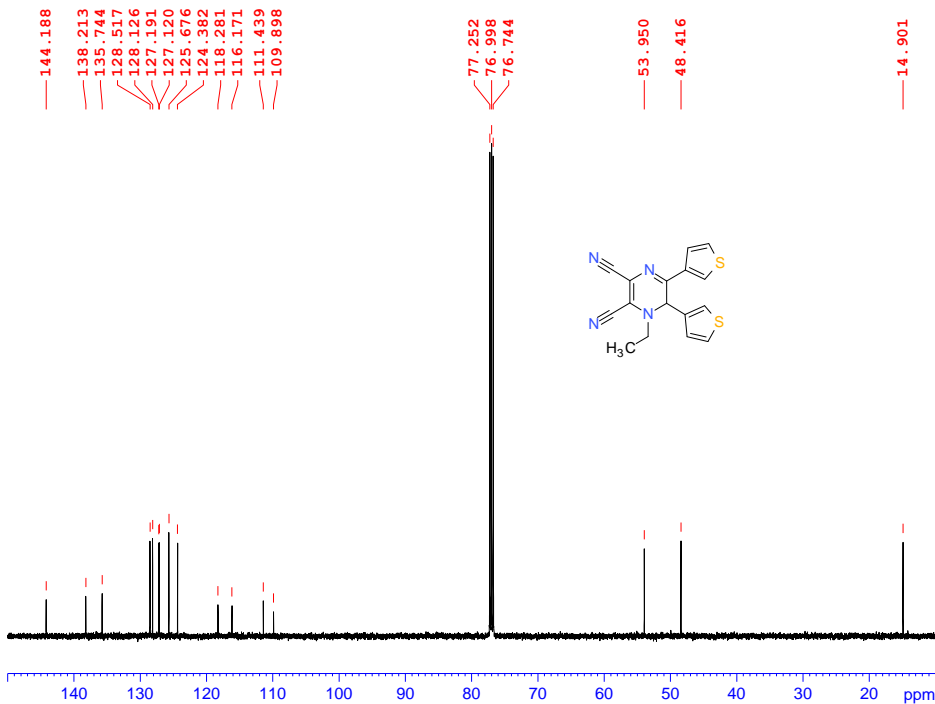
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 PROCNO 1

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 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 8  
 DS 2  
 AQ 2.7263477 sec  
 RG 101  
 TE 296.1 K  
 D1 1.0000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SF01 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300134 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 2.00

ema: A\*01723



<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of 12c.

Current Data Parameters  
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 PROCNO 1

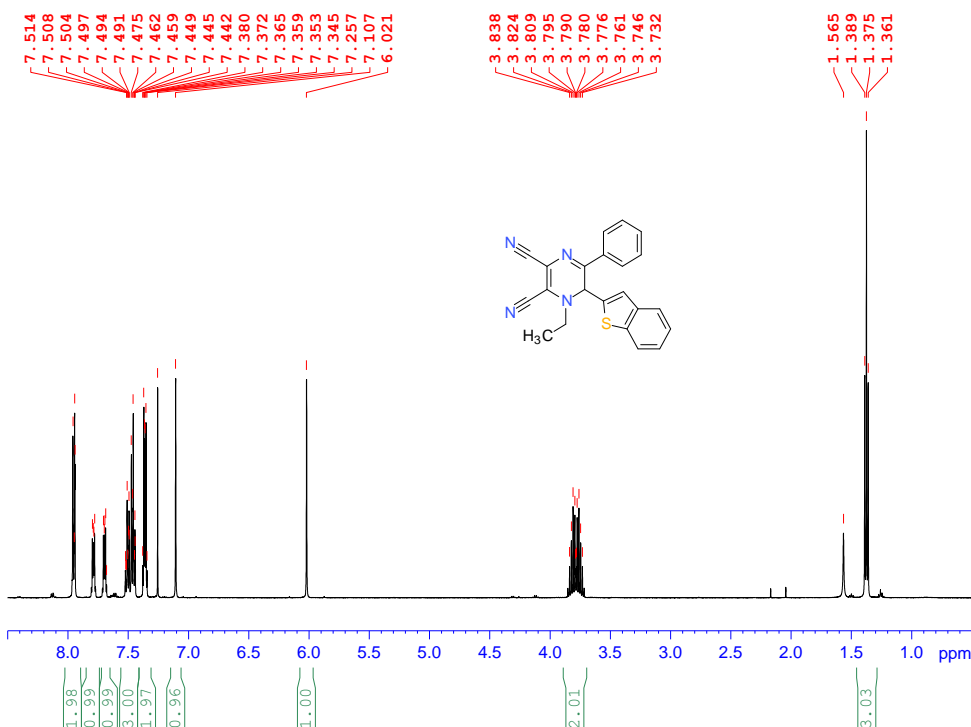
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 Time\_ 17.55  
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 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 512  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.6 K  
 D1 0.8000001 sec  
 D11 0.0300000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.2958563 W  
 SF01 125.7691072 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SF02 500.1320005 MHz

F2 - Processing parameters  
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 SF 125.7577936 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.80

ema: A\*01724



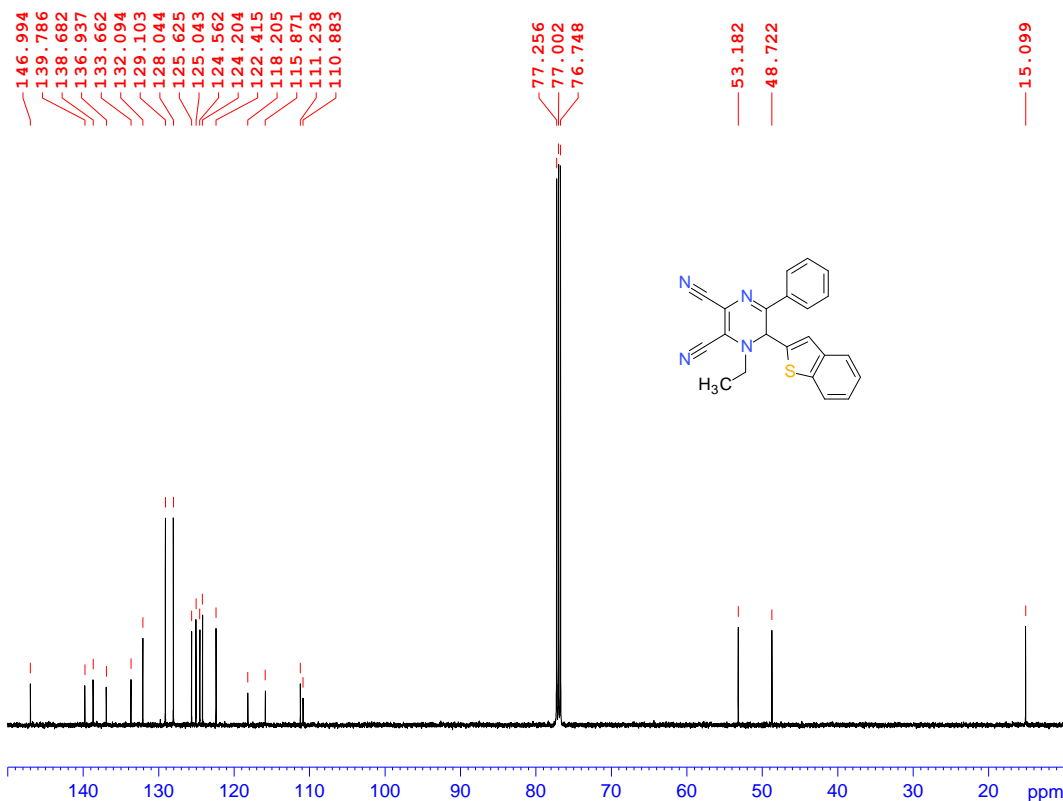
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 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 16  
 DS 2  
 AQ 2.7263477 sec  
 RG 203  
 TE 296.4 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300153 MHz  
 EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

ema: A\*02481

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 15a.

