

## Supporting Information

### **Synthesis of functionalized unsymmetrical 1,3-butadiene-3-yne derivatives from $\beta$ -halo styrene derivatives and its application for the synthesis of trisubstituted pyridines**

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## X-ray Crystallographic Structure of **4a**

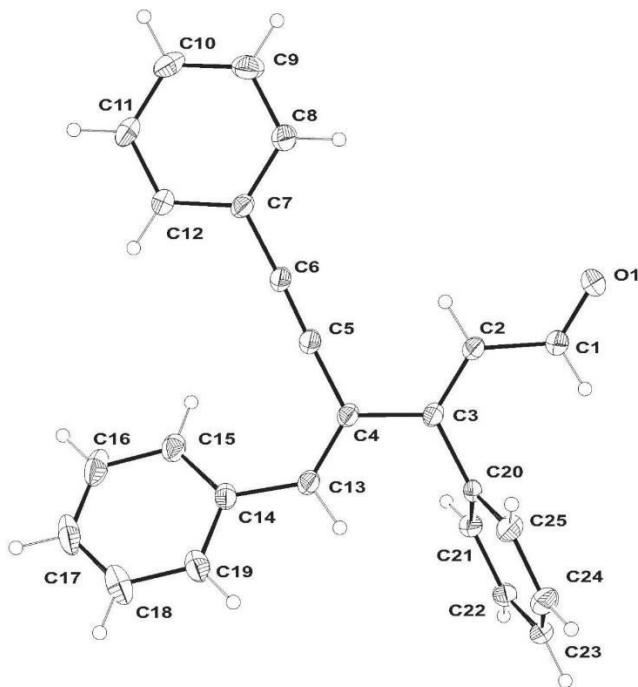


Table 1. Crystal data and structure refinement for ch15278.

Identification code	ch15278		
Empirical formula	C <sub>25</sub> H <sub>18</sub> O		
Formula weight	334.39		
Temperature	200(2) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	P 21/n		
Unit cell dimensions	a = 10.3643(11) Å	α= 90°.	
	b = 12.1725(13) Å	β= 97.592(4)°.	
	c = 14.7261(16) Å	γ = 90°.	
Volume	1841.6(3) Å <sup>3</sup>		
Z	4		
Density (calculated)	1.206 Mg/m <sup>3</sup>		
Absorption coefficient	0.072 mm <sup>-1</sup>		
F(000)	704		
Crystal size	0.78 x 0.78 x 0.24 mm <sup>3</sup>		
Theta range for data collection	2.18 to 25.07°.		

Index ranges	-11≤h≤12, -14≤k≤14, -13≤l≤17
Reflections collected	9099
Independent reflections	3202 [R(int) = 0.0414]
Completeness to theta = 25.07°	97.9 %
Absorption correction	multi-scan
Max. and min. transmission	0.9829 and 0.9460
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3202 / 0 / 235
Goodness-of-fit on F <sup>2</sup>	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0512, wR2 = 0.1279
R indices (all data)	R1 = 0.0736, wR2 = 0.1521
Largest diff. peak and hole	0.200 and -0.342 e.Å <sup>-3</sup>

## X-ray Crystallographic Structure of **6a**

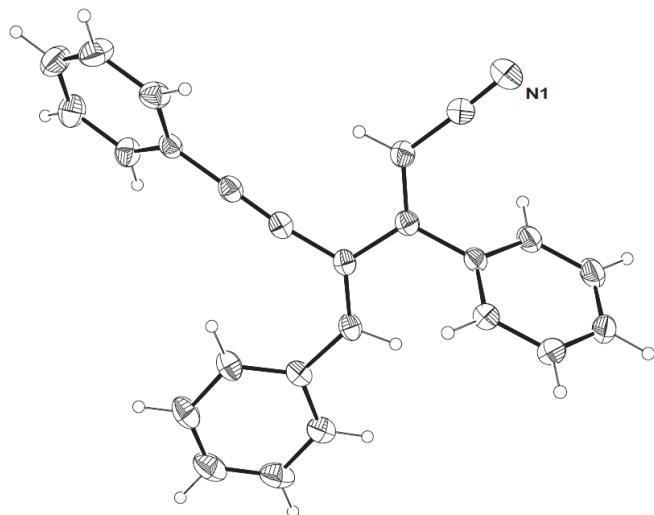


Table 2. Crystal data and structure refinement for a17319.

Identification code	a17319
Empirical formula	C <sub>25</sub> H <sub>17</sub> N
Formula weight	331.40
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	P 21/n	
Unit cell dimensions	a = 13.773(3) Å b = 7.1192(14) Å c = 19.135(4) Å	α= 90°. β= 96.972(4)°. γ = 90°.
Volume	1862.4(6) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.182 Mg/m <sup>3</sup>	
Absorption coefficient	0.068 mm <sup>-1</sup>	
F(000)	696	
Crystal size	0.79 x 0.08 x 0.03 mm <sup>3</sup>	
Theta range for data collection	1.94 to 25.13°.	
Index ranges	-16≤h≤16, -8≤k≤7, -21≤l≤22	
Reflections collected	11134	
Independent reflections	3313 [R(int) = 0.0579]	
Completeness to theta = 25.13°	99.0 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9980 and 0.9481	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3313 / 0 / 235	
Goodness-of-fit on F <sup>2</sup>	0.989	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.0958	
R indices (all data)	R1 = 0.0938, wR2 = 0.1114	
Largest diff. peak and hole	0.129 and -0.138 e.Å <sup>-3</sup>	

## X-ray Crystallographic Structure of 6'a

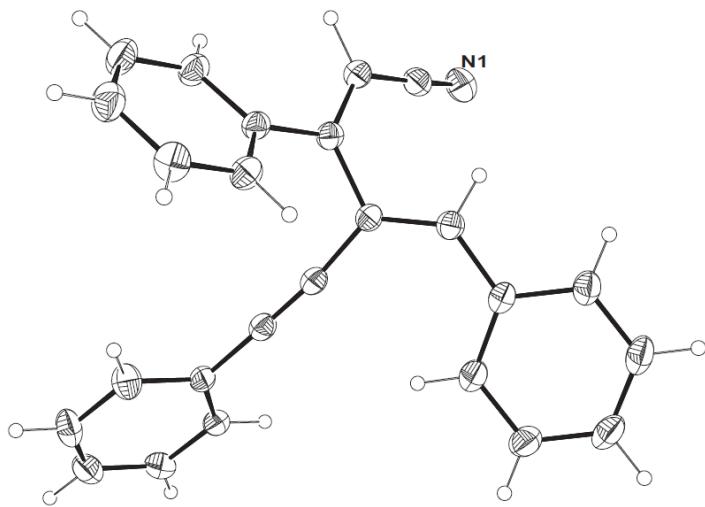


Table 3. Crystal data and structure refinement for a17293.

Identification code	a17293
Empirical formula	C <sub>25</sub> H <sub>17</sub> N
Formula weight	331.40
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	$a = 9.2568(4)$ Å $\alpha = 88.389(3)^\circ$ . $b = 10.0256(4)$ Å $\beta = 88.878(2)^\circ$ . $c = 11.0470(5)$ Å $\gamma = 66.498(2)^\circ$ .
Volume	939.76(7) Å <sup>3</sup>
Z	2
Density (calculated)	1.171 Mg/m <sup>3</sup>
Absorption coefficient	0.068 mm <sup>-1</sup>
F(000)	348
Crystal size	0.66 x 0.64 x 0.20 mm <sup>3</sup>
Theta range for data collection	1.84 to 25.00°.
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -13 ≤ l ≤ 13
Reflections collected	7953
Independent reflections	3200 [R(int) = 0.0525]

Completeness to theta = 24.80°	99.2 %
Absorption correction	multi-scan
Max. and min. transmission	0.9866 and 0.9567
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3200 / 0 / 235
Goodness-of-fit on F <sup>2</sup>	1.088
Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1294
R indices (all data)	R1 = 0.0575, wR2 = 0.1463
Largest diff. peak and hole	0.193 and -0.232 e.Å <sup>-3</sup>

### X-ray Crystallographic Structure of **8a**

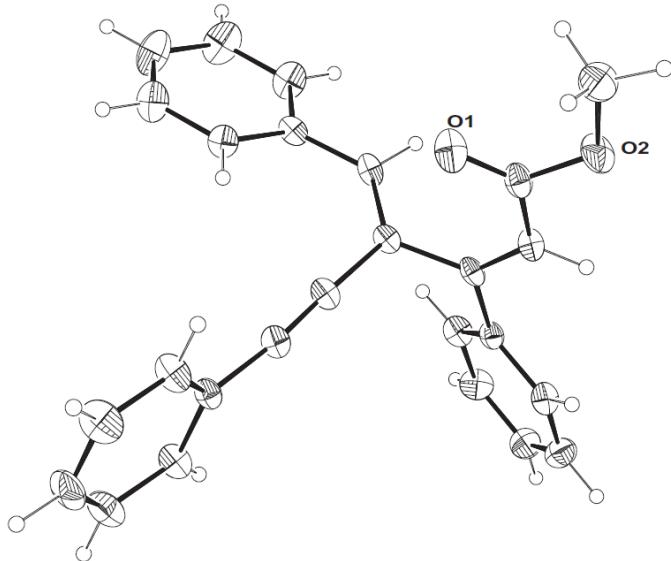


Table 4. Crystal data and structure refinement for a17448.

Identification code	a17448
Empirical formula	C <sub>26</sub> H <sub>20</sub> O <sub>2</sub>
Formula weight	364.42
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	$a = 12.480(3)$ Å $\alpha = 90^\circ$ . $b = 5.9054(12)$ Å $\beta = 94.720(18)^\circ$ . $c = 27.814(10)$ Å $\gamma = 90^\circ$ .

Volume	2042.9(10) Å <sup>3</sup>
Z	4
Density (calculated)	1.185 Mg/m <sup>3</sup>
Absorption coefficient	0.074 mm <sup>-1</sup>
F(000)	768
Crystal size	0.47 x 0.08 x 0.05 mm <sup>3</sup>
Theta range for data collection	1.47 to 25.06°.
Index ranges	-14<=h<=14, -6<=k<=6, -33<=l<=31
Reflections collected	12390
Independent reflections	3525 [R(int) = 0.1502]
Completeness to theta = 25.06°	97.7 %
Absorption correction	multi-scan
Max. and min. transmission	0.9963 and 0.9662
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3525 / 0 / 254
Goodness-of-fit on F <sup>2</sup>	1.029
Final R indices [I>2sigma(I)]	R1 = 0.1106, wR2 = 0.1654
R indices (all data)	R1 = 0.2411, wR2 = 0.2084
Extinction coefficient	0.012(2)
Largest diff. peak and hole	0.219 and -0.214 e.Å <sup>-3</sup>

## X-ray Crystallographic Structure of **10a**

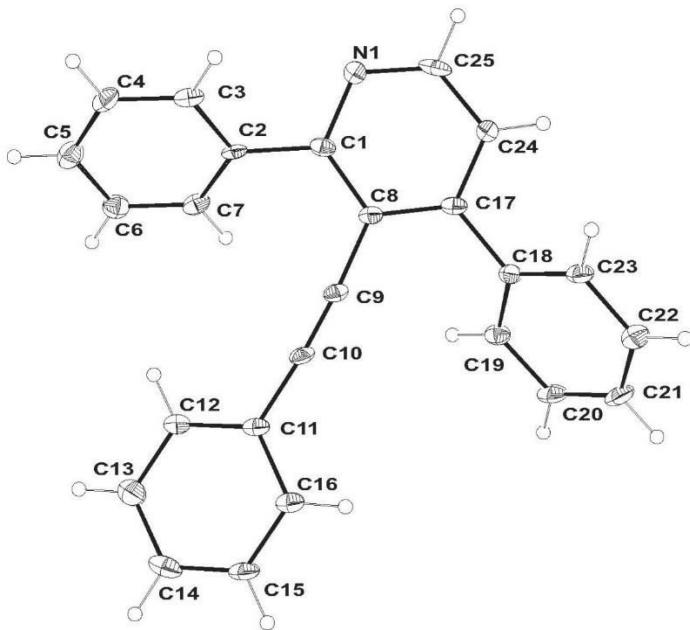


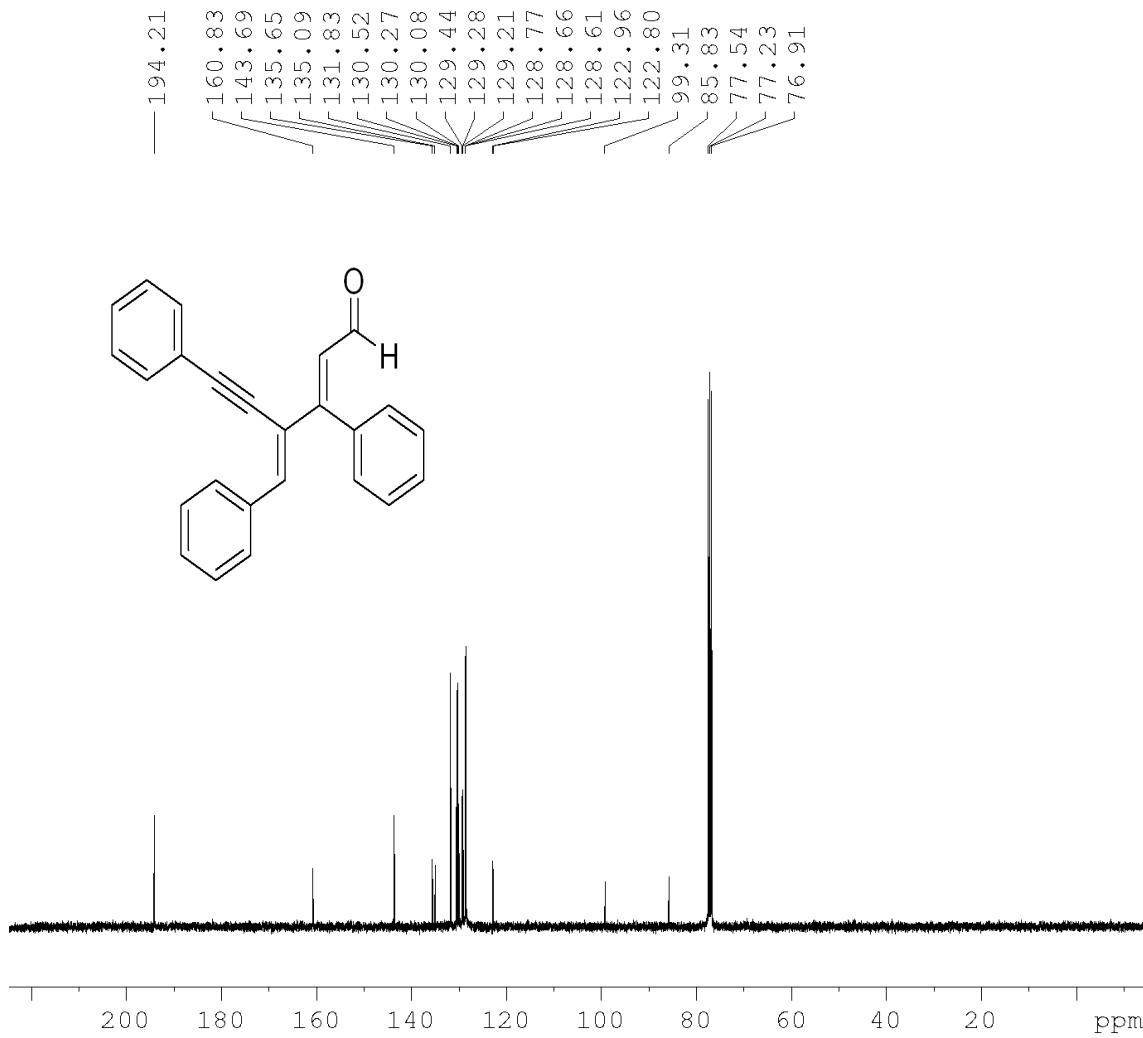
Table 5. Crystal data and structure refinement for 15371a. **N1, C24 50% disorder**

Identification code	15371a		
Empirical formula	C <sub>25</sub> H <sub>17</sub> N		
Formula weight	331.40		
Temperature	200(2) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	P 21/c		
Unit cell dimensions	a = 22.492(3) Å	α = 90°.	
	b = 3.9450(5) Å	β = 112.820(9)°.	
	c = 20.893(3) Å	γ = 90°.	
Volume	1708.8(4) Å <sup>3</sup>		
Z	4		
Density (calculated)	1.288 Mg/m <sup>3</sup>		
Absorption coefficient	0.074 mm <sup>-1</sup>		
F(000)	696		
Crystal size	0.34 x 0.14 x 0.03 mm <sup>3</sup>		
Theta range for data collection	0.98 to 25.02°.		

Index ranges	-26<=h<=26, -4<=k<=4, -24<=l<=24
Reflections collected	12026
Independent reflections	3009 [R(int) = 0.1490]
Completeness to theta = 25.02°	99.3 %
Absorption correction	multi-scan
Max. and min. transmission	0.9978 and 0.9752
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3009 / 0 / 218
Goodness-of-fit on F <sup>2</sup>	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0943, wR2 = 0.2358
R indices (all data)	R1 = 0.1852, wR2 = 0.2966
Largest diff. peak and hole	0.353 and -0.692 e.Å <sup>-3</sup>



(E)-4-((E)-benzylidene)-3,6-diphenylhex-2-en-5-ynal (4a)



Current Data Parameters

NAME lio-1  
EXPNO 102  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20130604  
Time 21.51  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 629  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 8192  
DW 20.800 use  
DE 6.50 use  
TE 301.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

NUC1 <sup>13</sup>C  
P1 9.40 use  
PL1 7.00 dB  
SFO1 100.6233325 MHz

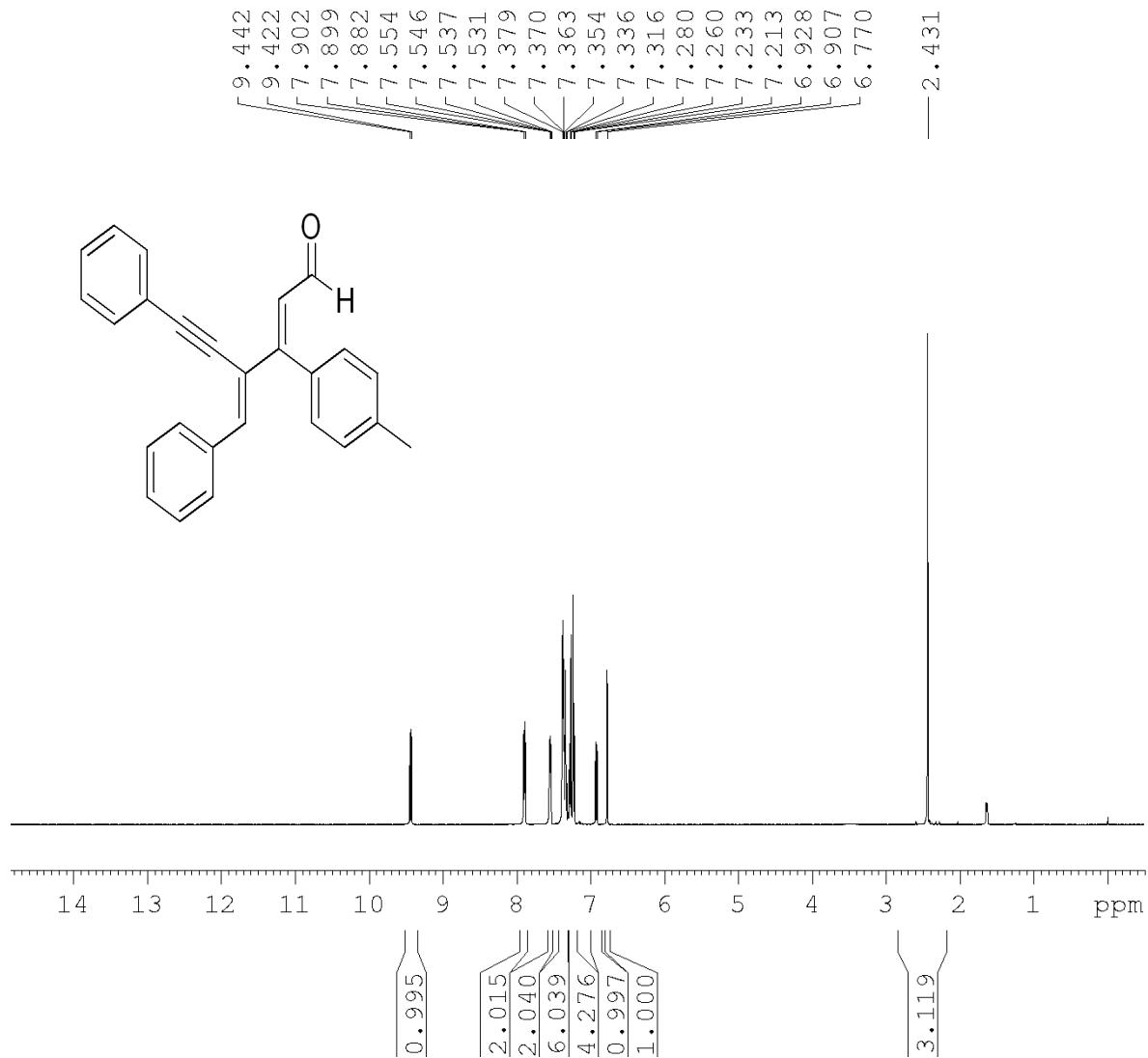
===== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 <sup>1</sup>H  
PCPD2 90.00 use  
PL2 3.00 dB  
PL12 20.70 dB  
PL13 23.70 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127484 MHz