Current Data Parameters  
 NAME VEV1079c  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120705  
 Time 14.24  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 1024  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.7 K  
 D1 0.8000001 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

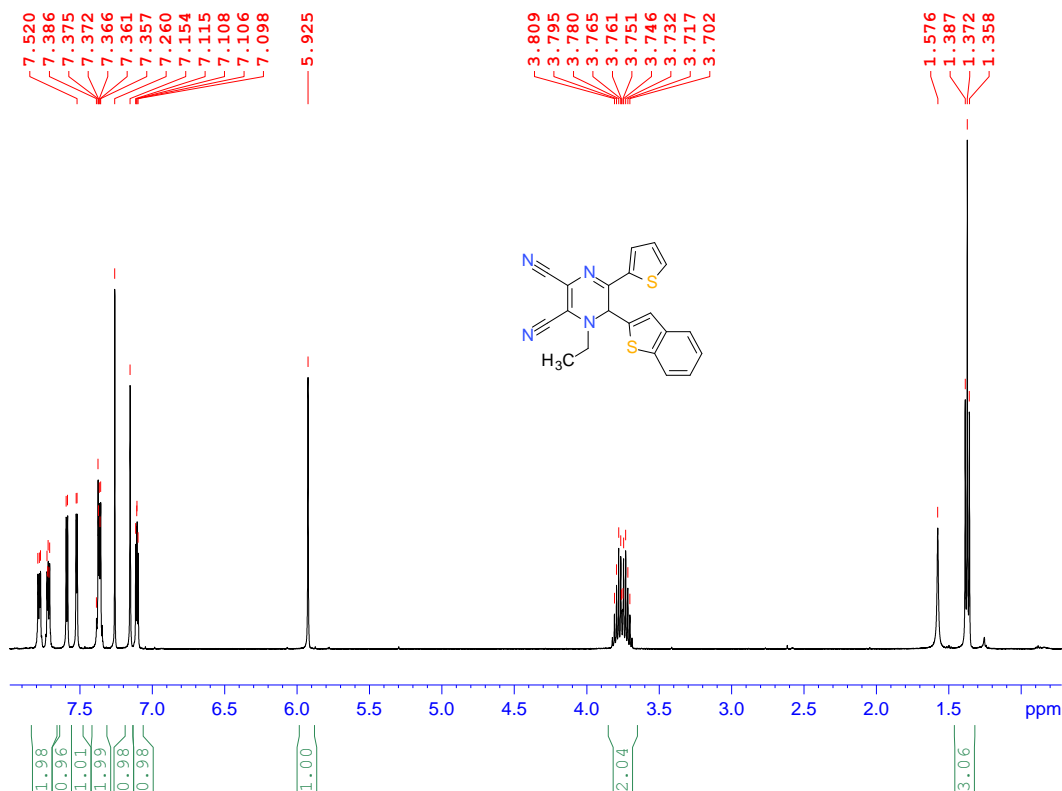
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 CPDPRG2 waltz16  
 NUC2 1H  
 FCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577929 MHz  
 EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.80

ema: A\*02482

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of 15a.





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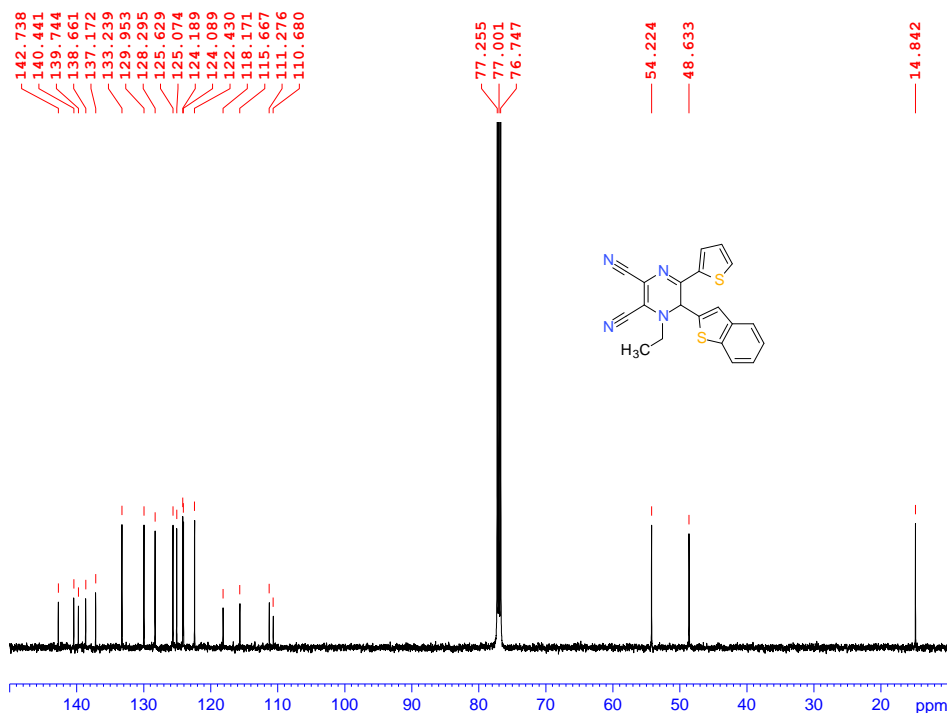
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NAME      VEV1077c
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20120629
Time     13.01
INSTRUM  AV500
PROBHD   5 mm PABBO BB-
PULPROG  zg30
SOLVENT  CDCl3
TD       32768
SW       12.0160 ppm
O1P      5.000 ppm
FIDRES   0.183399 Hz
NS        16
DS         2
AQ        2.7263477 sec
RG         203
TE         296.3 K
D1        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      1H
P1        12.00 usec
PL1       0 dB
PL1W     16.10176659 W
SFO1     500.1325007 MHz