(E)-4-((E)-benzylidene)-6-phenyl-3-(p-tolyl)hex-2-en-5-yneal (4b)



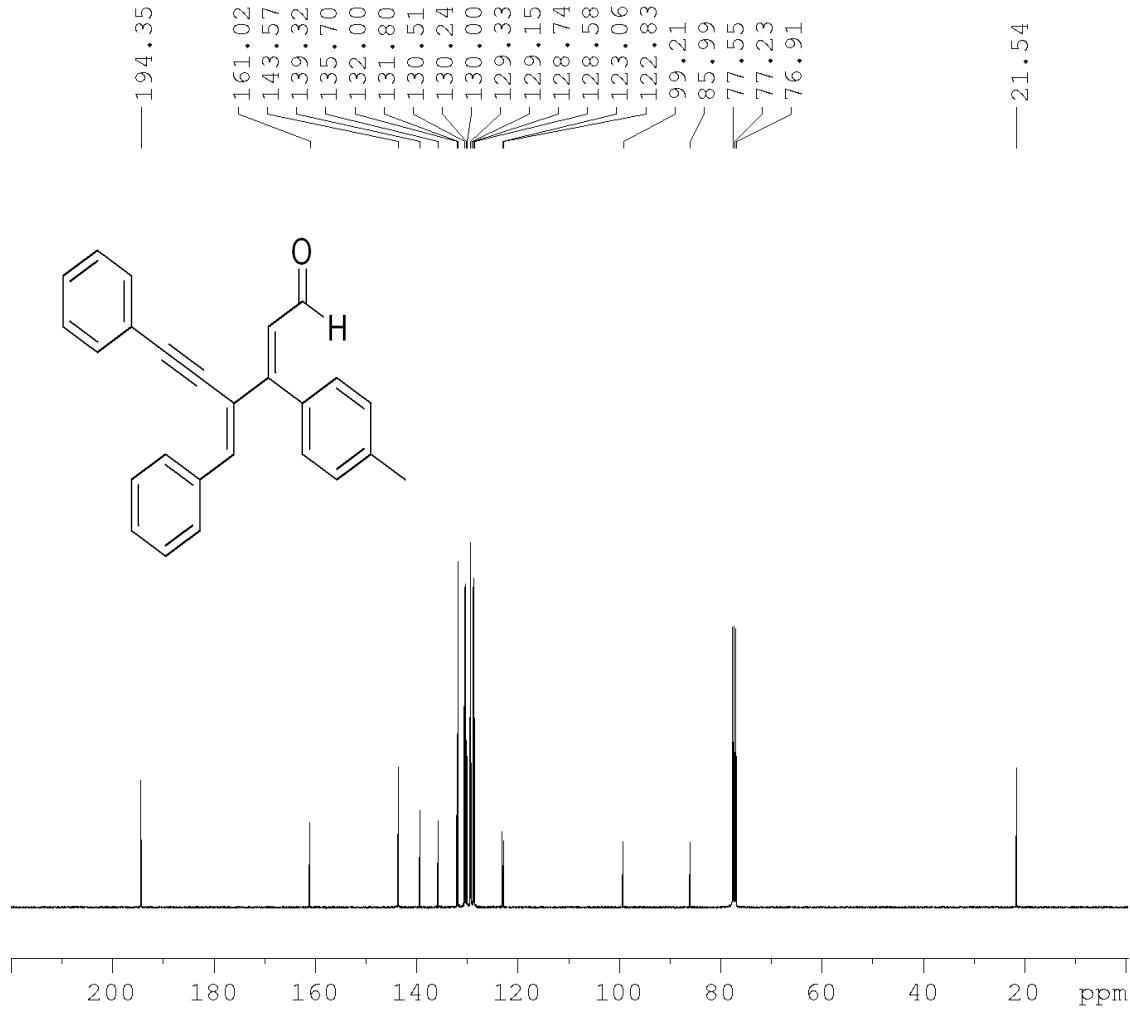
Current Data Parameters  
 NAME lio-1  
 EXPNO 125  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20131101  
 Time 1.01  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 114  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 300.4 K  
 D1 2.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.90 usec  
 PL1 3.00 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300213 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(E)-4-((E)-benzylidene)-6-phenyl-3-(p-tolyl)hex-2-en-5-yneal (4b)



Current Data Parameters

NAME lio-1  
EXPNO 126  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20131101  
Time 1.06  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 8159  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 8192  
DW 20.800 use  
DE 6.50 use  
TE 300.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

NUC1 13C  
P1 9.40 use  
PL1 7.00 dB  
SFO1 100.6233325 MHz

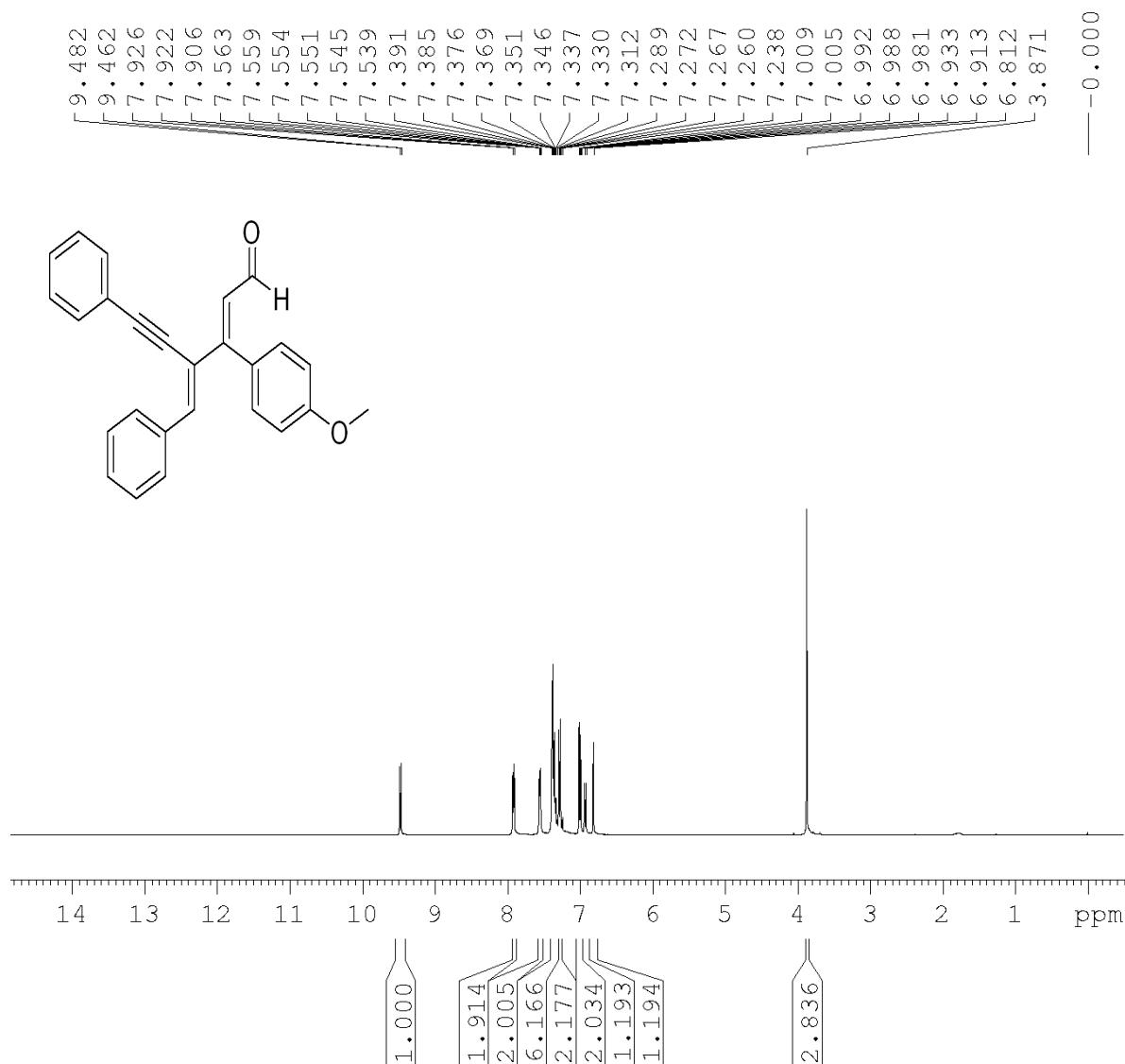
===== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 use  
PL2 3.00 dB  
PL12 20.70 dB  
PL13 23.70 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127517 MHz

(E)-4-((E)-benzylidene)-3-(4-methoxyphenyl)-6-phenylhex-2-en-5-ynal (4c)



Current Data Parameters

NAME lio-1  
EXPNO 127  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20131006  
Time 21.16  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 7246.377 Hz  
FIDRES 0.221142 Hz  
AQ 2.2609921 sec  
RG 40.3  
DW 69.000 usec  
DE 6.50 usec  
TE 299.3 K  
D1 2.0000000 sec  
TDO 1

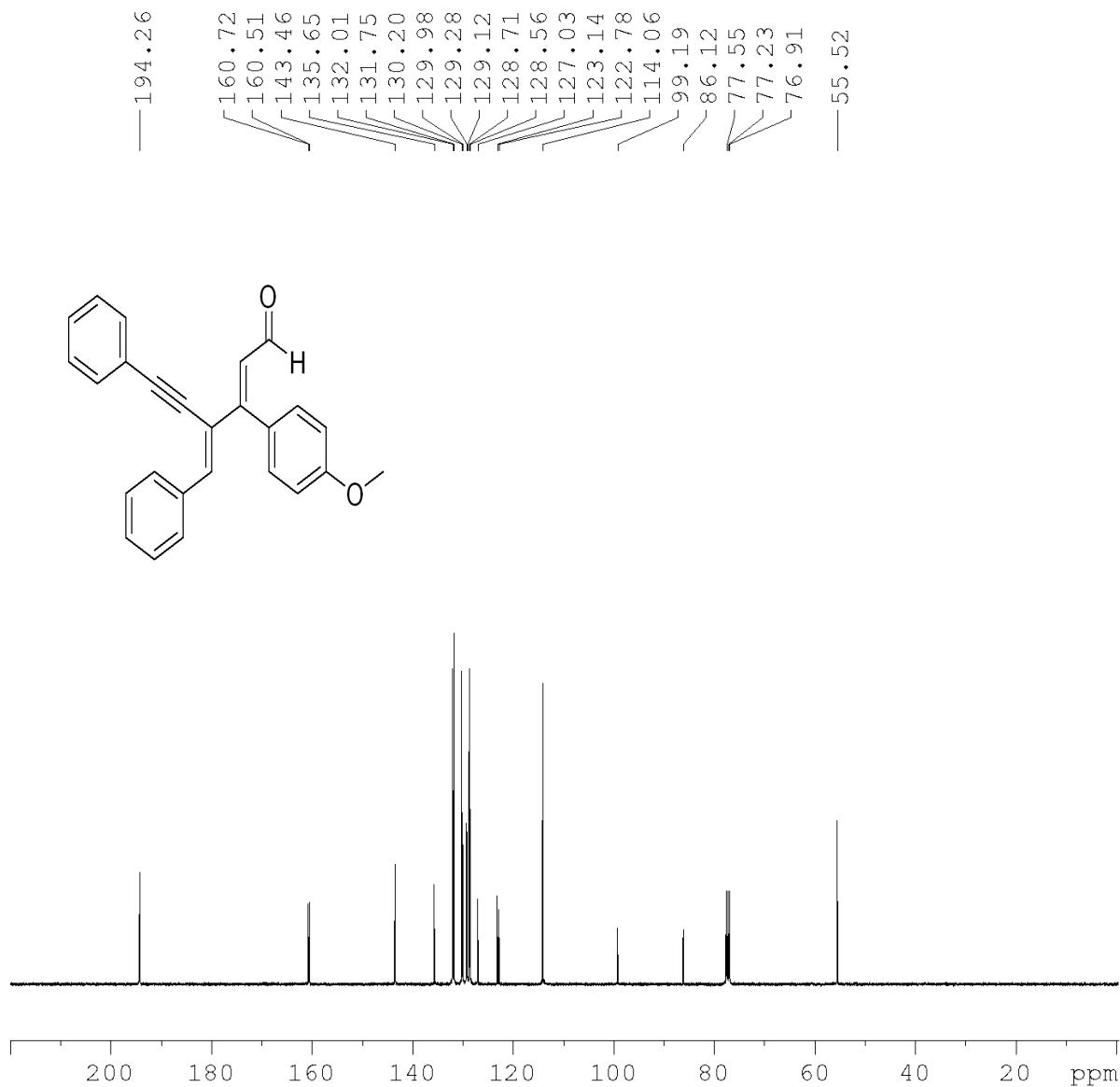
===== CHANNEL f1 =====

NUC1 1H  
P1 11.90 usec  
PL1 3.00 dB  
SFO1 400.1324008 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300180 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

(E)-4-((E)-benzylidene)-3-(4-methoxyphenyl)-6-phenylhex-2-en-5-ynal (4c)



Current Data Parameters

NAME	lio-1
EXPNO	128
PROCNO	1

F2 - Acquisition Parameters

Date_	20131006
Time	21.17
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl <sub>3</sub>
NS	1005
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6815744 sec
RG	8192
DW	20.800 use
DE	6.50 use
TE	299.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

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

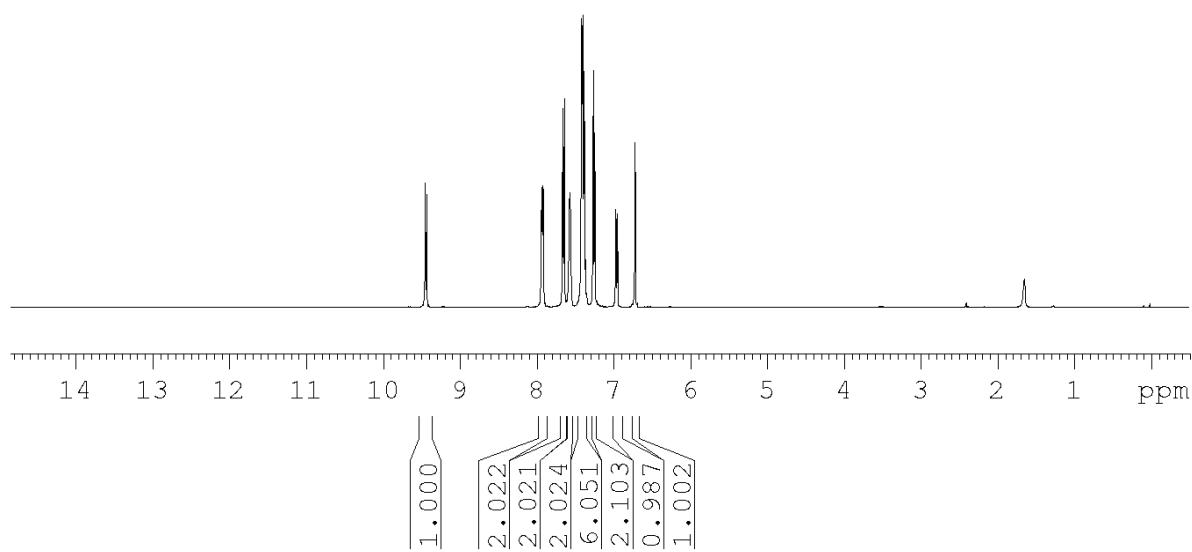
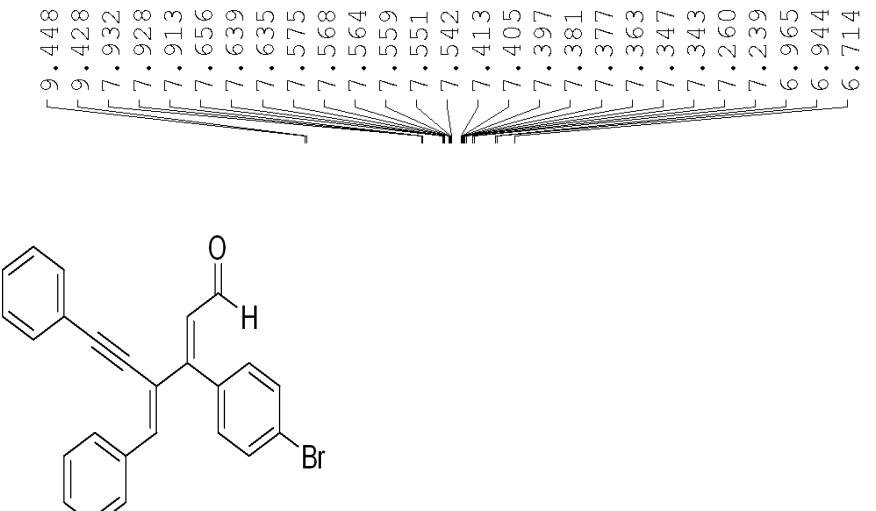
NUC1	<sup>13</sup> C
P1	9.40 use
PL1	7.00 dB
SFO1	100.6233325 MHz

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

CPDPRG[2]	waltz16
NUC2	<sup>1</sup> H
PCPD2	90.00 use
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

(E)-4-((E)-benzylidene)-3-(4-bromophenyl)-6-phenylhex-2-en-5-yneal (4d)



Current Data Parameters  
NAME lio-1  
EXPNO 117  
PROCNO 1

```

F2 - Acquisition Parameters
Date_          20130810
Time           22.19
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        zg30
TD             32768
SOLVENT        CDC13
NS              16
DS              0
SWH             7246.377 Hz
FIDRES        0.221142 Hz
AQ              2.2609921 sec
RG              114
DW              69.000 usec
DE              6.50 usec
TE              297.1 K
D1              2.00000000 sec
TD0              1

```

===== CHANNEL f1 =====  
NUC1 1H  
P1 11.90 usec  
PL1 3.00 dB  
SFO1 400.1324008 MHz