F2 - Processing parameters
SI        65536
SF        500.1300139 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC        4.00
  
```

ema: A\*02458

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **15b**.

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Current Data Parameters
NAME      VEV1077c
EXPNO    13
PROCNO   1

F2 - Acquisition Parameters
Date_    20120629
Time     13.30
INSTRUM  AV500
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
SOLVENT  CDCl3
TD       32768
SW       180.7063 ppm
O1P      90.000 ppm
FIDRES   0.693581 Hz
NS        2048
DS         8
AQ        0.7209460 sec
RG         203
TE         297.7 K
D1        0.80000001 sec
D11      0.03000000 sec
TDO       1

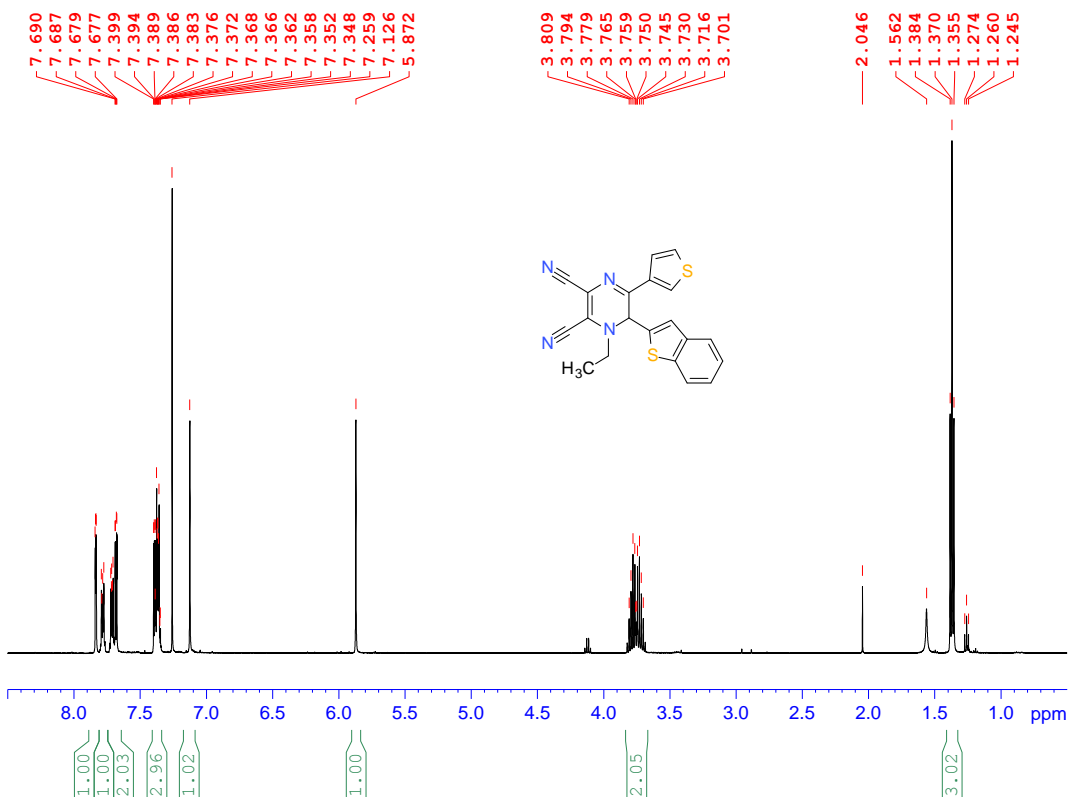
===== CHANNEL f1 =====
NUC1      13C
P1        9.00 usec
PL1       0 dB
PL1W     115.29558563 W
SFO1     125.7691072 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCFD2    75.00 usec
PL2      120.00 dB
PL12     17.00 dB
PL13     20.00 dB
PL2W     0 W
PL12W    0.40445811 W
PL13W    0.20270923 W
SFO2     500.1320005 MHz

F2 - Processing parameters
SI        125.7577922 MHz
WDW       EM
SSB       0
LB        2.00 Hz
GB        0
PC        0.80
  
```

ema: A\*02459

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **15b**.



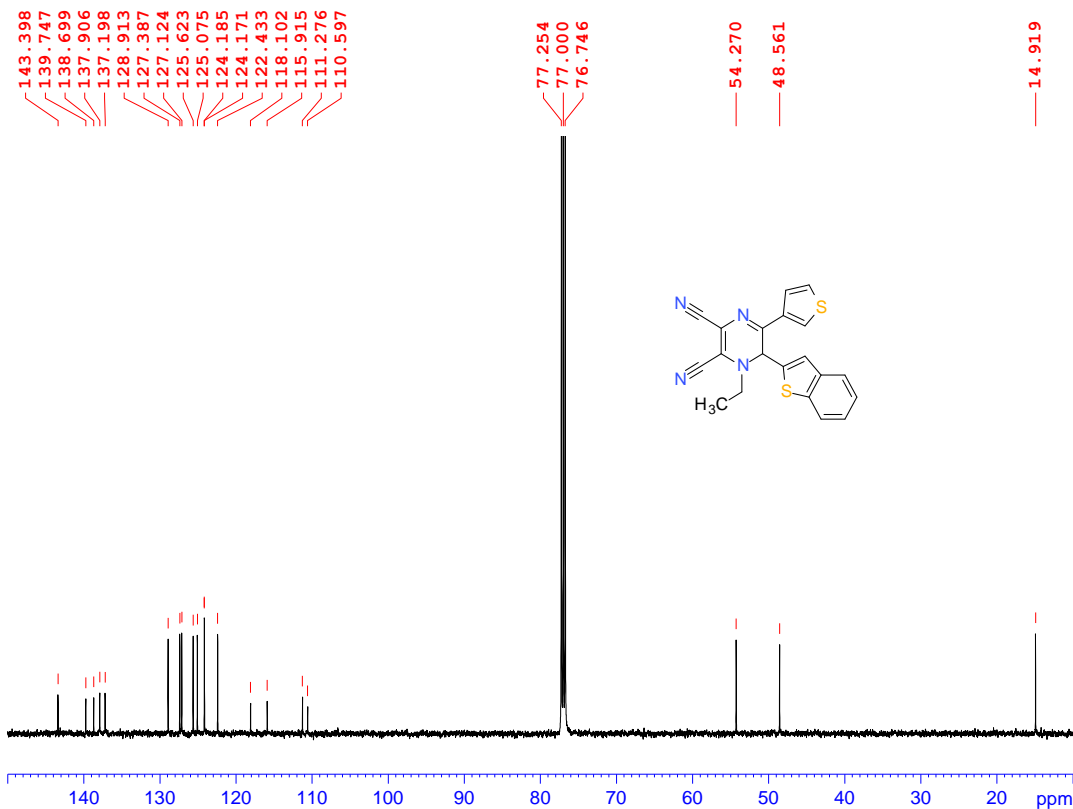
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 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120626  
 Time 14.39  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 16  
 DS 2  
 AQ 2.7263477 sec  
 RG 203  
 TE 295.7 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300140 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

ema: A\*02446

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **15c**.

Current Data Parameters  
 NAME VEVI075c  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120626  
 Time 14.46  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 2048  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 296.9 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TDO 1

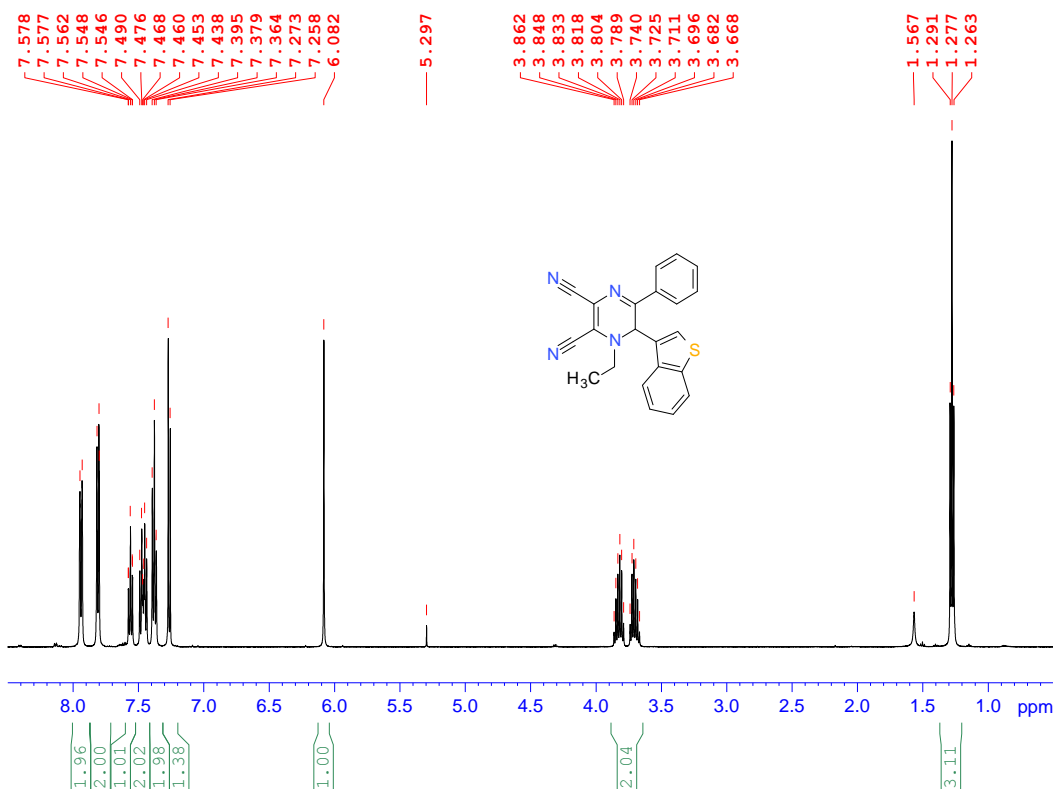
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 75.00 usec  
 PL12 120.00 dB  
 PL13 17.00 dB  
 PL14 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577921 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 0.80

ema: A\*02447

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **15c**.



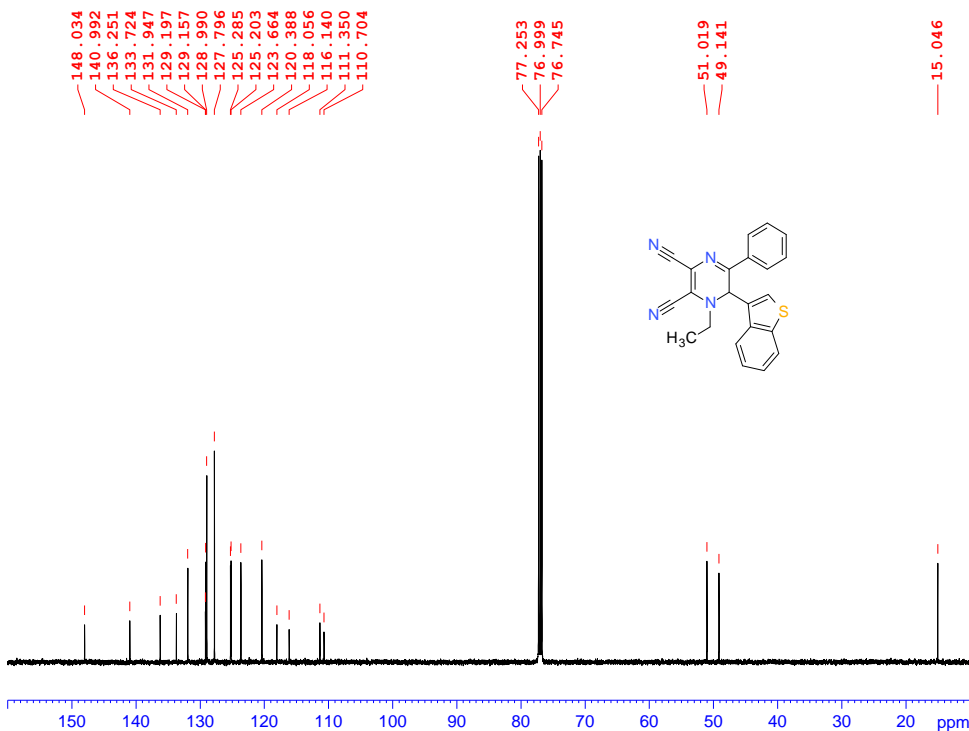
Current Data Parameters  
 NAME VEV1080c  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120710  
 Time 15.07  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 2  
 DS 16  
 AQ 2.7263477 sec  
 RG 128  
 TE 295.8 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300149 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

ema: A\*02484

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 16a.

Current Data Parameters  
 NAME VEV1080c  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120710  
 Time 15.12  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 1024  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.1 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TDO 1

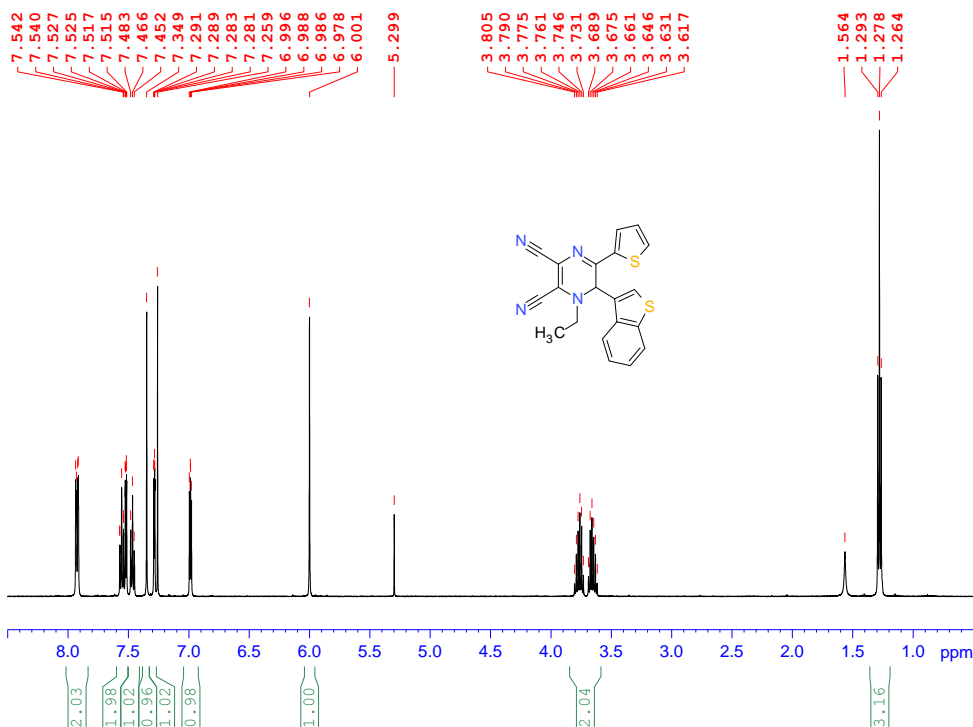
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577935 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.80

ema: A\*02485

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of 16a.



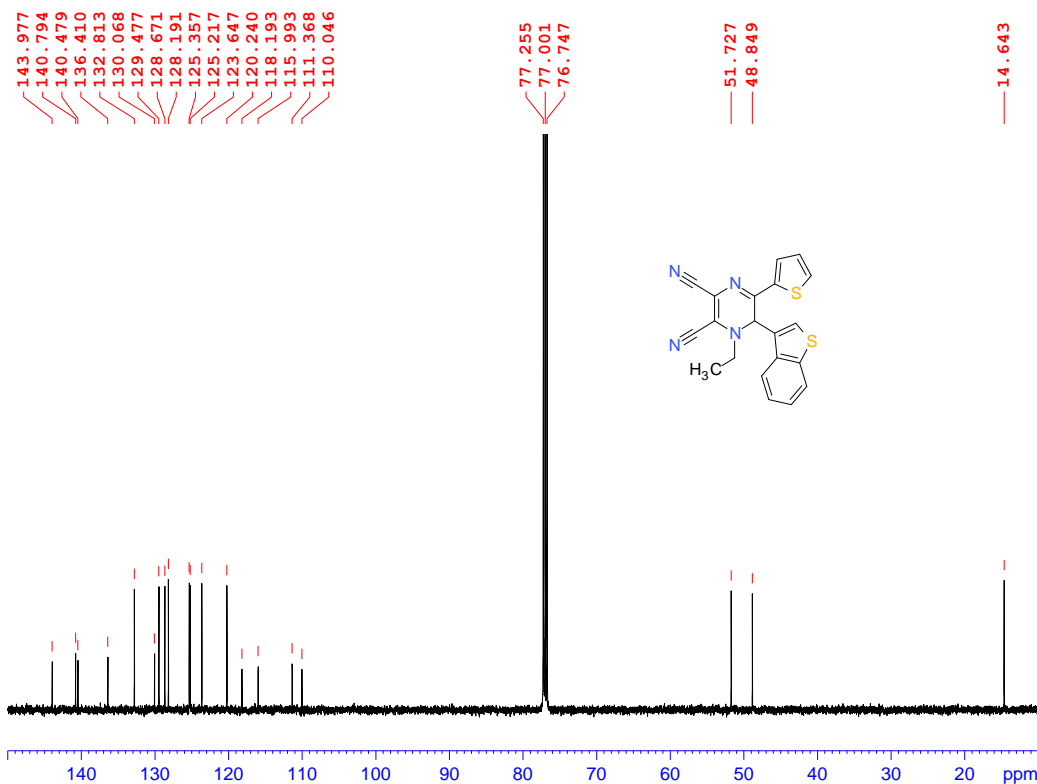
Current Data Parameters  
 NAME VEV1078c  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120704  
 Time 16.29  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 8  
 DS 2  
 AQ 2.7263477 sec  
 RG 203  
 TE 296.5 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300140 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 4.00