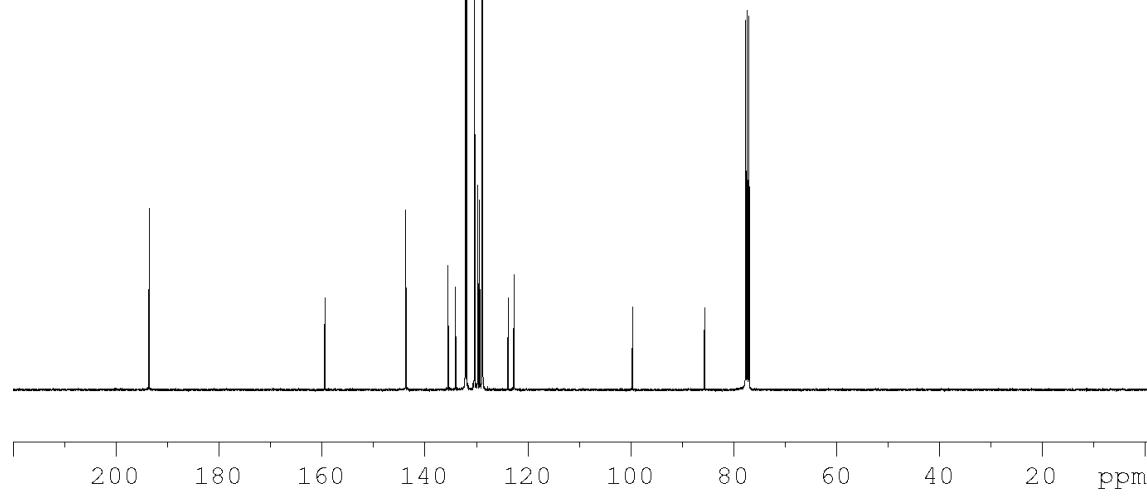
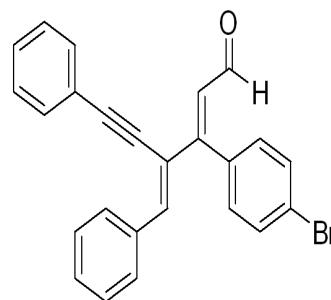
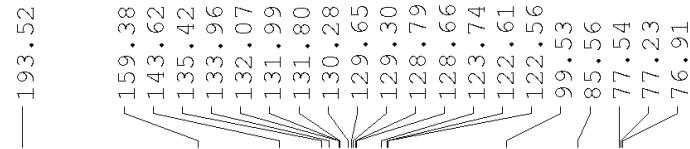
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F2 - Processing parameters
SI           16384
SF          400.1300098 MHz
WDW          EM
SSB           0
LB            0 Hz
GB           0
PC           1.00

```

(E)-4-((E)-benzylidene)-3-(4-bromophenyl)-6-phenylhex-2-en-5-yneal (4d)

Current Data Parameters  
 NAME lio-1  
 EXPNO 118  
 PROCNO 1



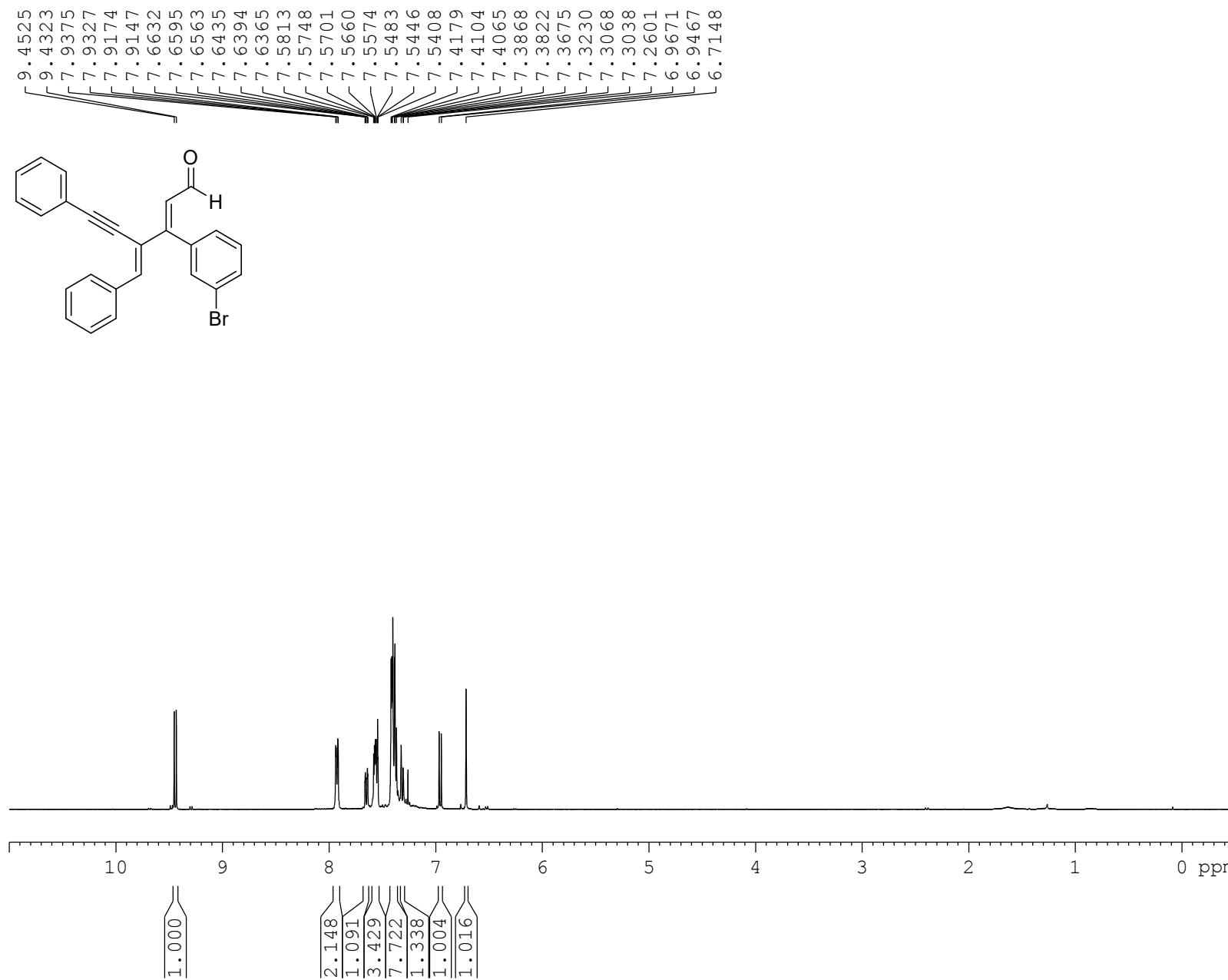
F2 - Acquisition Parameters  
 Date\_ 20130810  
 Time 22.20  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 15099  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 8192  
 DW 20.800 use  
 DE 6.50 use  
 TE 297.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 9.40 use  
 PL1 7.00 dB  
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====  
 CPDPRG[2 waltz16  
 NUC2 1H  
 PCPD2 90.00 use  
 PL2 3.00 dB  
 PL12 20.70 dB  
 PL13 23.70 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127525 MHz

(2E, 4E)-4-benzylidene-3-(3-bromophenyl)-6-phenylhex-2-en-5-yneal (4e)



Current Data Parameters  
NAME TRY  
EXPNO 594  
PROCNO 1

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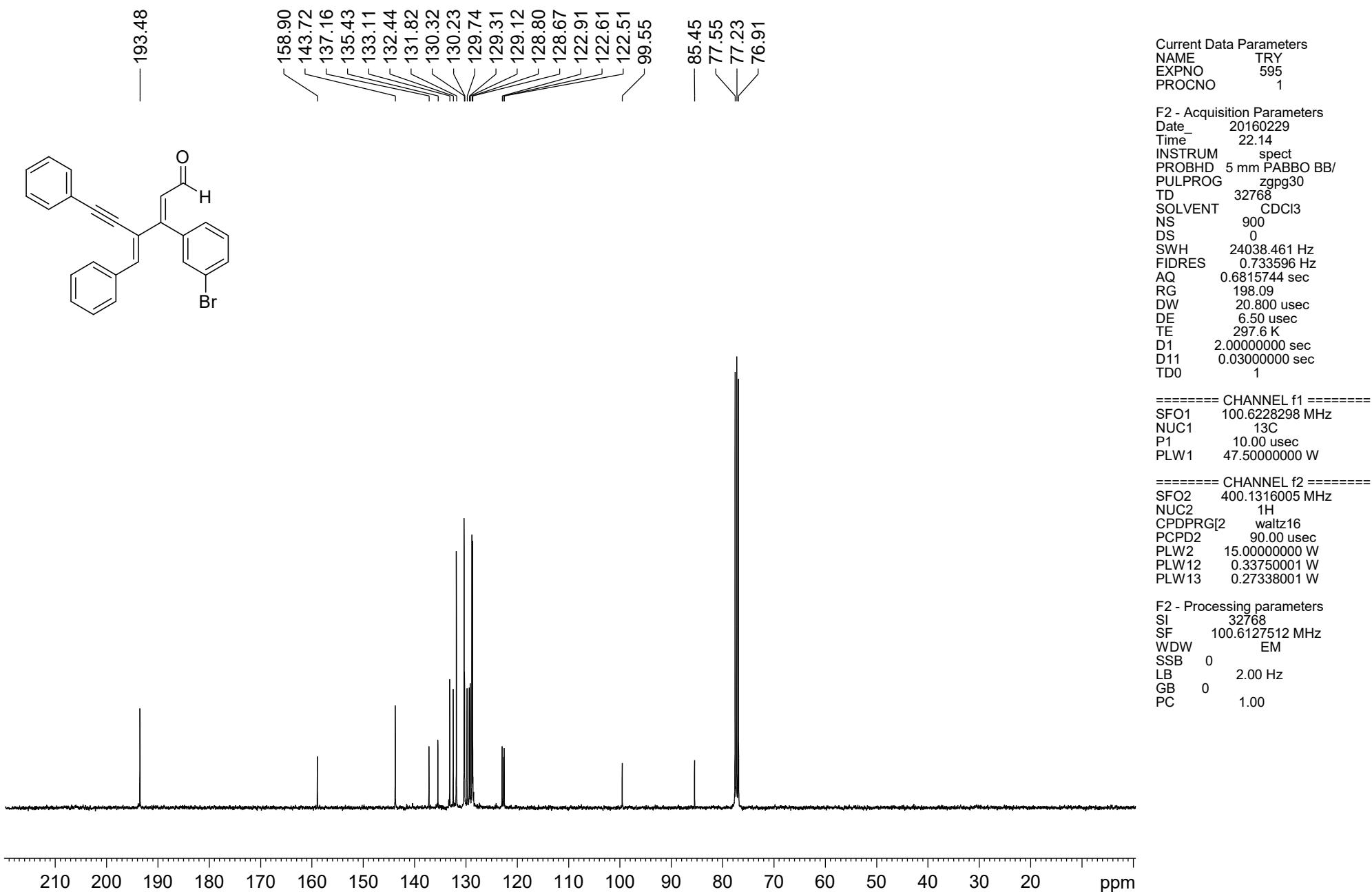
F2 - Acquisition Parameters
Date_      20160229
Time       22.07
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD        32768
SOLVENT   CDCl3
NS         64
DS         0
SWH       7211.539 Hz
FIDRES   0.220079 Hz
AQ        2.2719147 sec
RG        78.51
DW        69.333 usec
DE        10.50 usec
TE        296.9 K
D1        2.0000000 sec
TD0           1

```

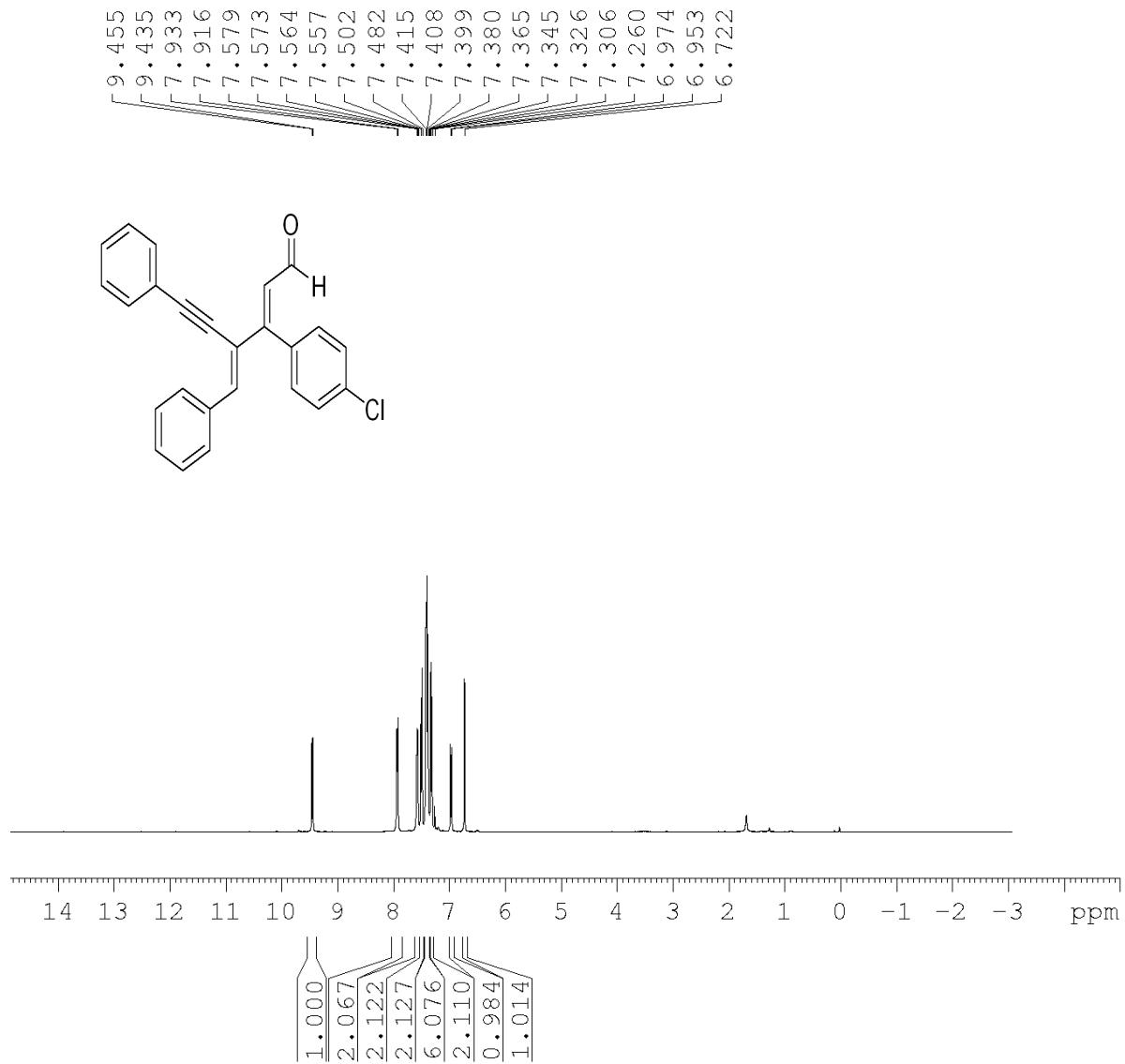
===== CHANNEL f1 =====  
SFO1 400.1324008 MHz  
NUC1 1H  
P1 12.90 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1300097 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

(2E, 4E)-4-benzylidene-3-(3-bromophenyl)-6-phenylhex-2-en-5-ynal (4e)



(E)-4-((E)-benzylidene)-3-(4-chlorophenyl)-6-phenylhex-2-en-5-yneal (4f)



Current Data Parameters  
 NAME lio-1  
 EXPNO 119  
 PROCNO 1

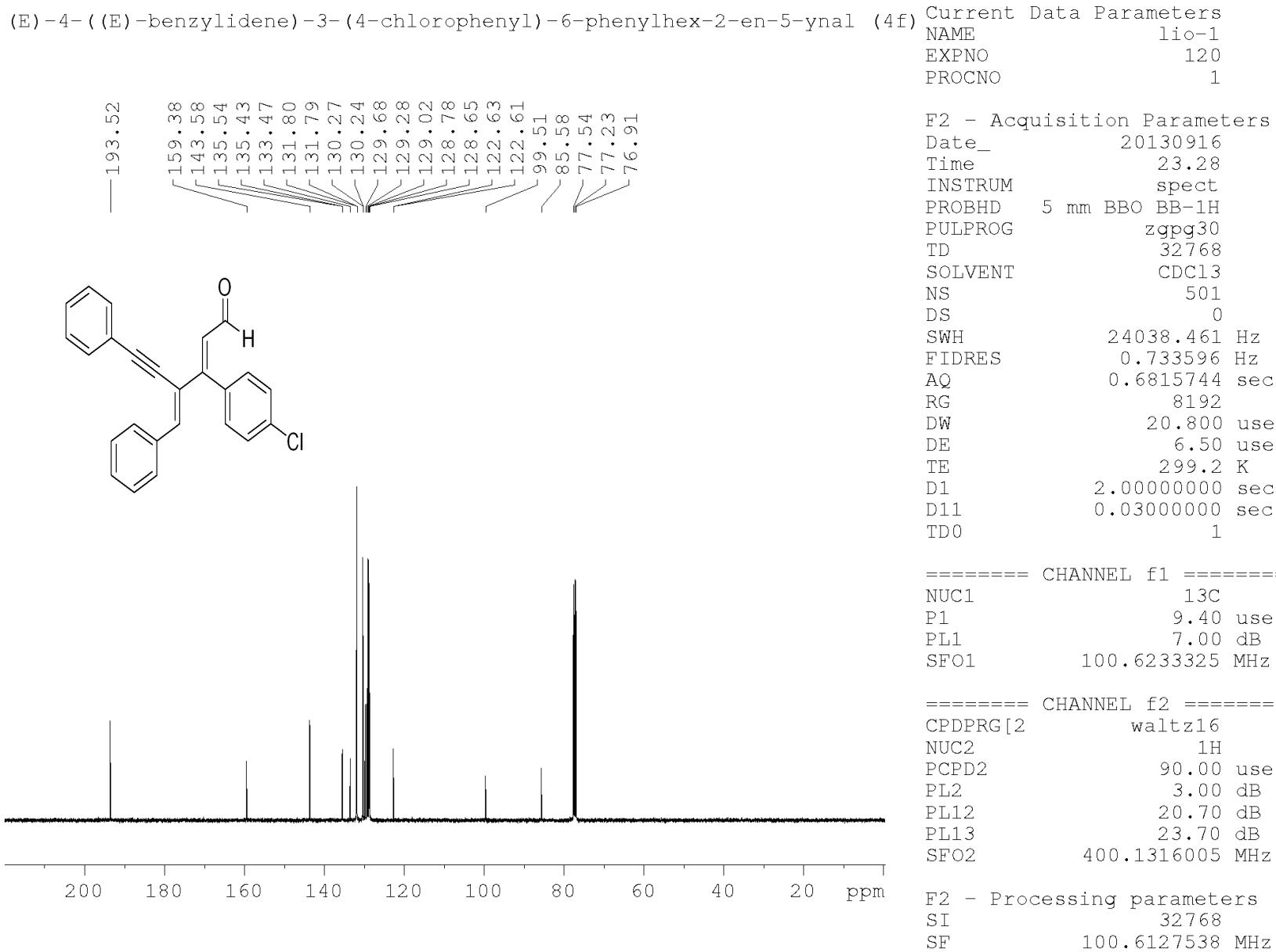
F2 - Acquisition Parameters  
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 Time 23.27  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 8  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 114  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 2.00000000 sec  
 TDO 1