ema: A\*02477

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **16b**.

Current Data Parameters  
 NAME VEV1078c  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120704  
 Time 16.44  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 1024  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 298.0 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TDO 1

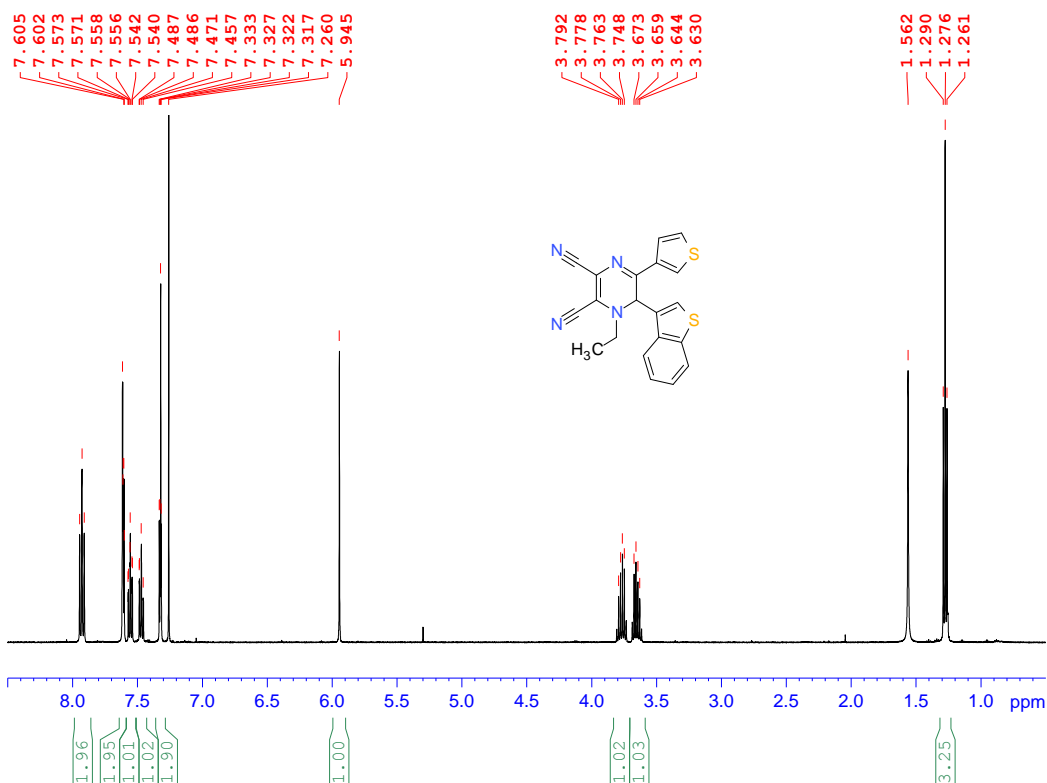
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 FCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577924 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 0.80

ema: A\*02478

<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **16b**.



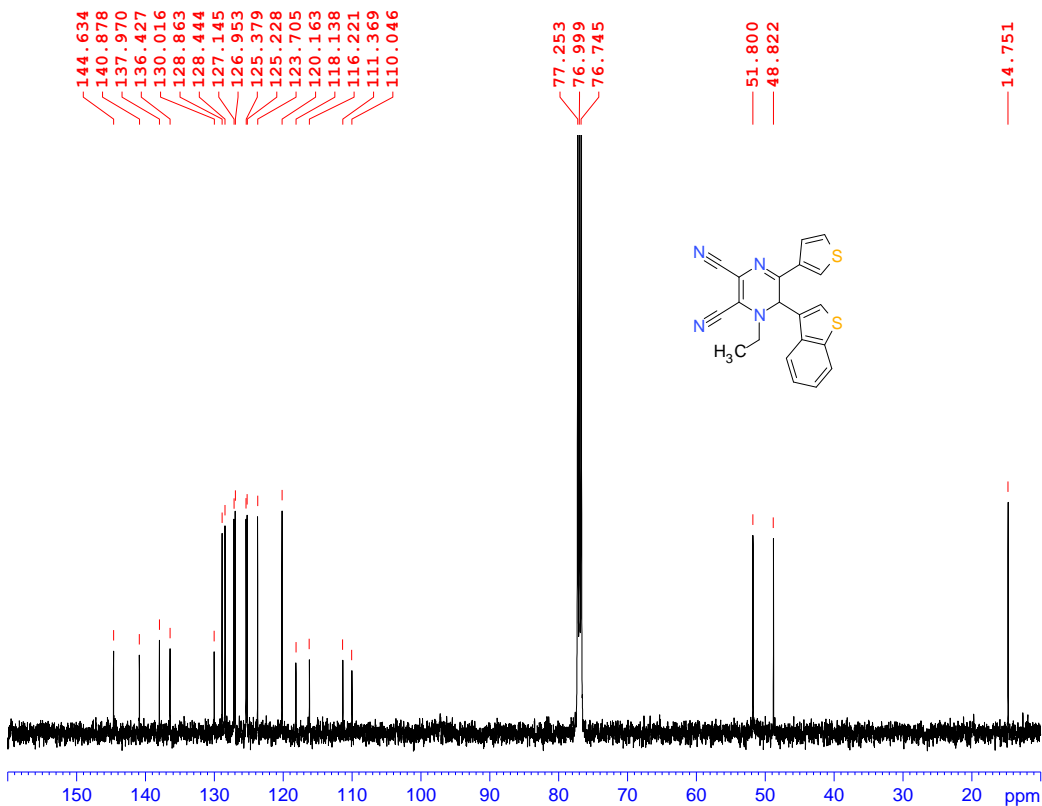
Current Data Parameters  
 NAME VEVI076c  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120621  
 Time 16.01  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 12.0160 ppm  
 O1P 5.000 ppm  
 FIDRES 0.183399 Hz  
 NS 16  
 DS 2  
 AQ 2.7263477 sec  
 RG 203  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 1.00 dB  
 PL1W 16.10176659 W  
 SFO1 500.1325007 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.1300137 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 4.00

ema: A\*02420

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 16c.

Current Data Parameters  
 NAME VEVI076c  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120621  
 Time 16.10  
 INSTRUM AV500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 SOLVENT CDCl3  
 TD 32768  
 SW 180.7063 ppm  
 O1P 90.000 ppm  
 FIDRES 0.693581 Hz  
 NS 2048  
 DS 8  
 AQ 0.7209460 sec  
 RG 203  
 TE 297.1 K  
 D1 0.80000001 sec  
 D11 0.03000000 sec  
 TD0 1

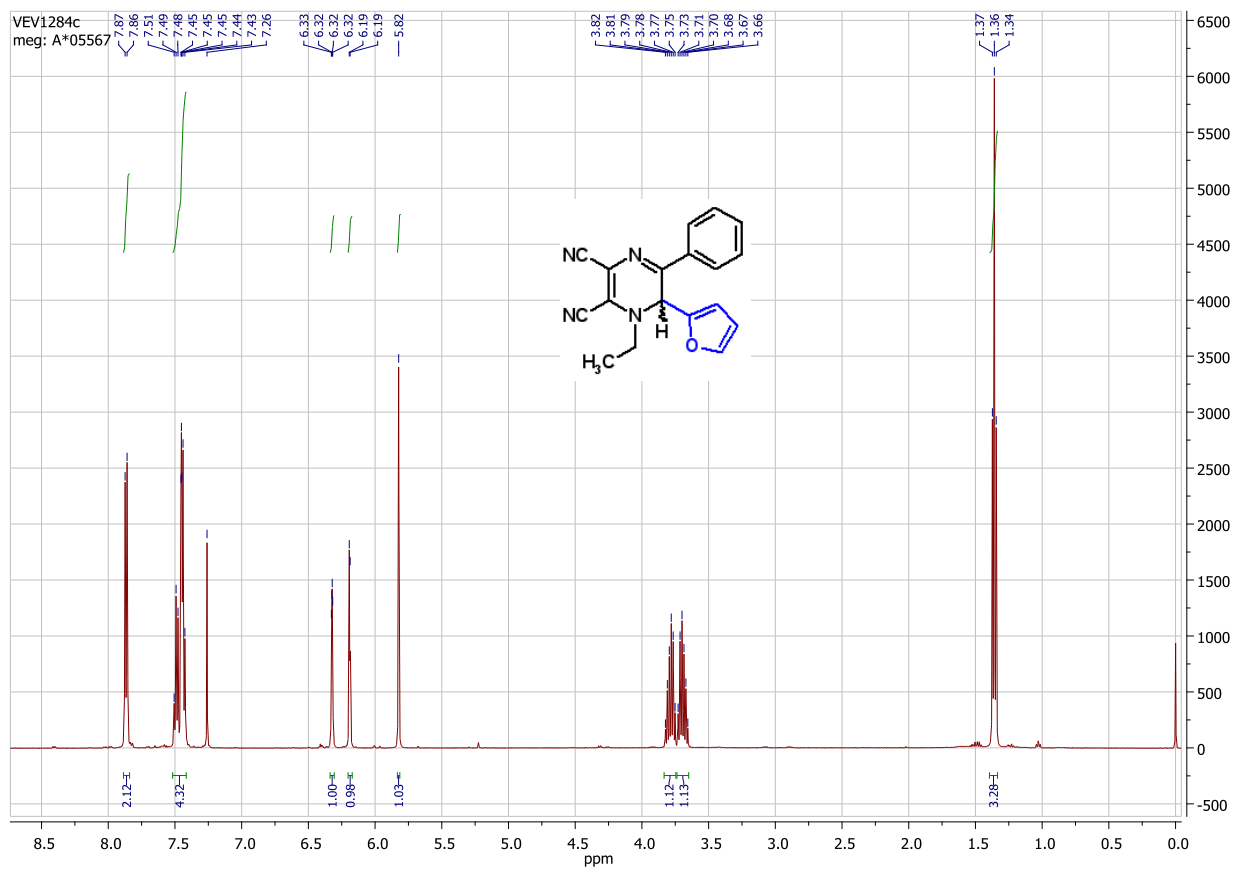
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0 dB  
 PL1W 115.29558563 W  
 SFO1 125.7691072 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 75.00 usec  
 PL2 120.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 PL2W 0 W  
 PL12W 0.40445811 W  
 PL13W 0.20270923 W  
 SFO2 500.1320005 MHz

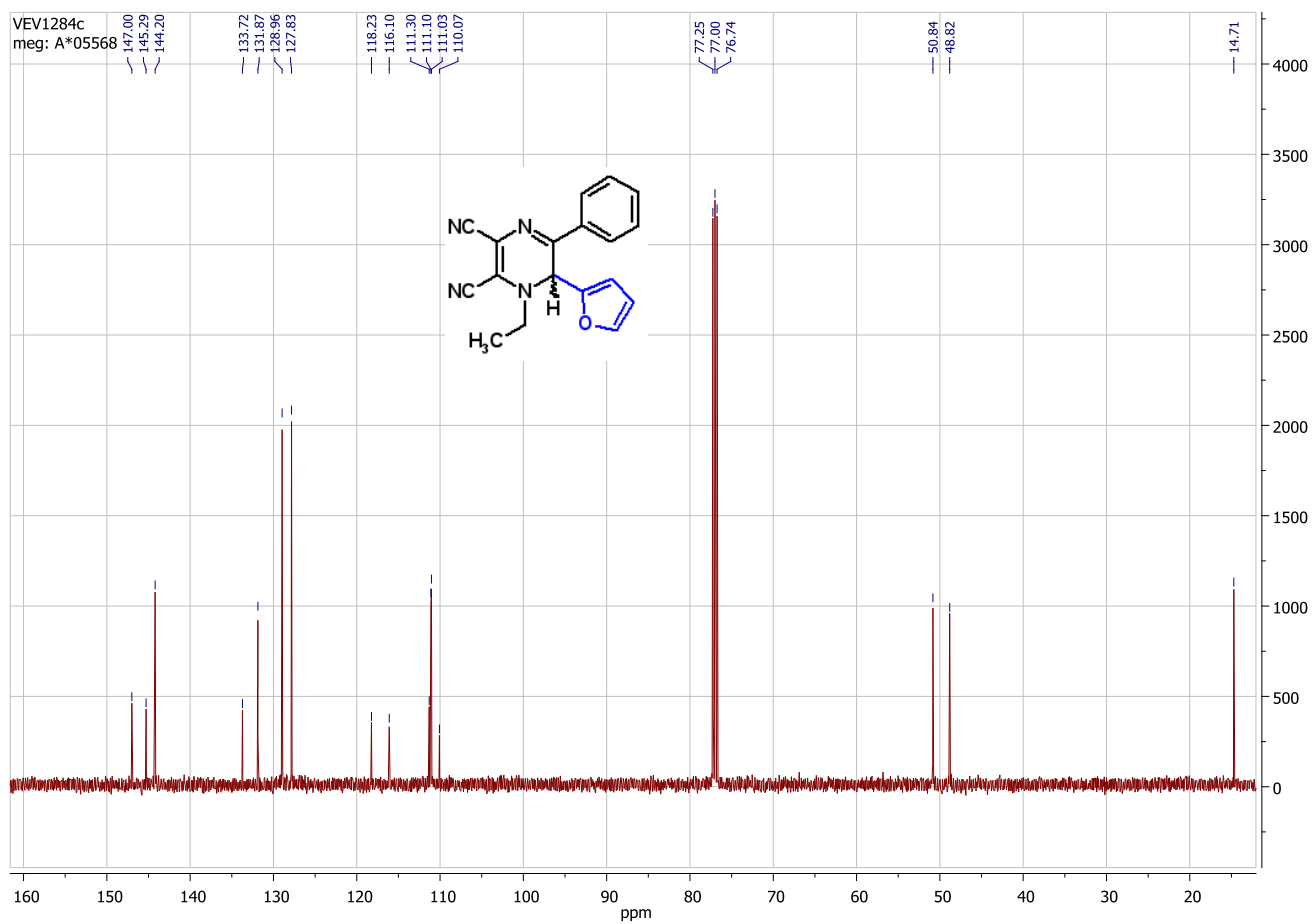
F2 - Processing parameters  
 SI 32768  
 SF 125.7577914 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 0.80