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

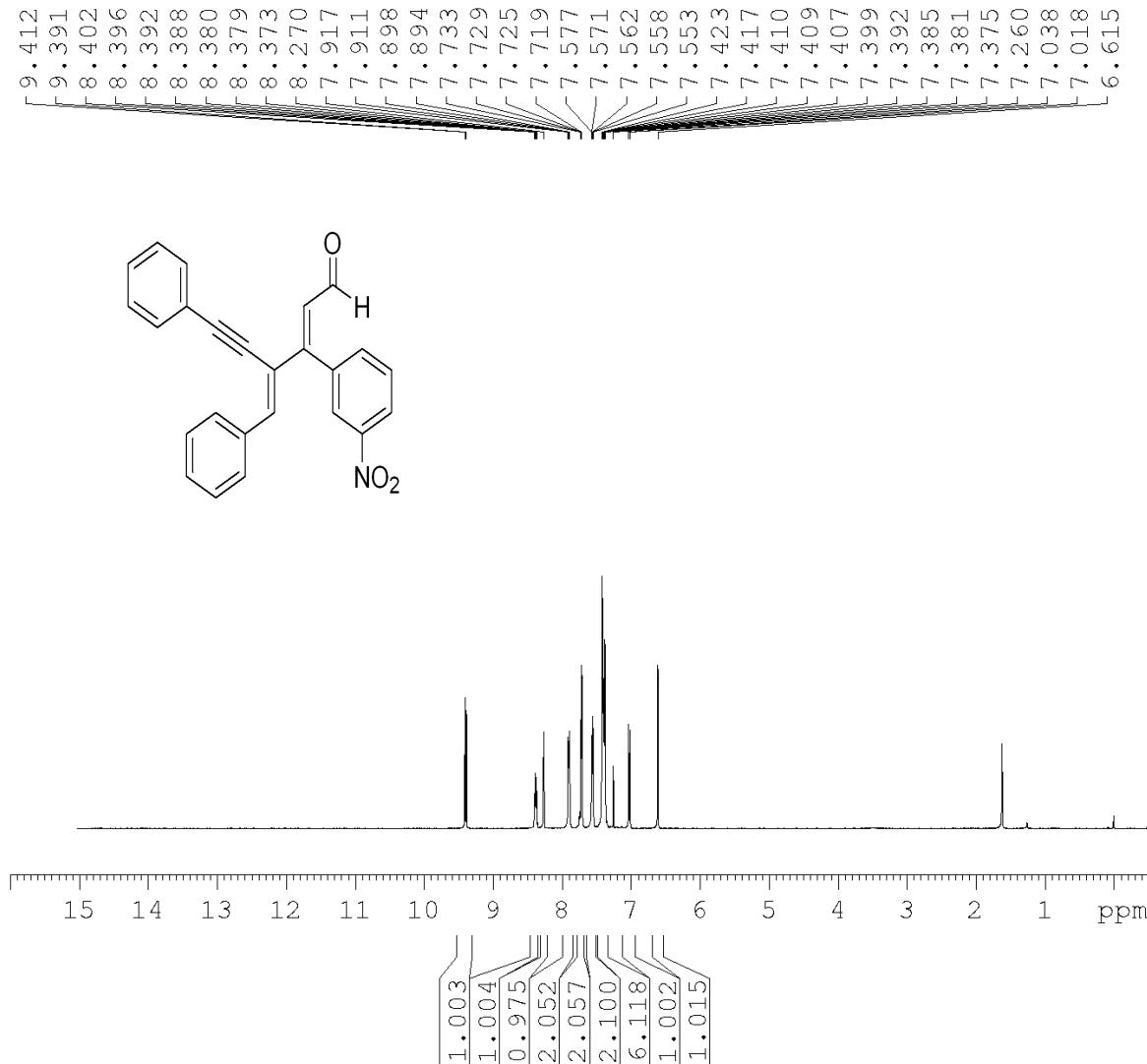
NUC1 1H  
 P1 11.90 usec  
 PL1 3.00 dB  
 SF01 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300095 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(E)-4-((E)-benzylidene)-3-(4-chlorophenyl)-6-phenylhex-2-en-5-yneal (4f)



(E)-4-((E)-benzylidene)-3-(3-nitrophenyl)-6-phenylhex-2-en-5-yneal (4g)



#### Current Data Parameters

NAME lio-1  
EXPNO 111  
PROCNO 1

#### F2 - Acquisition Parameters

Date 20130916  
Time 23.55  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 0  
SWH 7246.377 Hz  
FIDRES 0.221142 Hz  
AQ 2.2609921 sec  
RG 161.3  
DW 69.000 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.00000000 sec  
TD0 1

#### ===== CHANNEL f1 =====

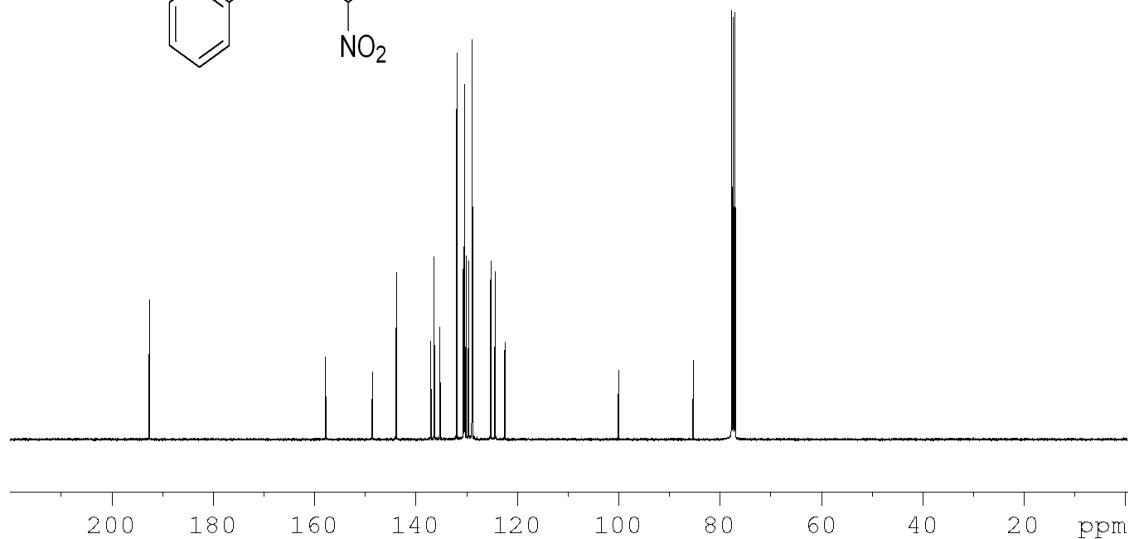
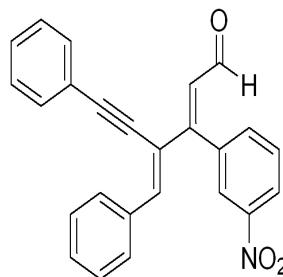
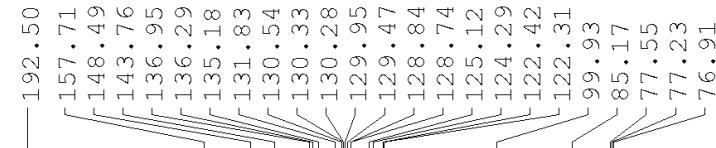
NUC1 1H  
P1 11.90 usec  
PL1 3.00 dB  
SFO1 400.1324008 MHz

#### F2 - Processing parameters

SI 16384  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

(E)-4-( (E)-benzylidene)-3-(3-nitrophenyl)-6-phenylhex-2-en-5-yneal (4g)

Current Data Parameters  
NAME lio-1  
EXPNO 112  
PROCNO 1



F2 - Acquisition Parameters

Date\_ 20130916  
Time 23.56  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 11915  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 8192  
DW 20.800 use  
DE 6.50 use  
TE 299.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

NUC1 13C  
P1 9.40 use  
PL1 7.00 dB  
SFO1 100.6233325 MHz

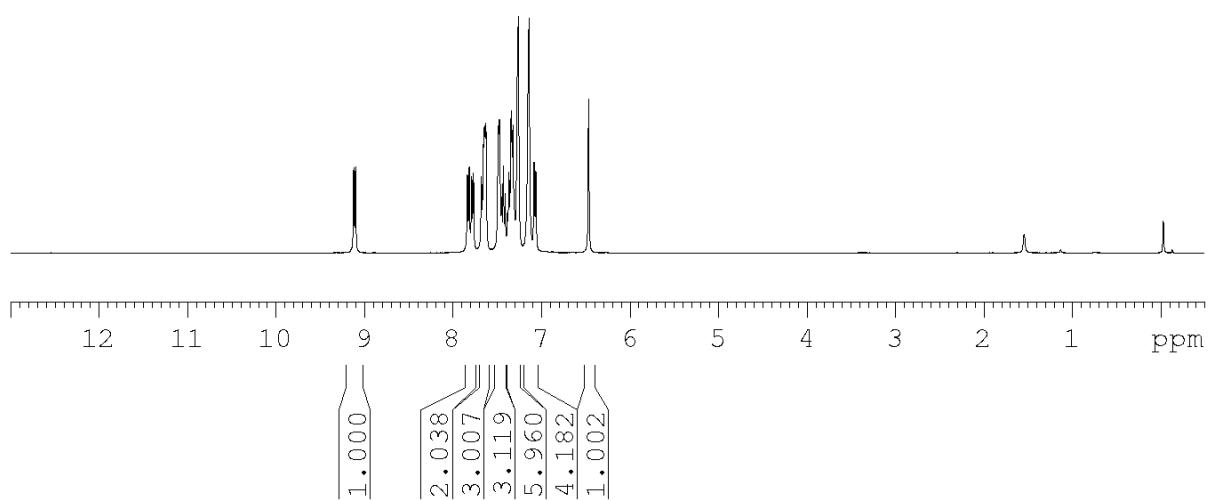
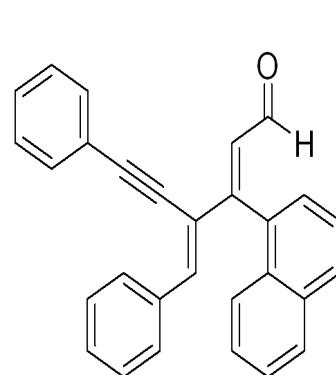
===== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 use  
PL2 3.00 dB  
PL12 20.70 dB  
PL13 23.70 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127503 MHz

(Z)-4-((E)-benzylidene)-3-(naphthalen-1-yl)-6-phenylhex-2-en-5-ynal (4h)



Current Data Parameters	
NAME	lio-1
EXPNO	103
PROCNO	1

```

F2 - Acquisition Parameters
Date_          20131101
Time           0.18
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        zg30
TD             32768
SOLVENT        CDC13
NS              8
DS              0
SWH             7246.377 Hz
FIDRES        0.221142 Hz
AQ             2.2609921 sec
RG              57
DW             69.000 usec
DE              6.50  usec
TE              300.4 K
D1             2.00000000 sec
TD0              1

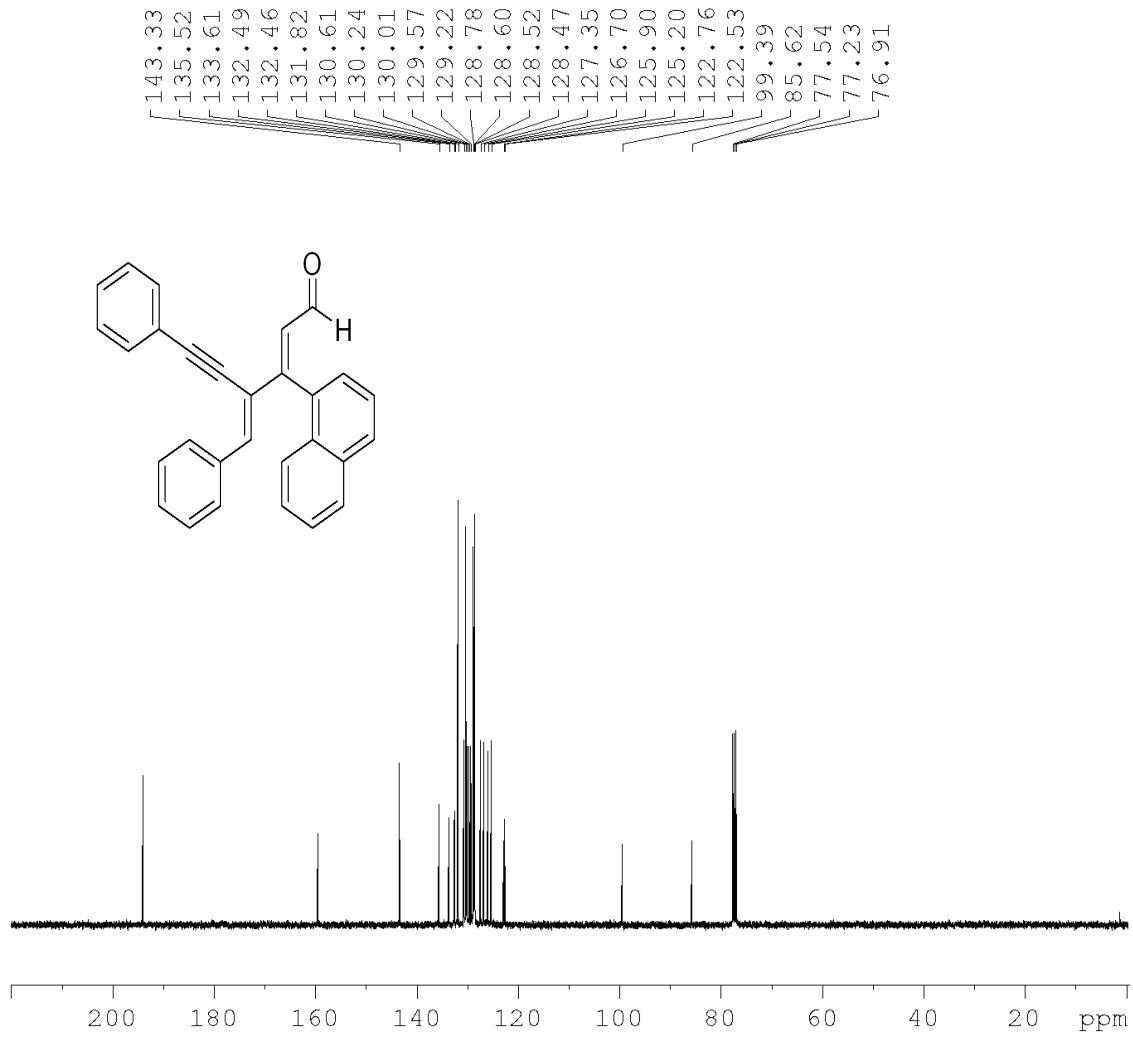
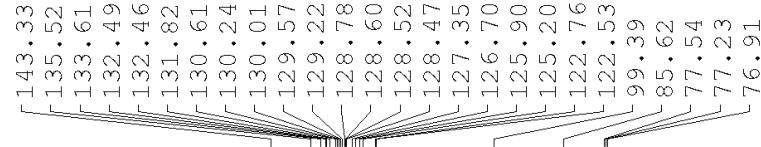
```

===== CHANNEL f1 =====  
NUC1 1H  
P1 11.90 usec  
PL1 3.00 dB  
SEQ1 400.1324008 MHz

(Z)-4-((E)-benzylidene)-3-(naphthalen-1-yl)-6-phenylhex-2-en-5-ynal (4h)

Current Data Parameters

NAME	lio-1
EXPNO	104
PROCNO	1



F2 - Acquisition Parameters

Date_	20131101
Time	0.32
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	300
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6815744 sec
RG	8192
DW	20.800 use
DE	6.50 use
TE	300.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

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

NUC1	13C
P1	9.40 use
PL1	7.00 dB
SFO1	100.6233325 MHz

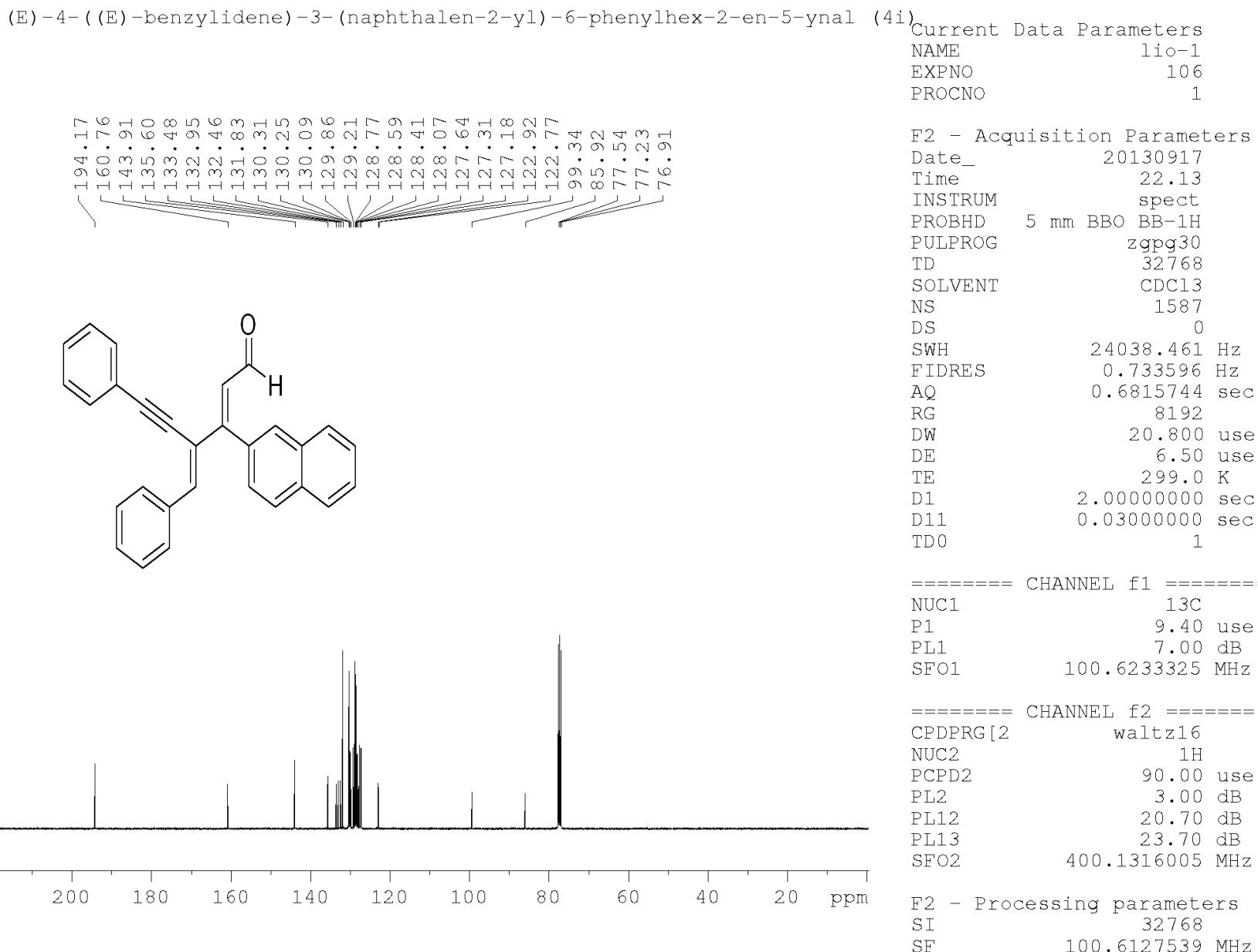
===== CHANNEL f2 =====

CPDPG[2]	waltz16
NUC2	1H
PCPD2	90.00 use
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz

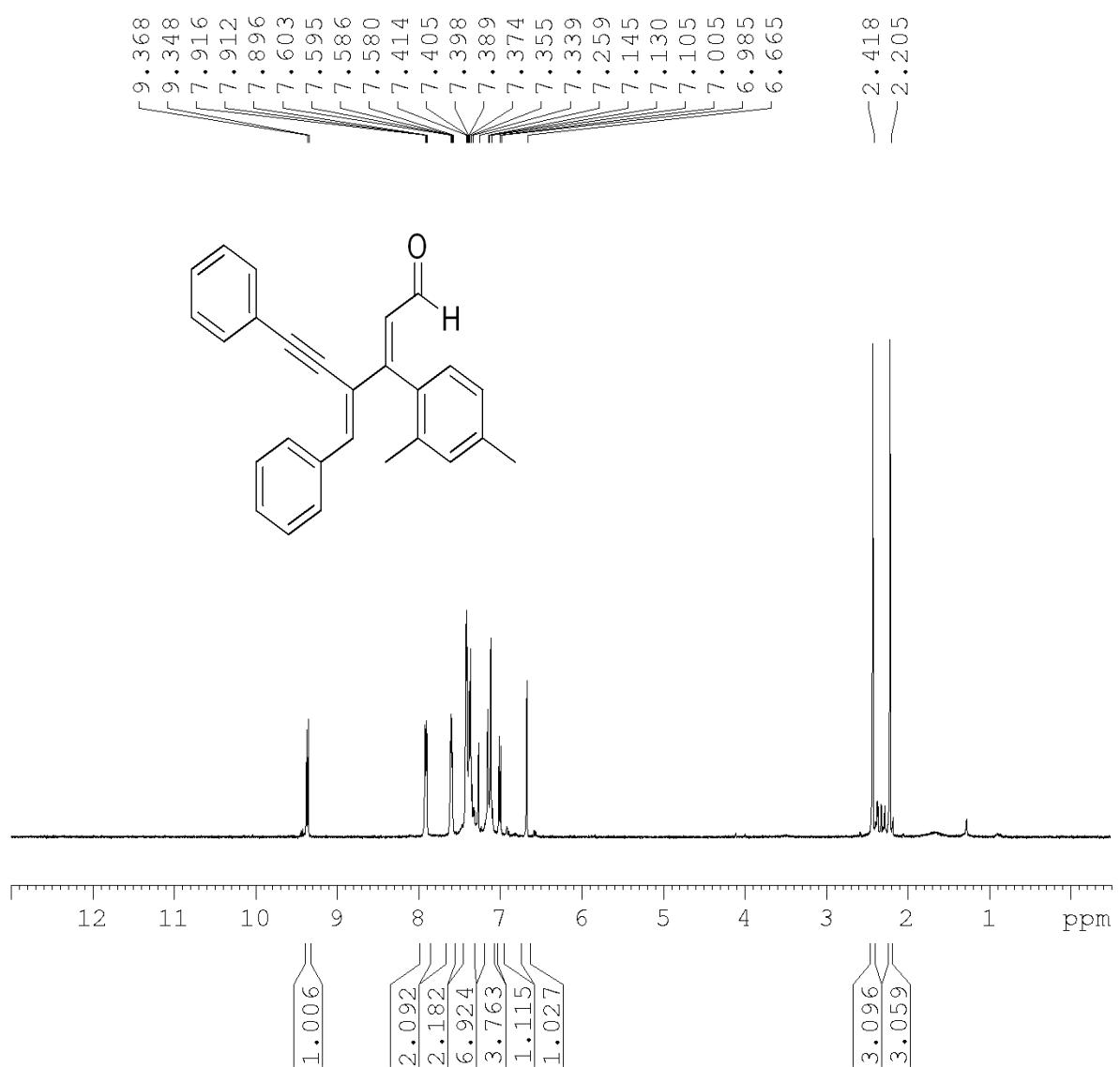
F2 - Processing parameters

SI	32768
SF	100.6127587 MHz





(E)-4-((E)-benzylidene)-3-(2,4-dimethylphenyl)-6-phenylhex-2-en-5-ynal (4j)



Current Data Parameters  
NAME lio-1  
EXPNO 107  
PROCNO 1

```

F2 - Acquisition Parameters
Date_           20131115
Time            2.02
INSTRUM        spect
PROBHD         5 mm BBO BB-1H
PULPROG        zg30
TD              32768
SOLVENT         CDC13
NS              1
DS              0
SWH             7246.377 Hz
FIDRES         0.221142 Hz
AQ              2.2609921 sec
RG              161.3
DW              69.000 usec
DE              6.50 usec
TE              300.3 K
D1              2.00000000 sec
TD0              1

```

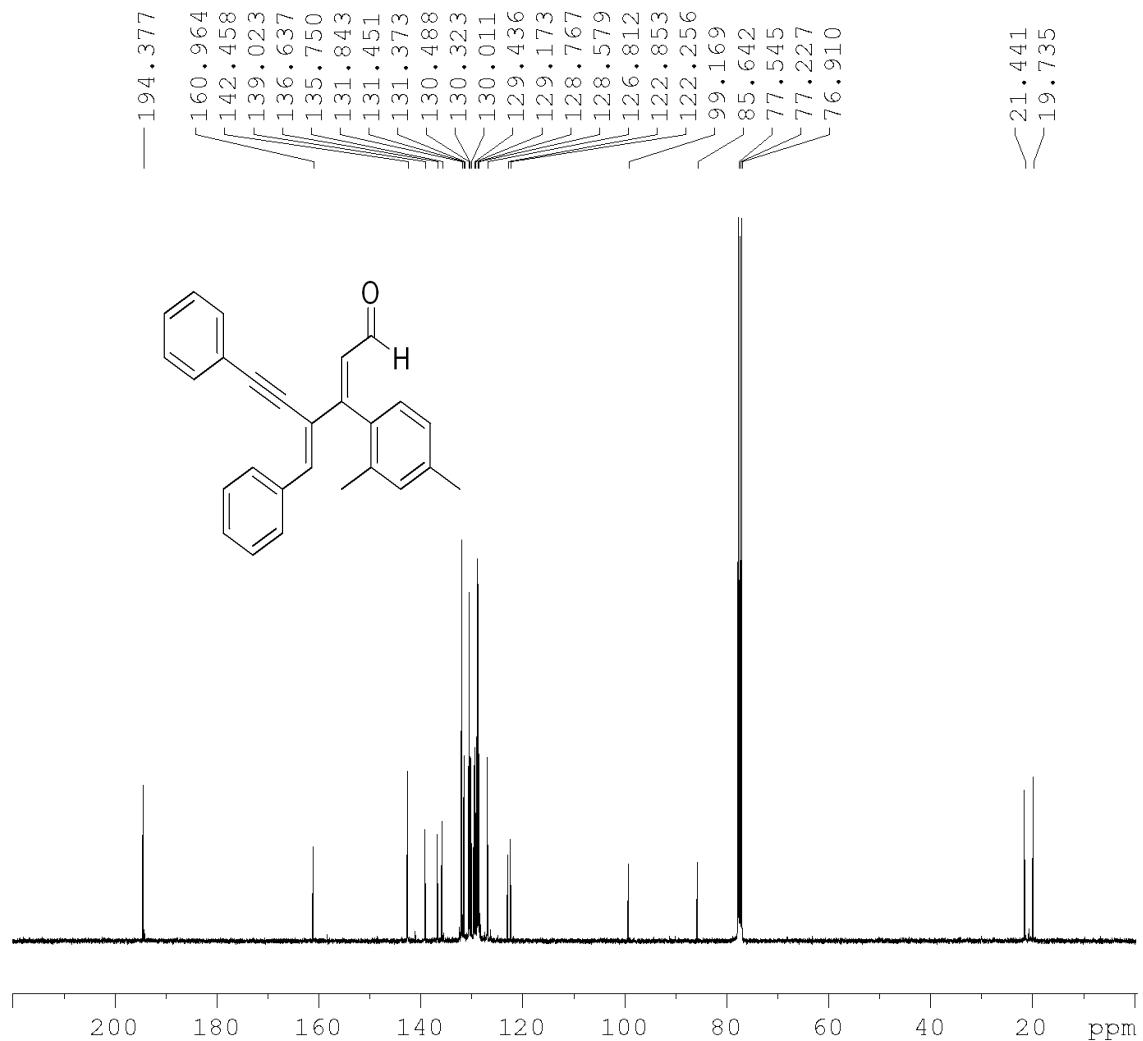
===== CHANNEL f1 =====  
NUC1 1H  
P1 11.90 usec  
PL1 3.00 dB  
SFO1 400.1324008 MHz

```

F2 - Processing parameters
SI           16384
SF          400.1300094 MHz
WDW          EM
SSB           0
LB            0 Hz
GB           0
PC           1.00

```

(E)-4-((E)-benzylidene)-3-(2,4-dimethylphenyl)-6-phenylhex-2-en-5-yneal (4j)



Current Data Parameters

NAME lio-1  
EXPNO 108  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20131115  
Time 2.03  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 7901  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 46341  
DW 20.800 use  
DE 6.50 use  
TE 300.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

NUC1 13C  
P1 9.40 use  
PL1 7.00 dB  
SFO1 100.6233325 MHz

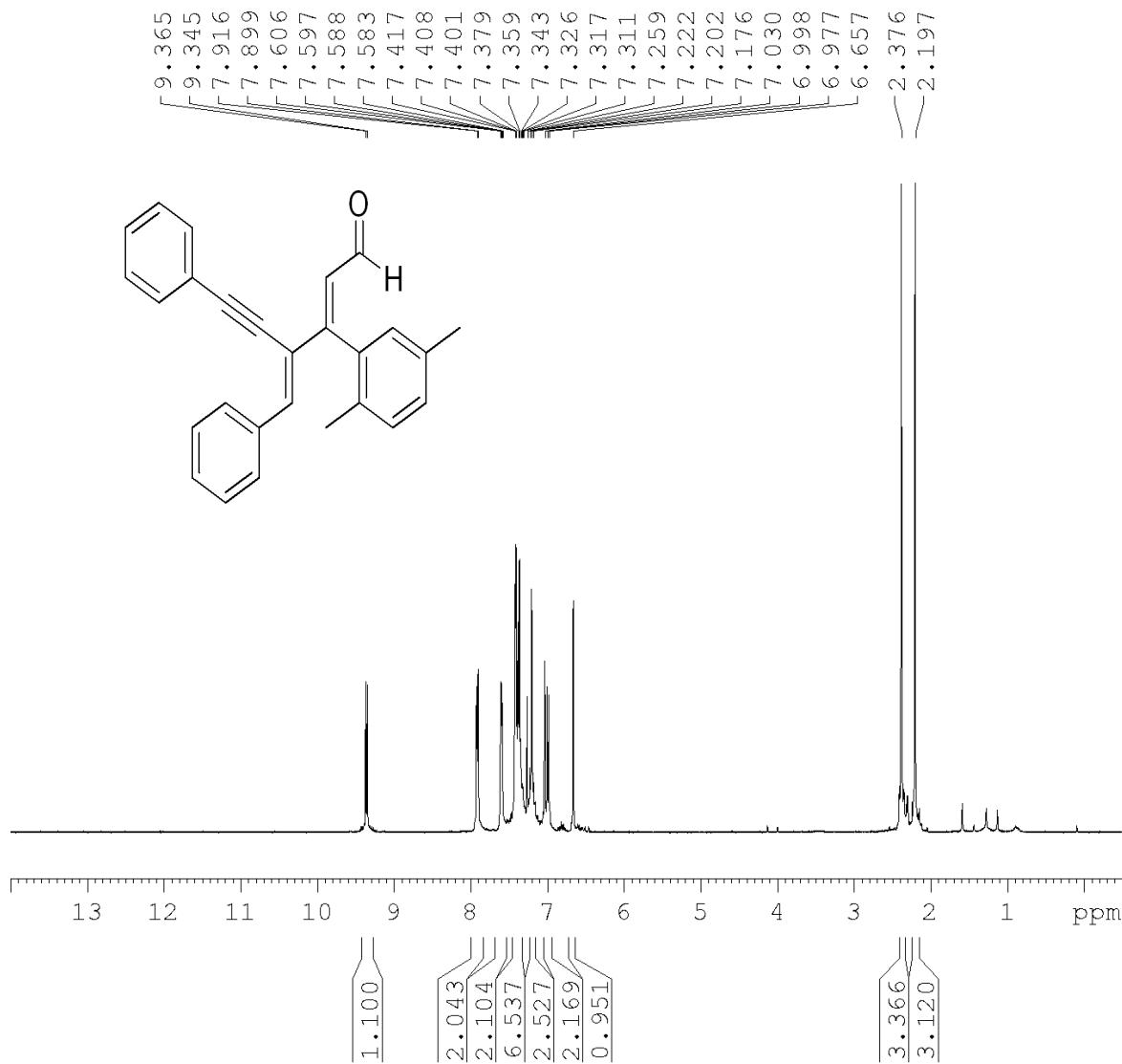
===== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 use  
PL2 3.00 dB  
PL12 20.70 dB  
PL13 23.70 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127492 MHz

(E)-4-((E)-benzylidene)-3-(2,5-dimethylphenyl)-6-phenylhex-2-en-5-yneal (4k)



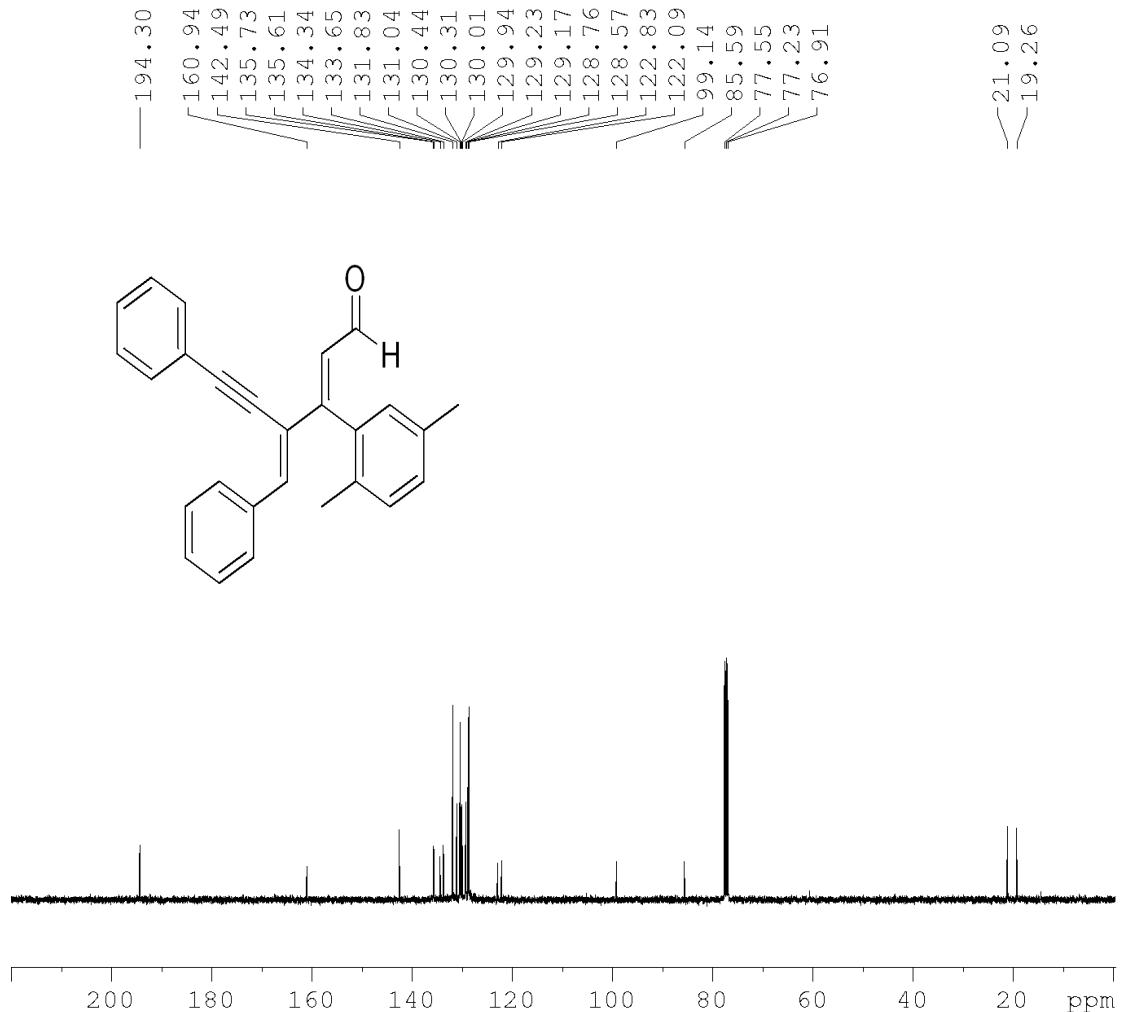
Current Data Parameters  
 NAME lio-1  
 EXPNO 109  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20131107  
 Time 22.09  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 181  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 TDO 1

===== CHANNEL f1 ======  
 NUC1 1H  
 P1 11.90 usec  
 PL1 3.00 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300098 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(E)-4-( (E)-benzylidene)-3-(2,5-dimethylphenyl)-6-phenylhex-2-en-5-ynal (4k)



Current Data Parameters  
 NAME lio-1  
 EXPNO 110  
 PROCNO 1

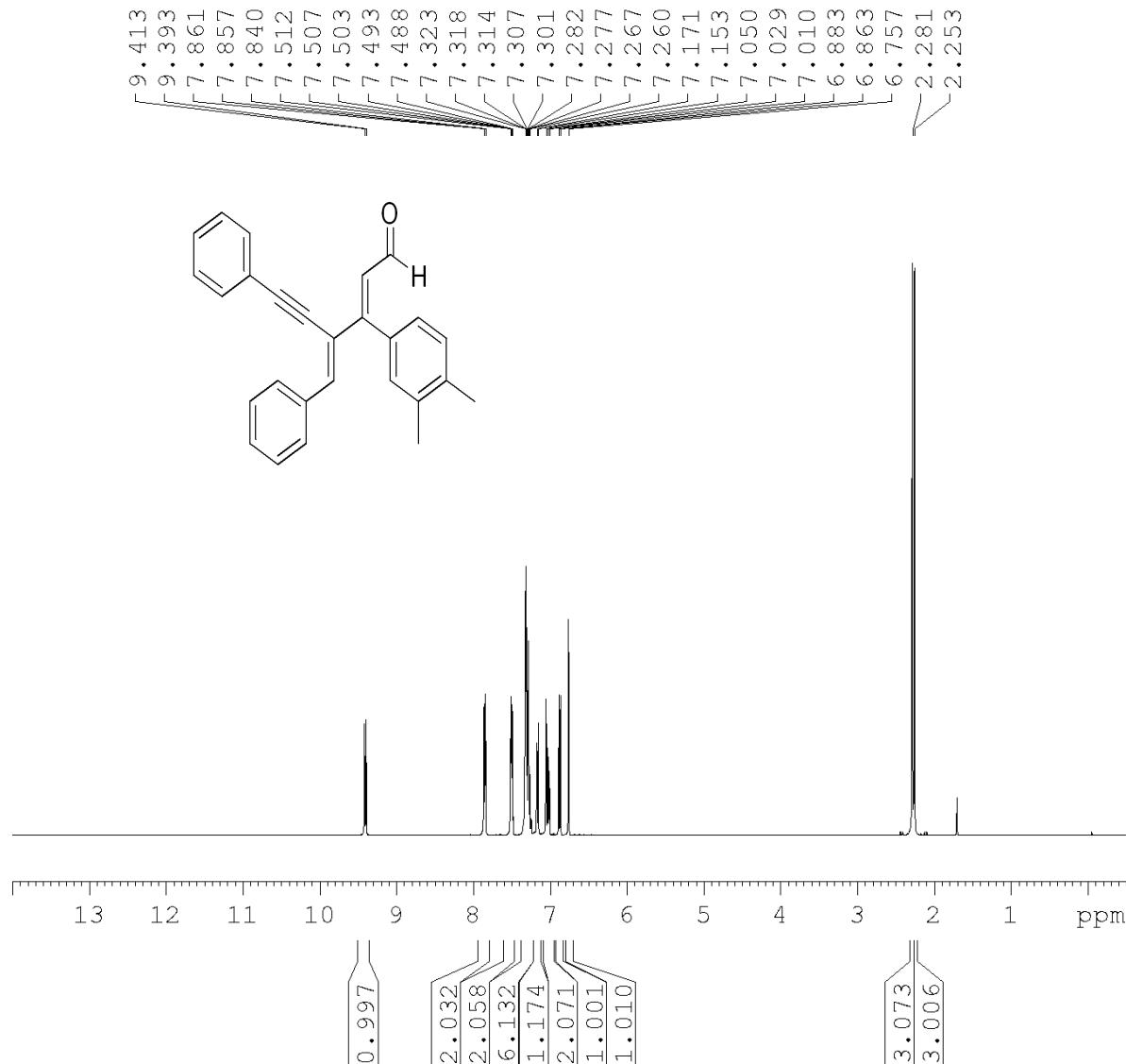
F2 - Acquisition Parameters  
 Date\_ 20131107  
 Time 22.19  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 205  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 8192  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.50 usec  
 PL1 7.00 dB  
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -0.60 dB  
 PL12 15.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127518 MHz