ema: A\*02421

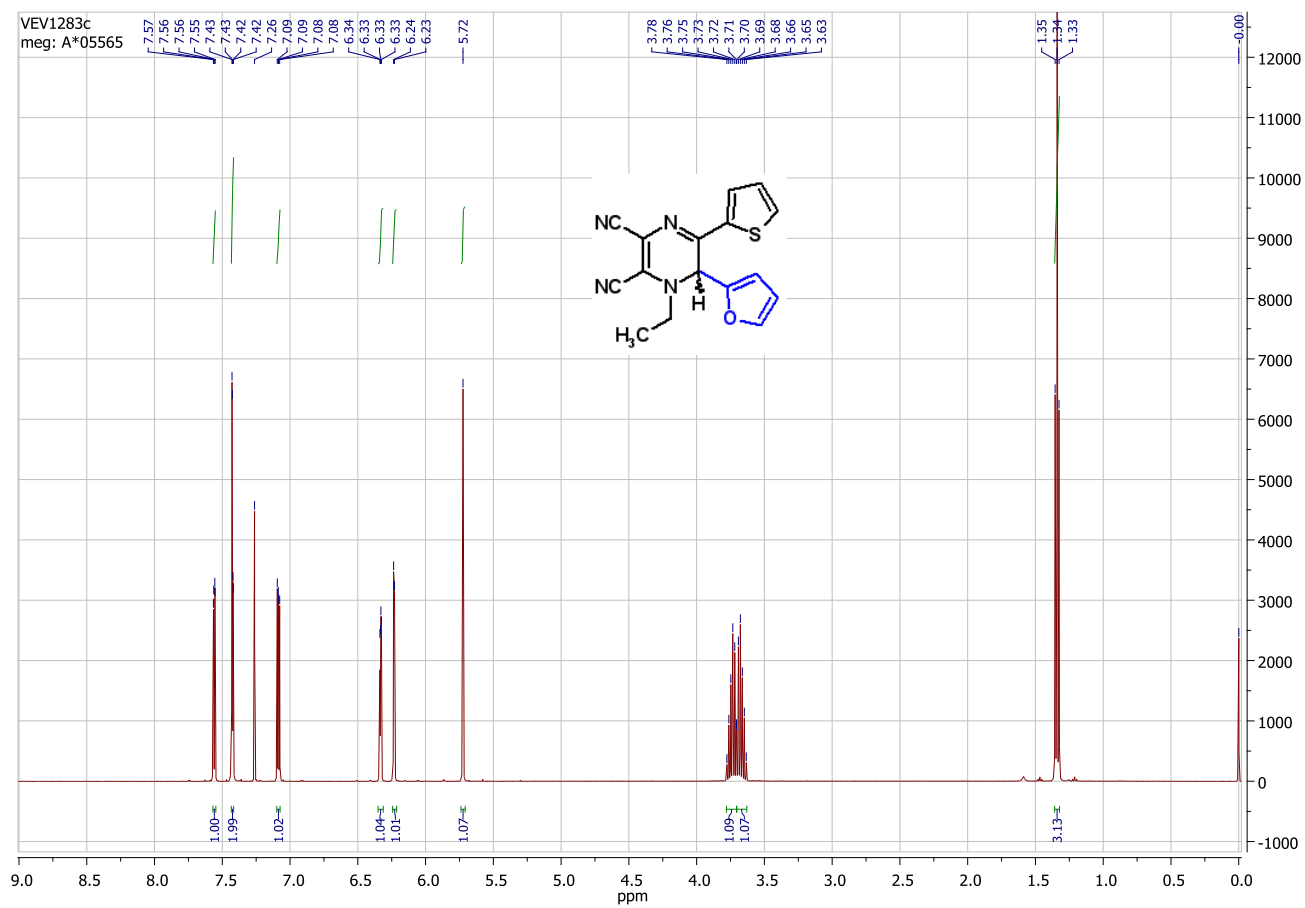
<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of 16c.



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **18a**.

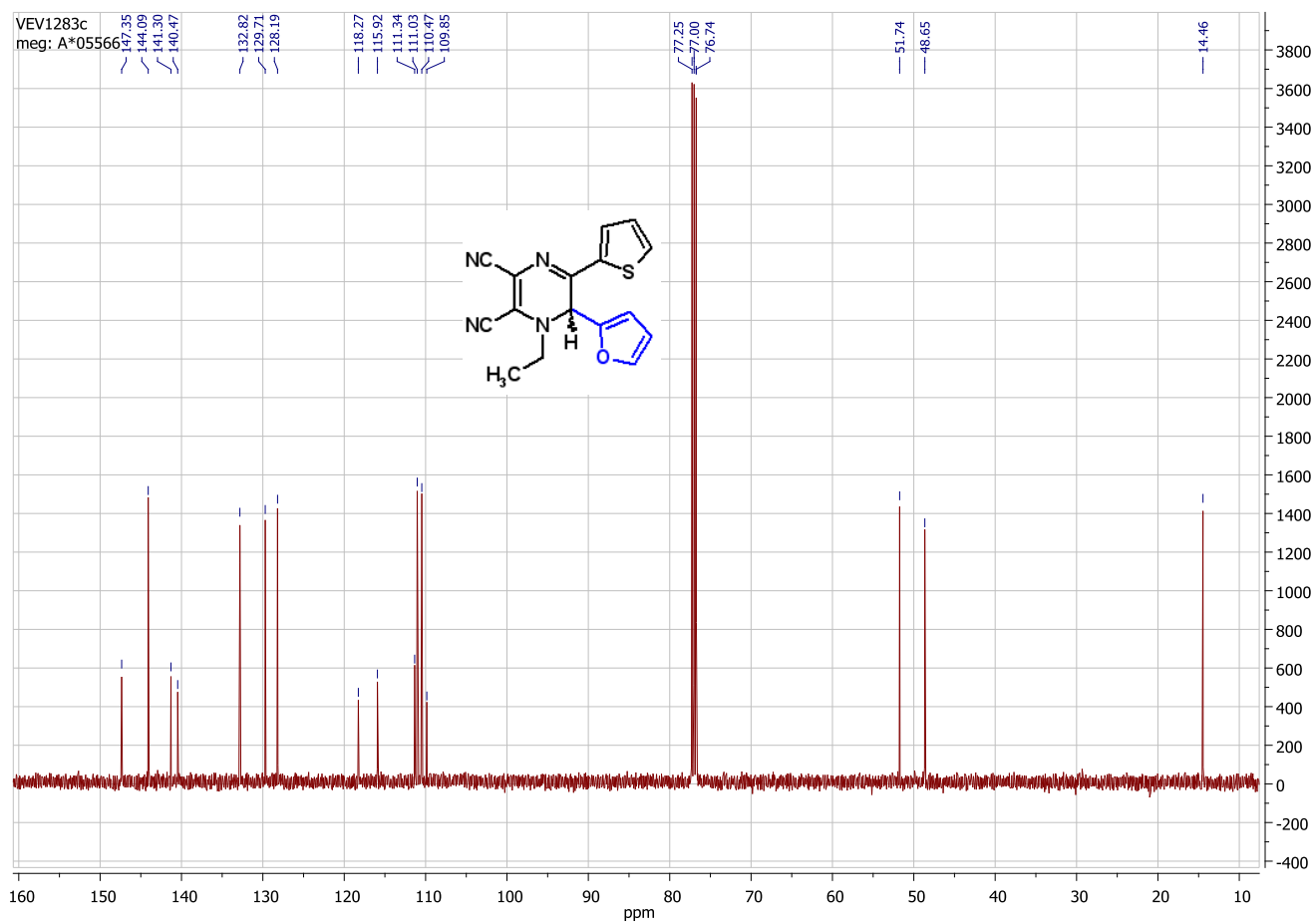


$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **18a**.