(E)-4-((E)-benzylidene)-3-(3,4-dimethylphenyl)-6-phenylhex-2-en-5-yneal (41)



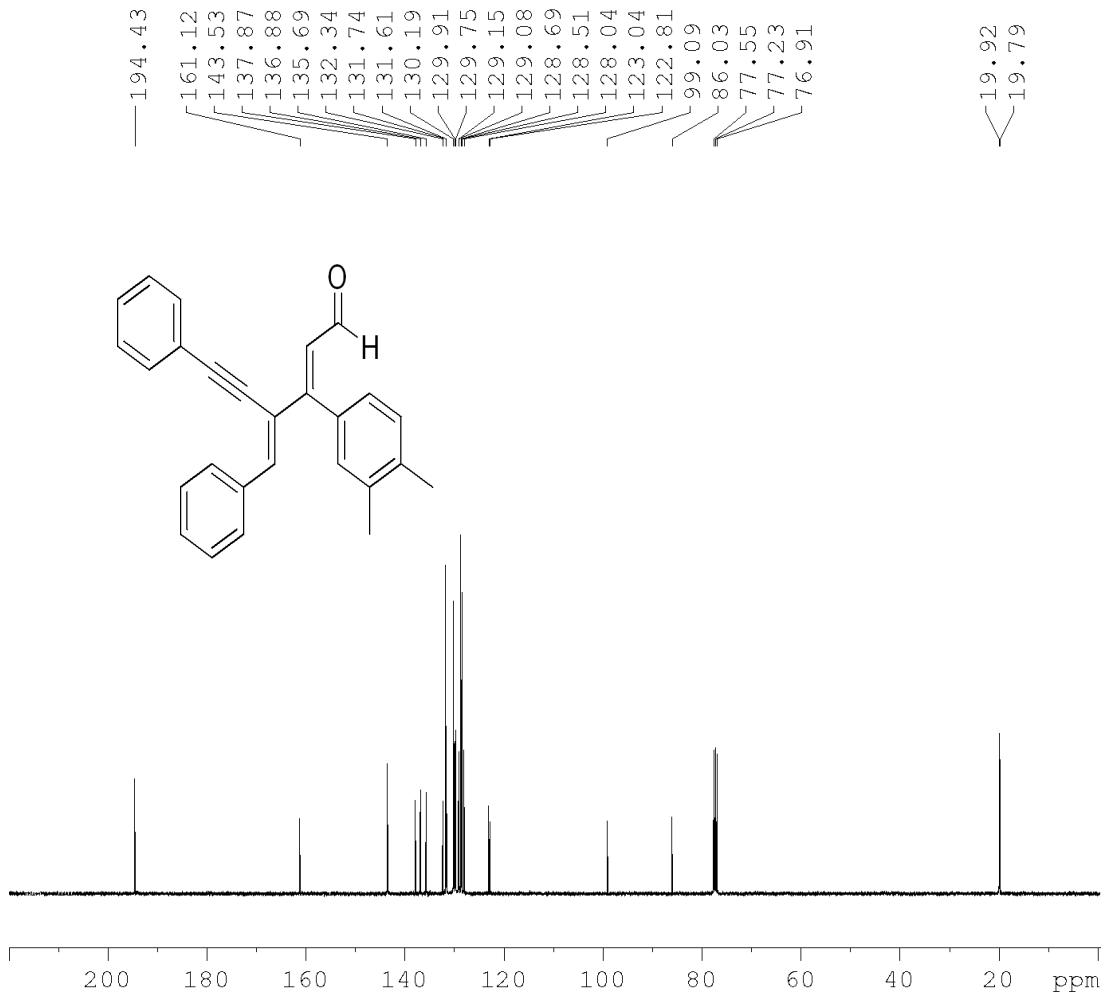
Current Data Parameters  
 NAME lio-1  
 EXPNO 113  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20131101  
 Time 0.56  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 8  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 45.3  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 300.6 K  
 D1 2.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.90 usec  
 PL1 3.00 dB  
 SF01 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300460 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(E)-4-( (E)-benzylidene)-3-(3,4-dimethylphenyl)-6-phenylhex-2-en-5-ynal (41)



Current Data Parameters

NAME lio-1  
EXPNO 114  
PROCNO 1

F2 - Acquisition Parameters

Date 20131101  
Time 0.54  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 300  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 8192  
DW 20.800 use  
DE 6.50 use  
TE 300.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

NUC1 13C  
P1 9.40 use  
PL1 7.00 dB  
SFO1 100.6233325 MHz

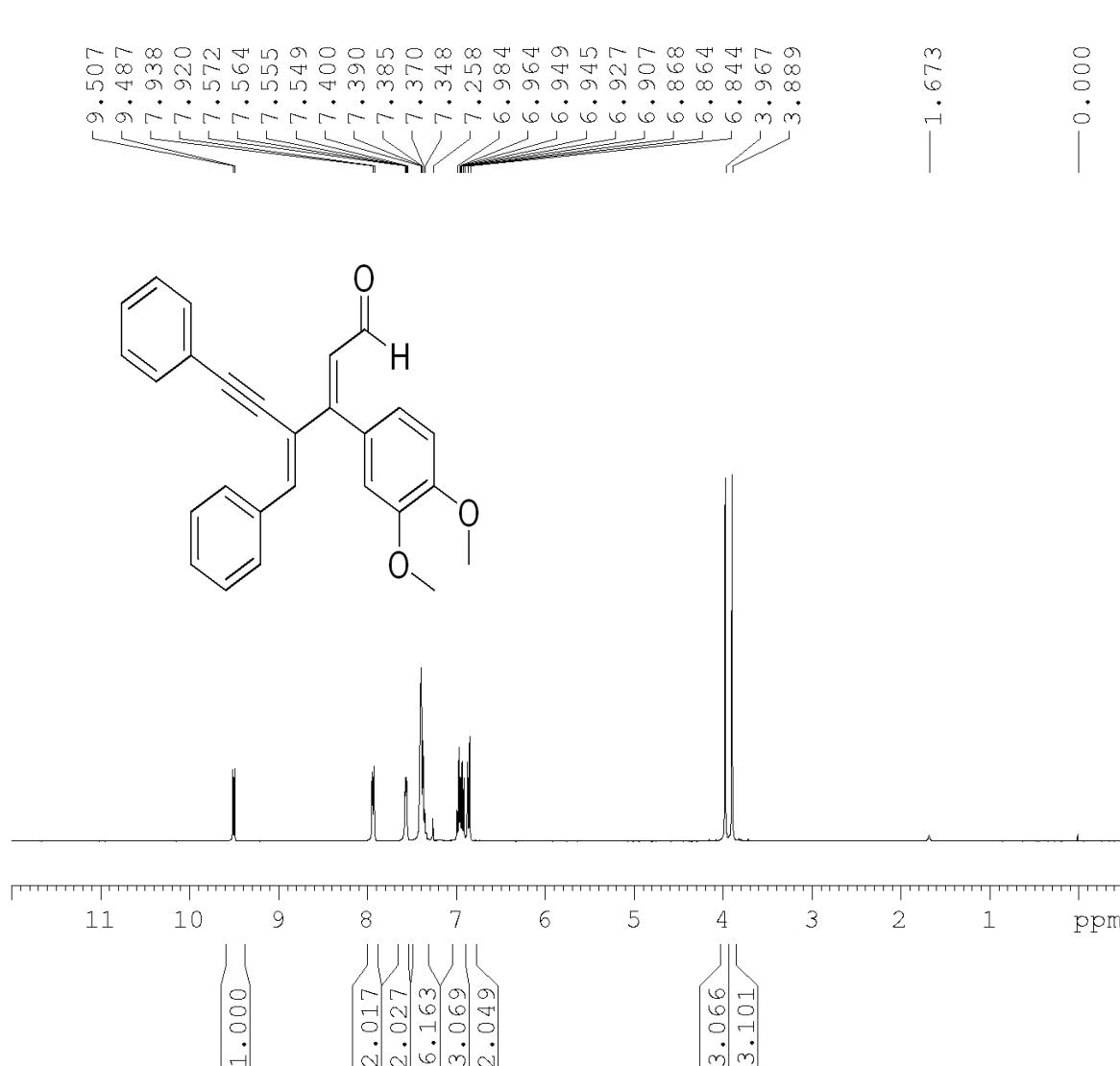
===== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 use  
PL2 3.00 dB  
PL12 20.70 dB  
PL13 23.70 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127598 MHz

(E)-4-((E)-benzylidene)-3-(3,4-dimethoxyphenyl)-6-phenylhex-2-en-5-ynal (4m)



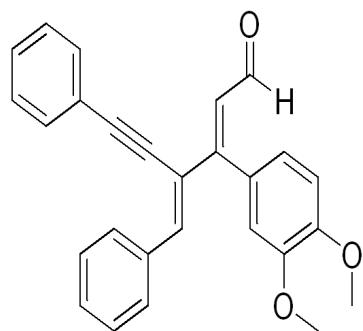
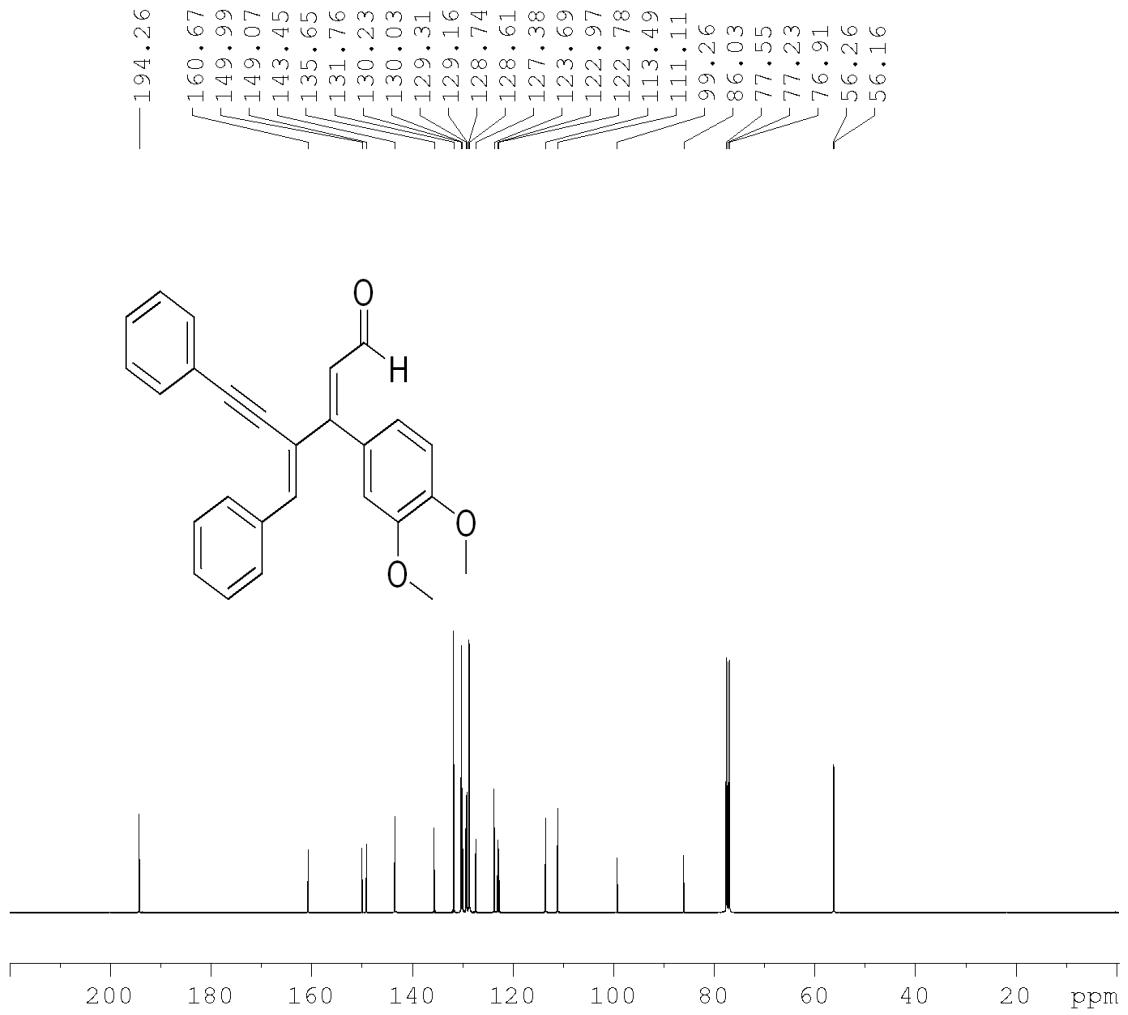
Current Data Parameters  
 NAME lio-1  
 EXPNO 115  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20131006  
 Time 21.06  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 114  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 299.3 K  
 D1 2.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 11.90 usec  
 PL1 3.00 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300102 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(E)-4-((E)-benzylidene)-3-(3,4-dimethoxyphenyl)-6-phenylhex-2-en-5-yneal (4m)



Current Data Parameters  
 NAME lio-1  
 EXPNO 116  
 PROCNO 1

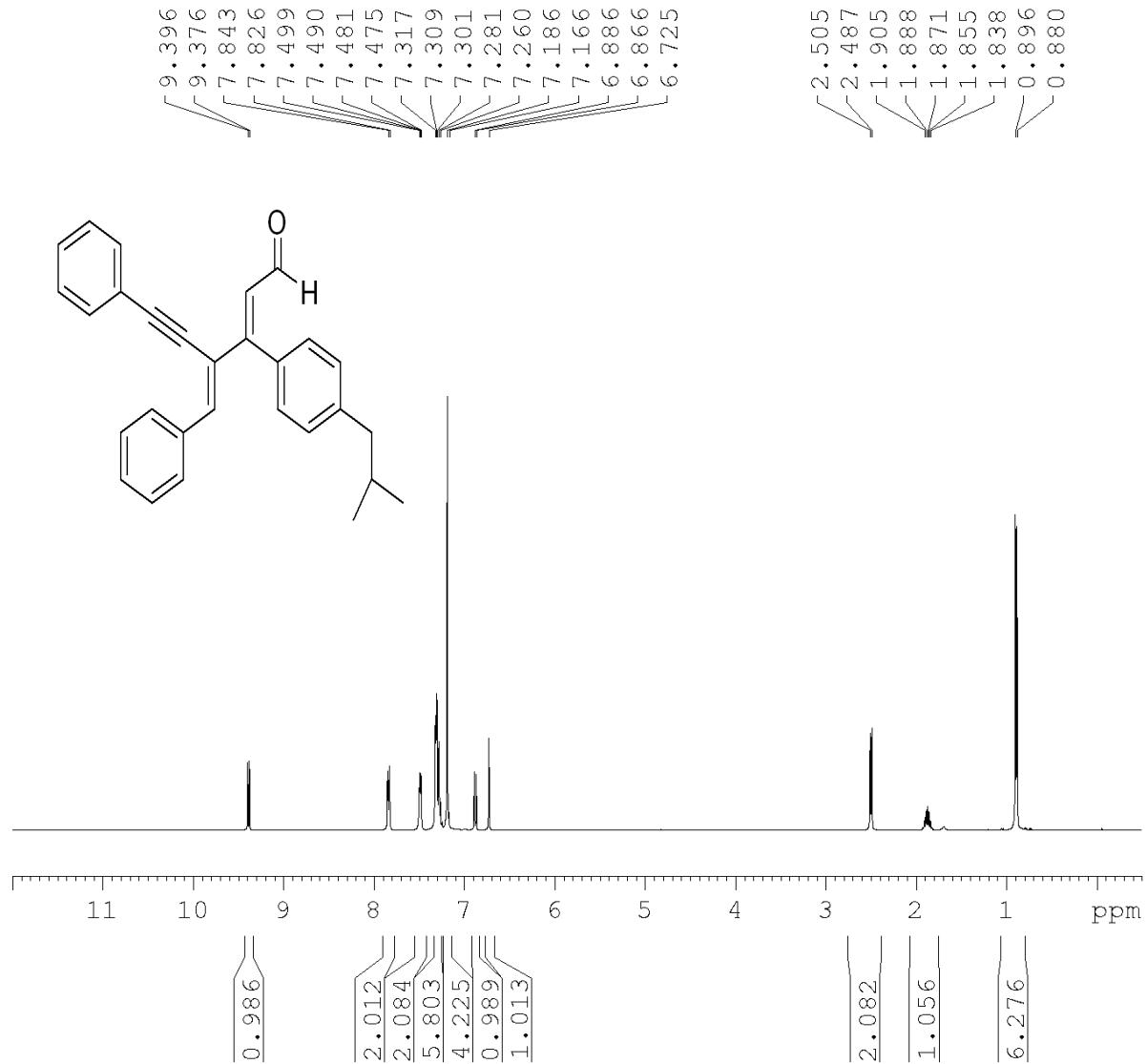
F2 - Acquisition Parameters  
 Date\_ 20131006  
 Time 23.47  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 11118  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 8192  
 DW 20.800 use  
 DE 6.50 use  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====:  
 NUC1 <sup>13</sup>C  
 P1 10.50 use:  
 PL1 7.00 dB  
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====:  
 CPDPRG[2] waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 90.00 use  
 PL2 -0.60 dB  
 PL12 15.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127532 MHz

(E)-4-((E)-benzylidene)-3-(4-isobutylphenyl)-6-phenylhex-2-en-5-ynal (4n)



Current Data Parameters

NAME lio-1  
EXPNO 121  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20130917  
Time 23.31  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 0  
SWH 7246.377 Hz  
FIDRES 0.221142 Hz  
AQ 2.2609921 sec  
RG 35.9  
DW 69.000 usec  
DE 6.50 usec  
TE 299.2 K  
D1 2.0000000 sec  
TDO 1