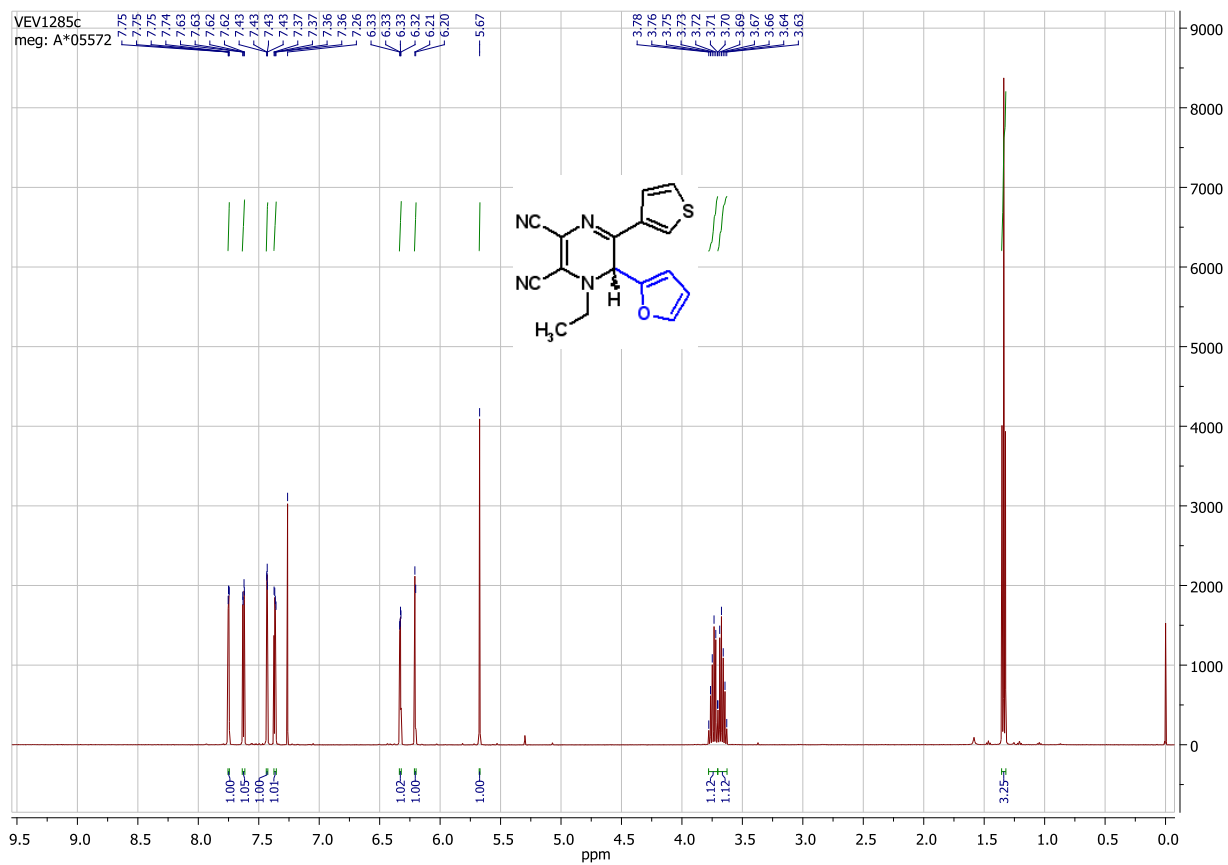


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **18b**.

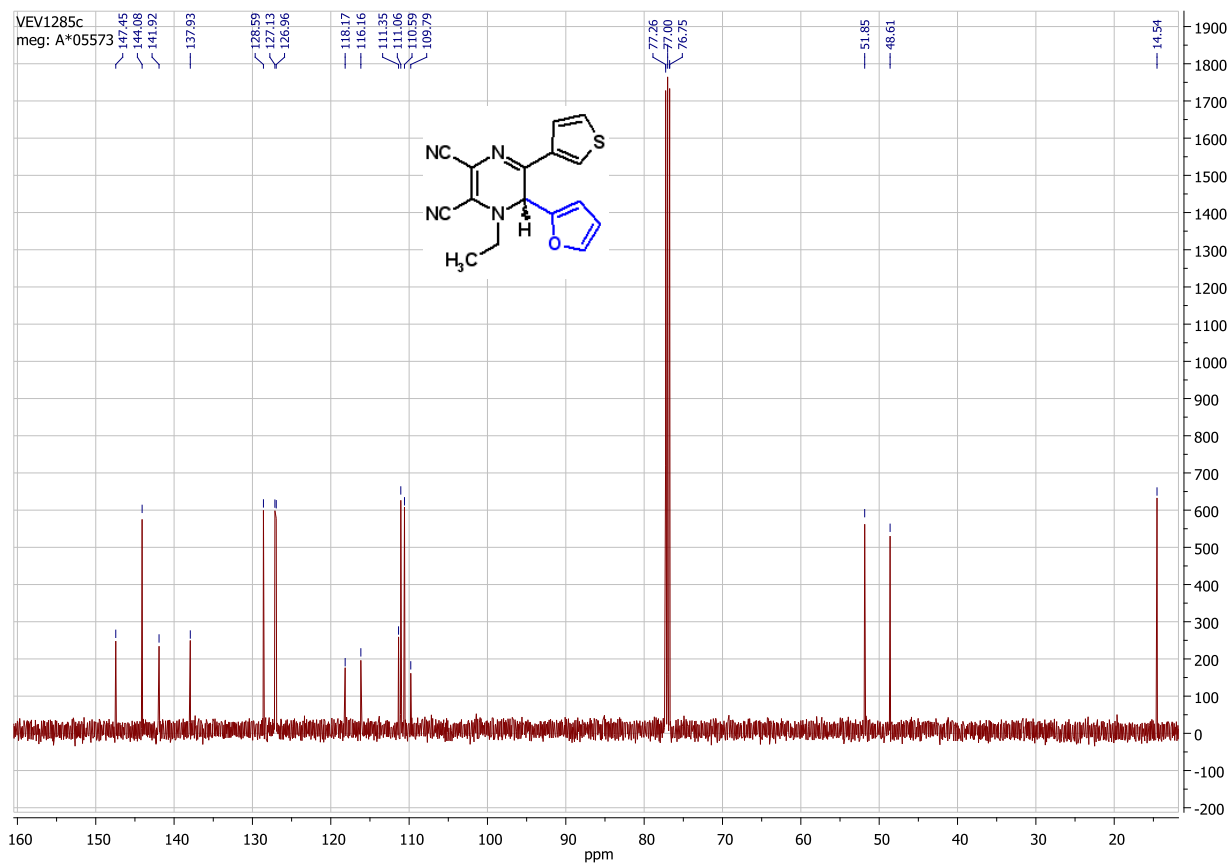




$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **18b**.



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **18c**.



$^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **18c**.