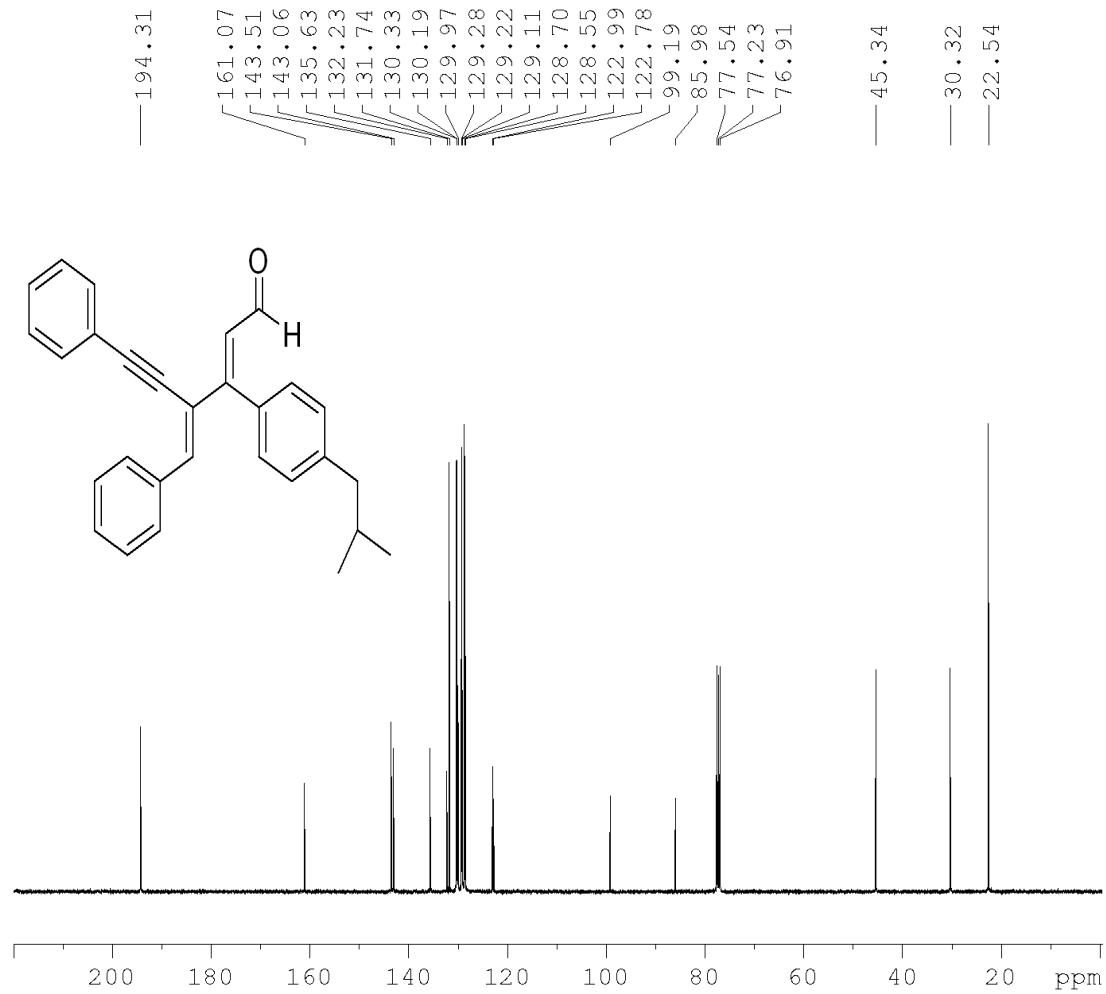
===== CHANNEL f1 =====

NUC1 1H  
P1 11.90 usec  
PL1 3.00 dB  
SFO1 400.1324008 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300468 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

(E)-4-((E)-benzylidene)-3-(4-isobutylphenyl)-6-phenylhex-2-en-5-yneal (4n)



Current	Data	Parameters
NAME		lio-1
EXPNO		122
PROCNO		1

```

F2 - Acquisition Parameters
Date_          20130917
Time           23.32
INSTRUM        spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD             32768
SOLVENT        CDCl3
NS              592
DS                 0
SWH            24038.461 Hz
FIDRES        0.733596 Hz
AQ             0.6815744 sec
RG               8192
DW             20.800 usec
DE               6.50 usec
TE              299.2 K
D1      2.00000000 sec
D11             0.03000000 sec
TDO                 1

```

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.40 use  
PL1 7.00 dB  
SEQ1 100.6233325 MHz

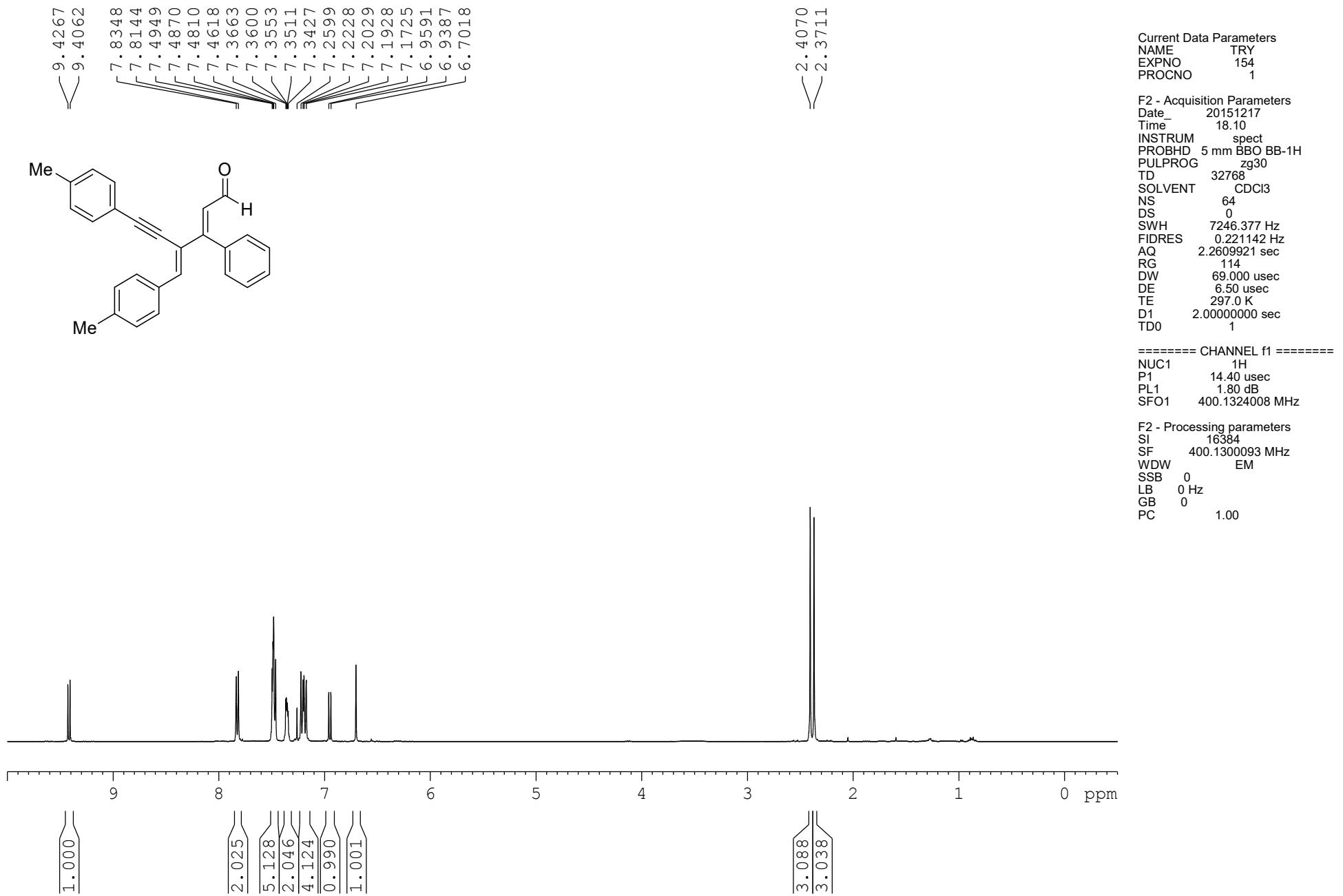
```

===== CHANNEL f2 =====
CPDPRG[2          waltz16
NUC2              1H
PCPD2             90.00 use
PL2               3.00 dB
PL12              20.70 dB
PL13              23.70 dB
SFO2             400.1316005 MHz

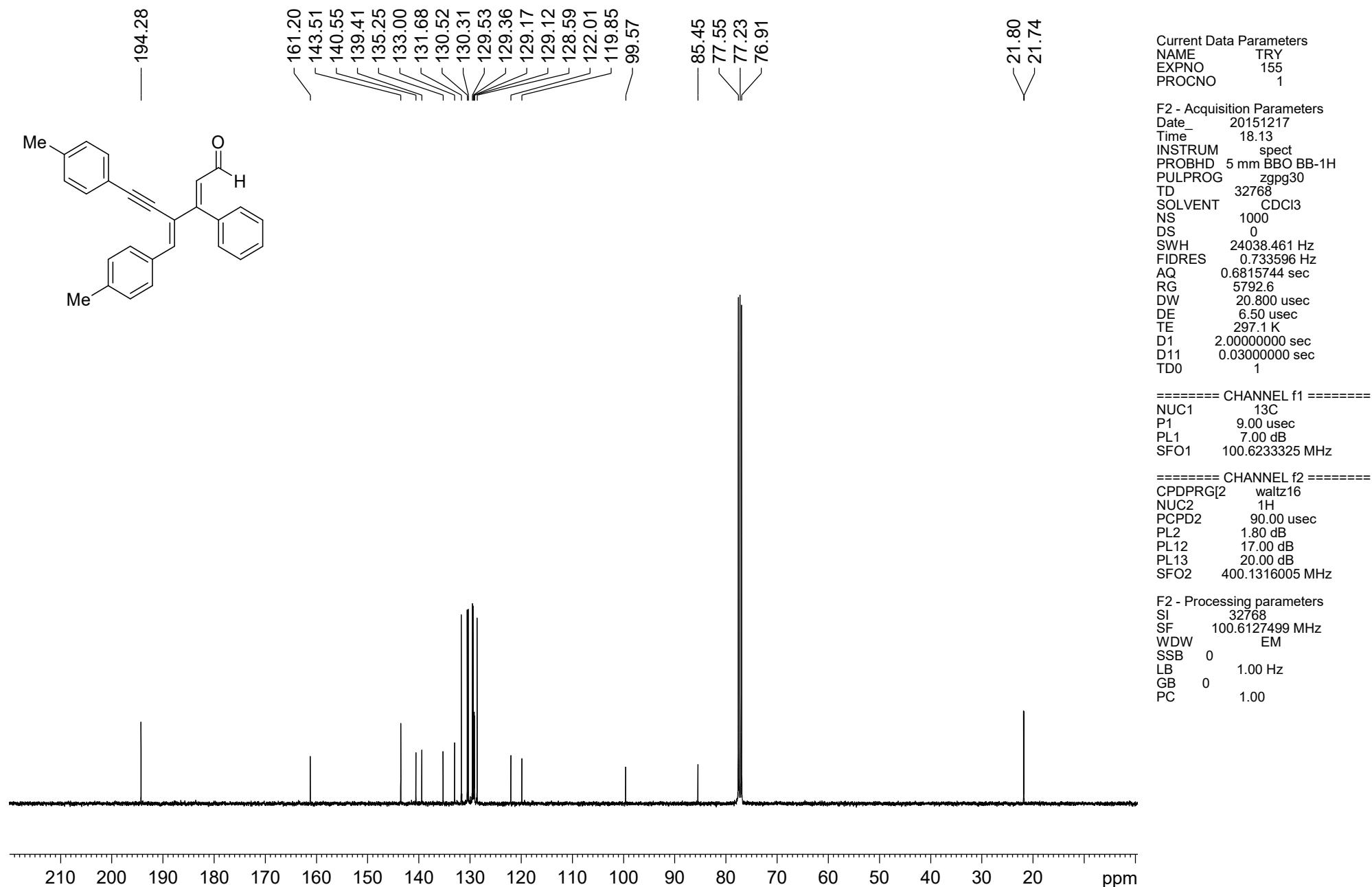
```

F2 - Processing parameters  
SI 32768  
SF 100.6127587 MHz

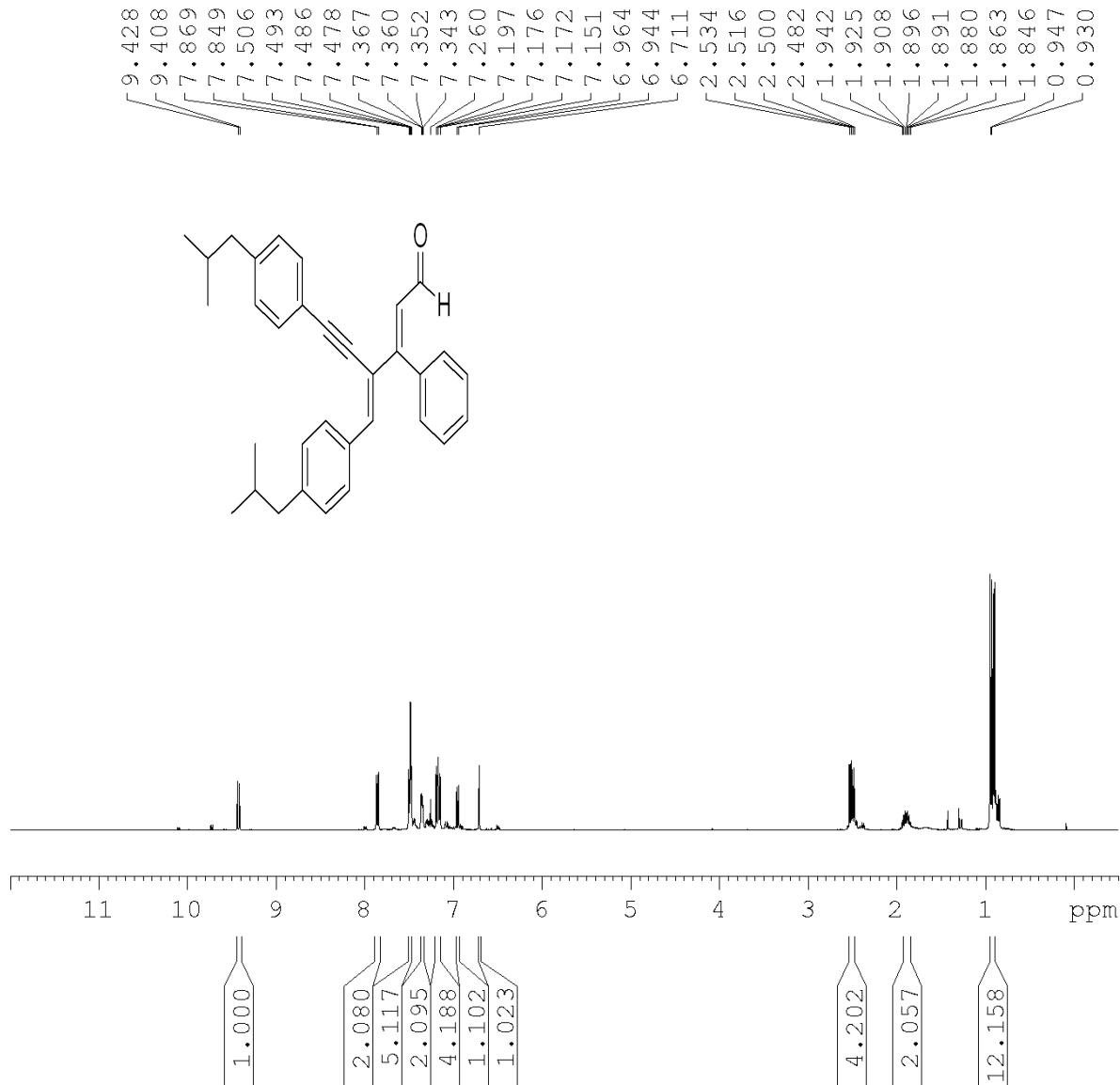
(2E,4E)-4-(4-methylbenzylidene)-3-phenyl-6-(p-tolyl)hex-2-en-5-ynal (4o)



(2E, 4E)-4-(4-methylbenzylidene)-3-phenyl-6-(p-tolyl)hex-2-en-5-yneal (4o)



(E)-4-((E)-4-isobutylbenzylidene)-6-(4-isobutylphenyl)-3-phenylhex-2-en-5-yneal (4p)



Current	Data	Parameters
NAME	v1	
EXPNO	689	
PROCNO	1	

```

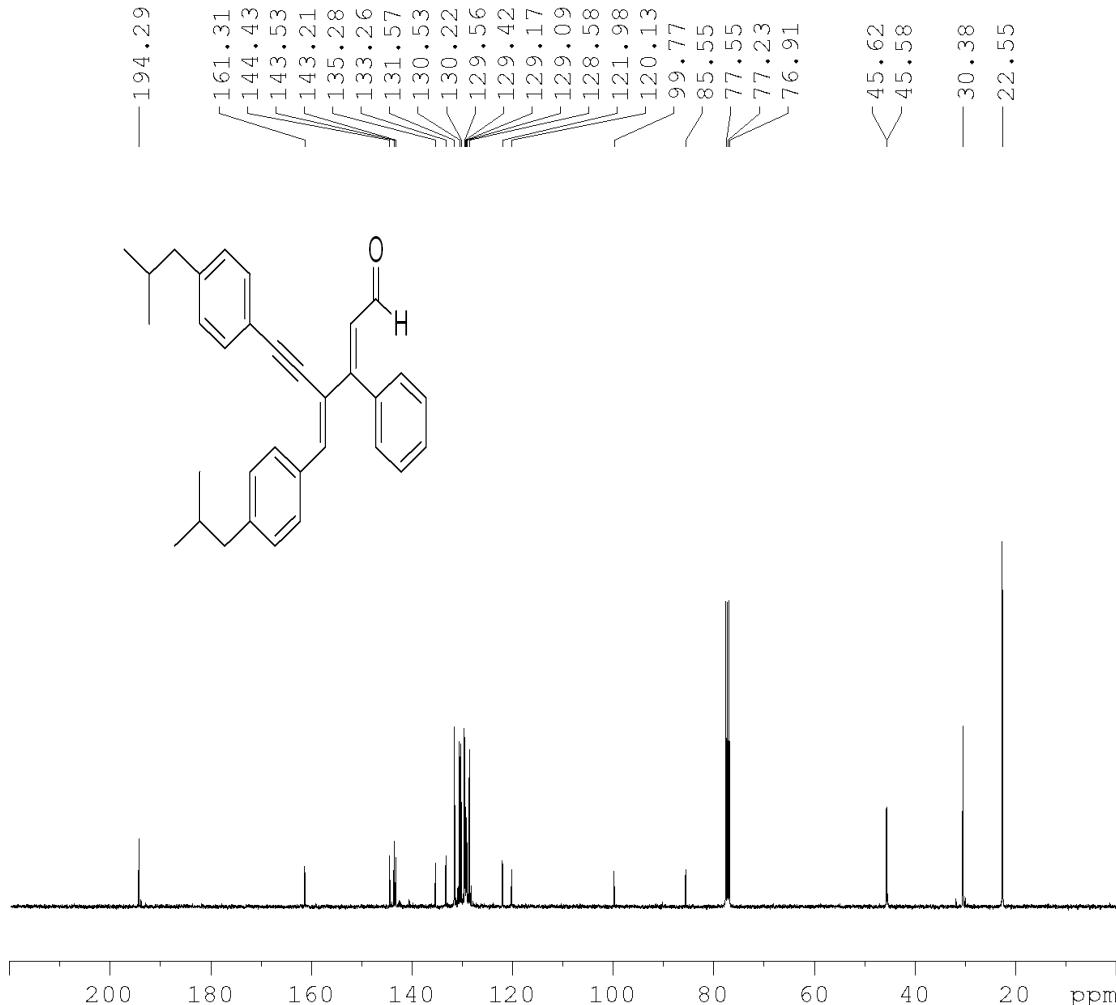
F2 - Acquisition Parameters
Date_          20160828
Time           22.53
INSTRUM        spect
PROBHD         5 mm PABBO BB/
PULPROG        zg30
TD             32768
SOLVENT        CDC13
NS              4
DS              0
SWH             7211.539 Hz
FIDRES         0.220079 Hz
AQ              2.2719147 sec
RG              57.42
DW              69.333 usec
DE              10.50 usec
TE              298.3 K
D1              2.00000000 sec
TD0              1

```

===== CHANNEL f1 =====  
SFO1 400.1324008 MHz  
NUC1 1H  
P1 12.90 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1300102 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

(E)-4-((E)-4-isobutylbenzylidene)-6-(4-isobutylphenyl)-3-phenylhex-2-en-5-yneal (4p)



Current Data Parameters

NAME vl  
EXPNO 690  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20160828  
Time 22.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 800  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 198.09  
DW 20.800 use  
DE 6.50 use  
TE 298.4 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TDO 1

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

SFO1 100.6228298 MHz  
NUC1 13C  
P1 10.00 use  
PLW1 47.50000000 W

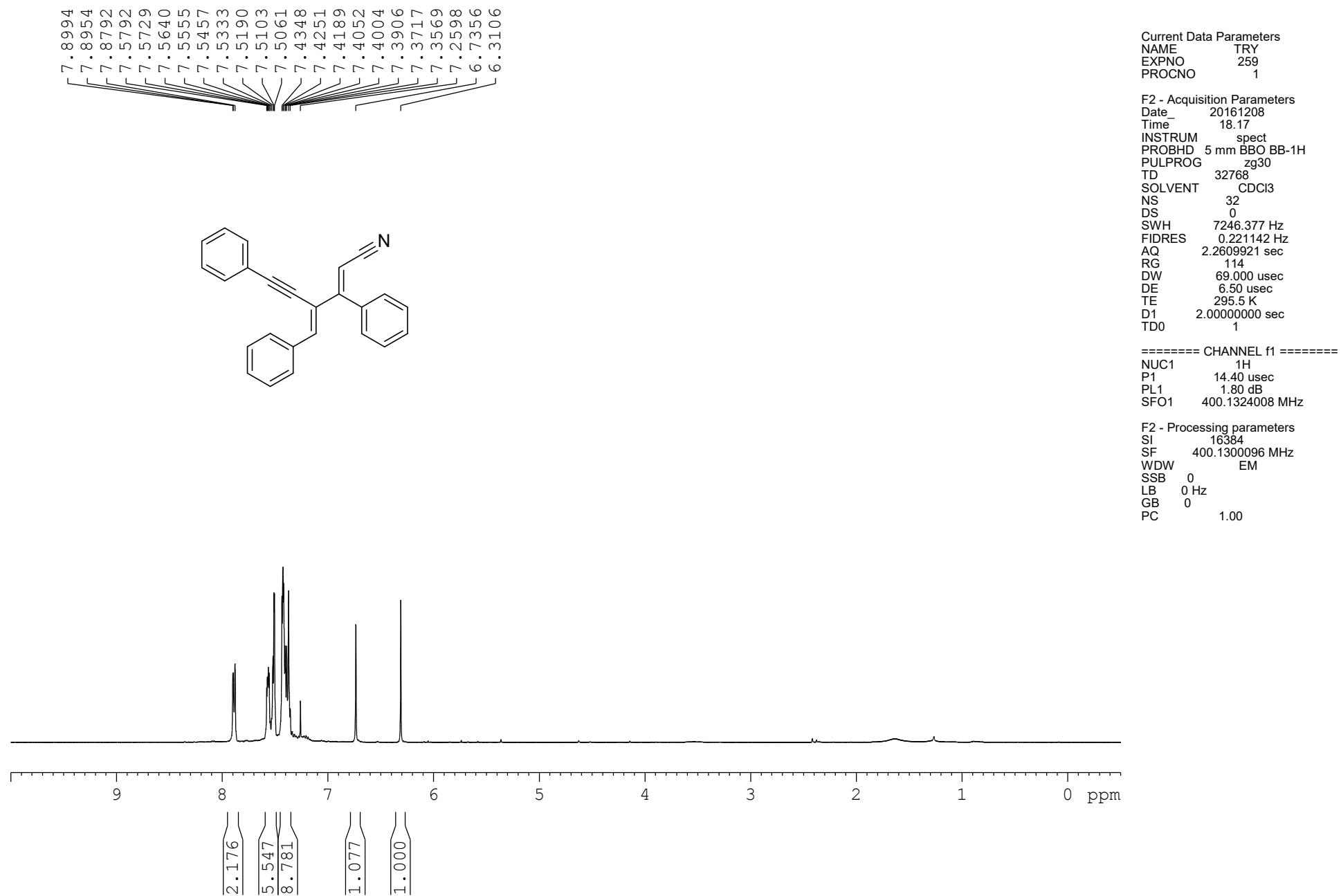
===== CHANNEL f2 =====

SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 use  
PLW2 15.00000000 W  
PLW12 0.33750001 W  
PLW13 0.27338001 W

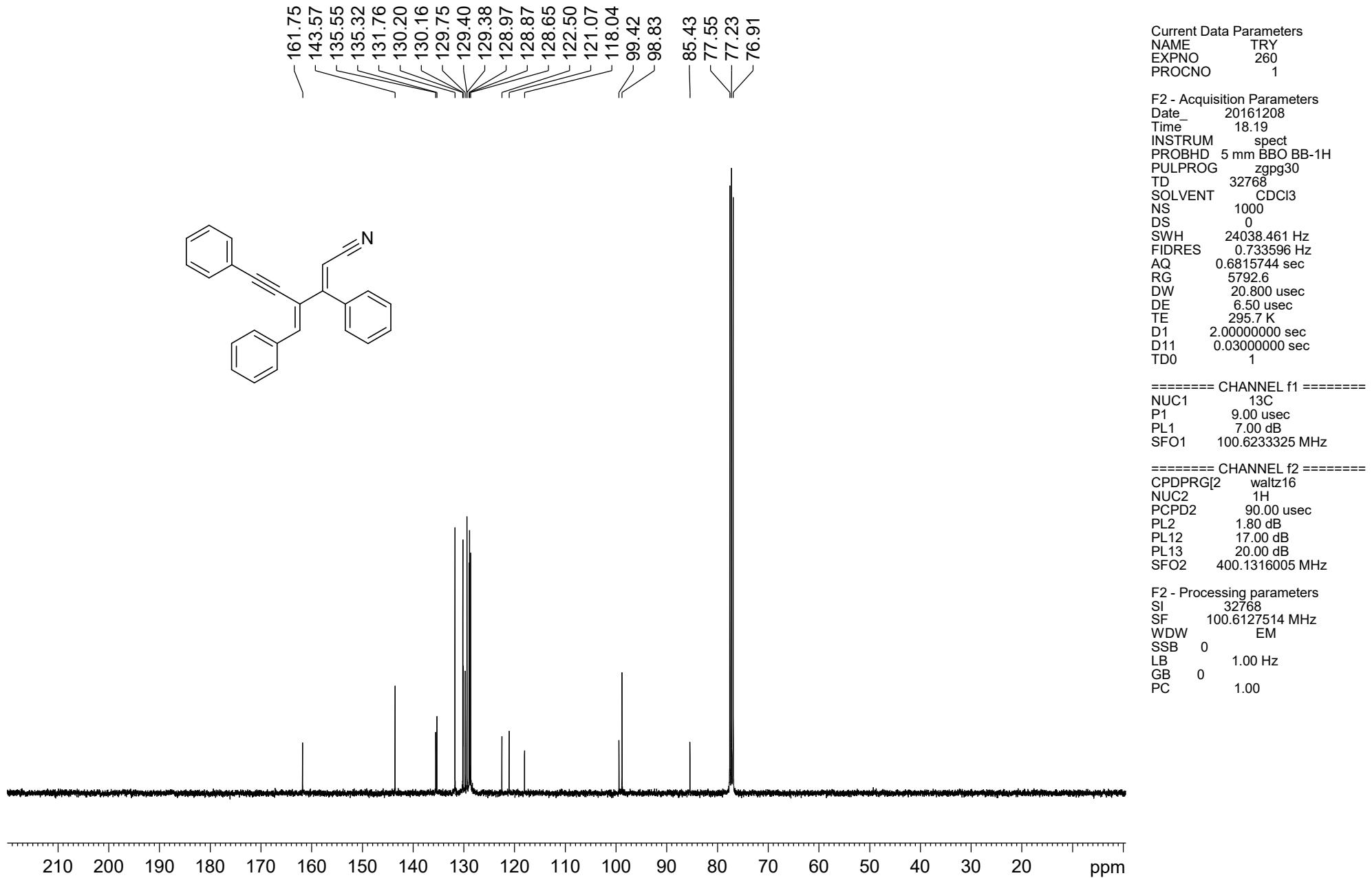
F2 - Processing parameters

SI 32768  
SF 100.6127501 MHz

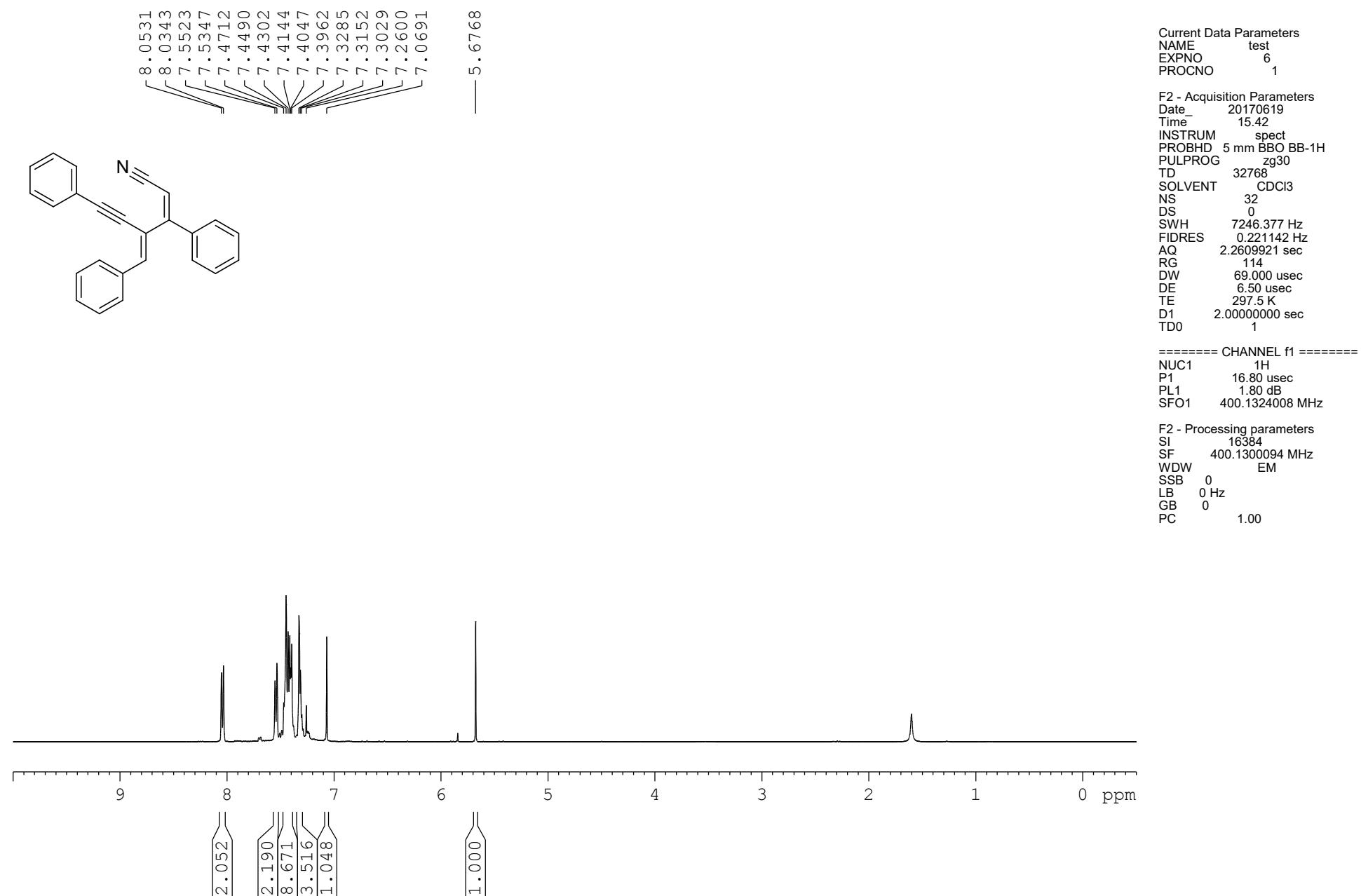
(2E,4E)-4-benzylidene-3,6-diphenylhex-2-en-5-yenenitrile (6a)



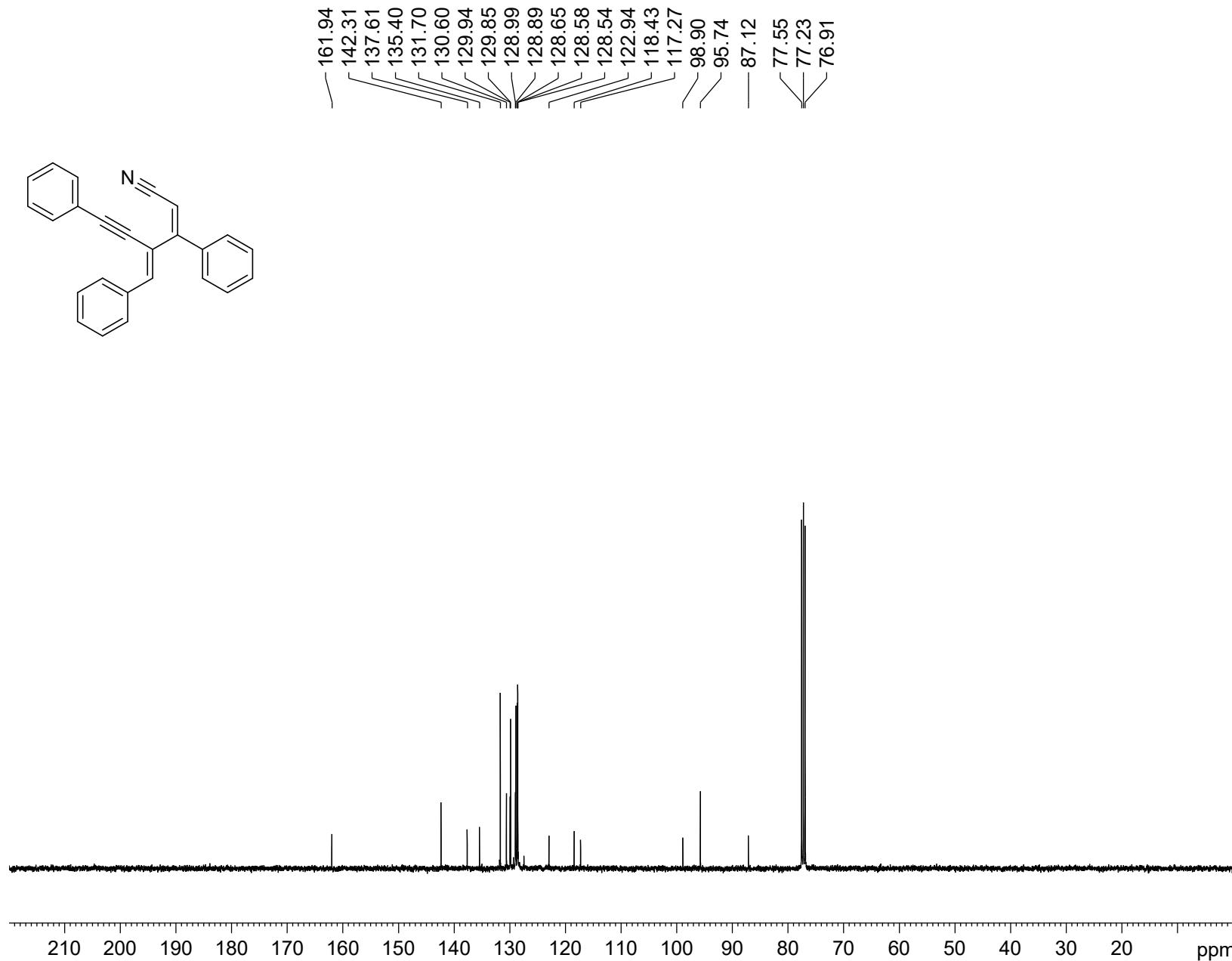
(2E,4E)-4-benzylidene-3,6-diphenylhex-2-en-5-ynenitrile (6a)



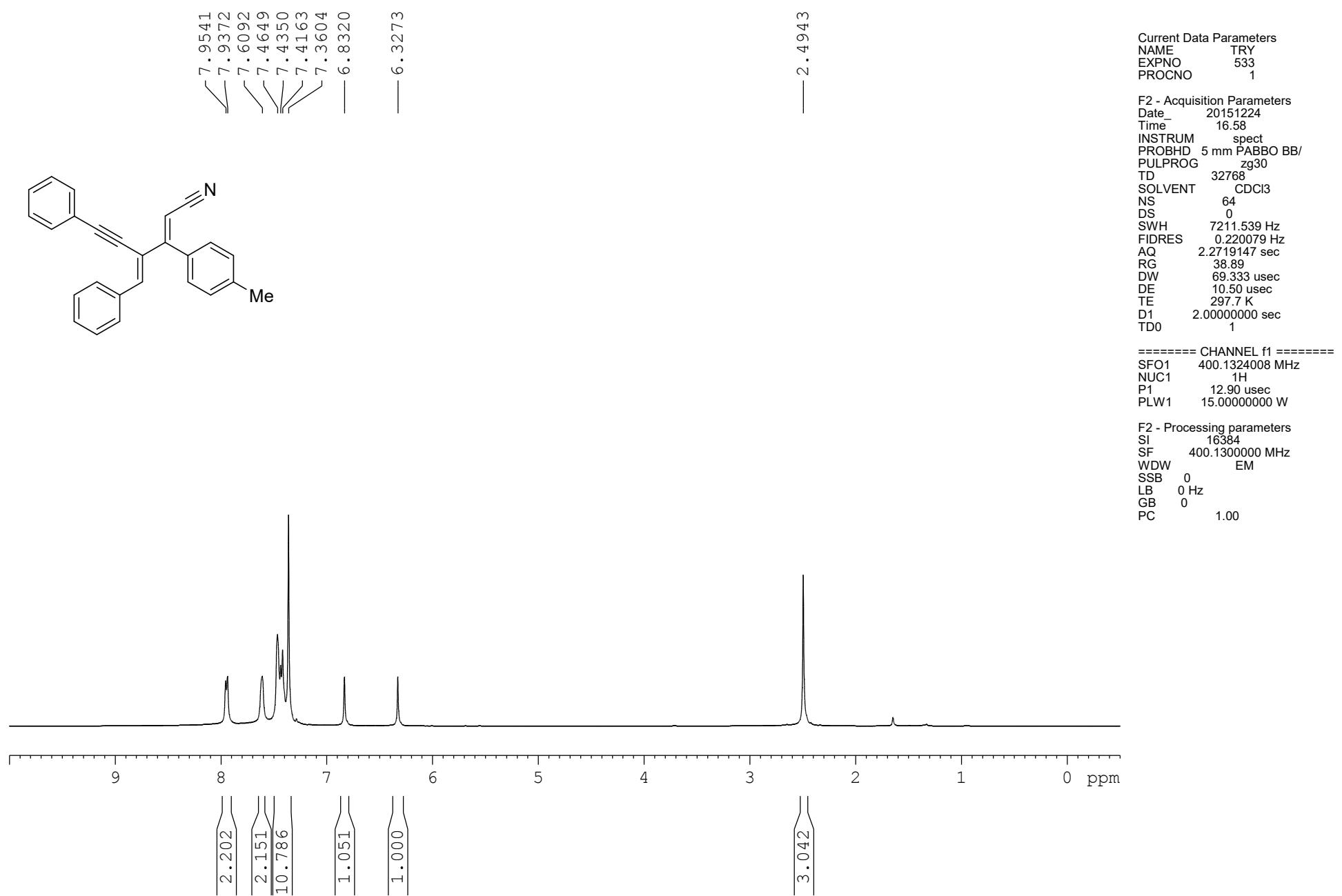
(2Z,4E)-4-benzylidene-3,6-diphenylhex-2-en-5-ynenitrile (6'a)



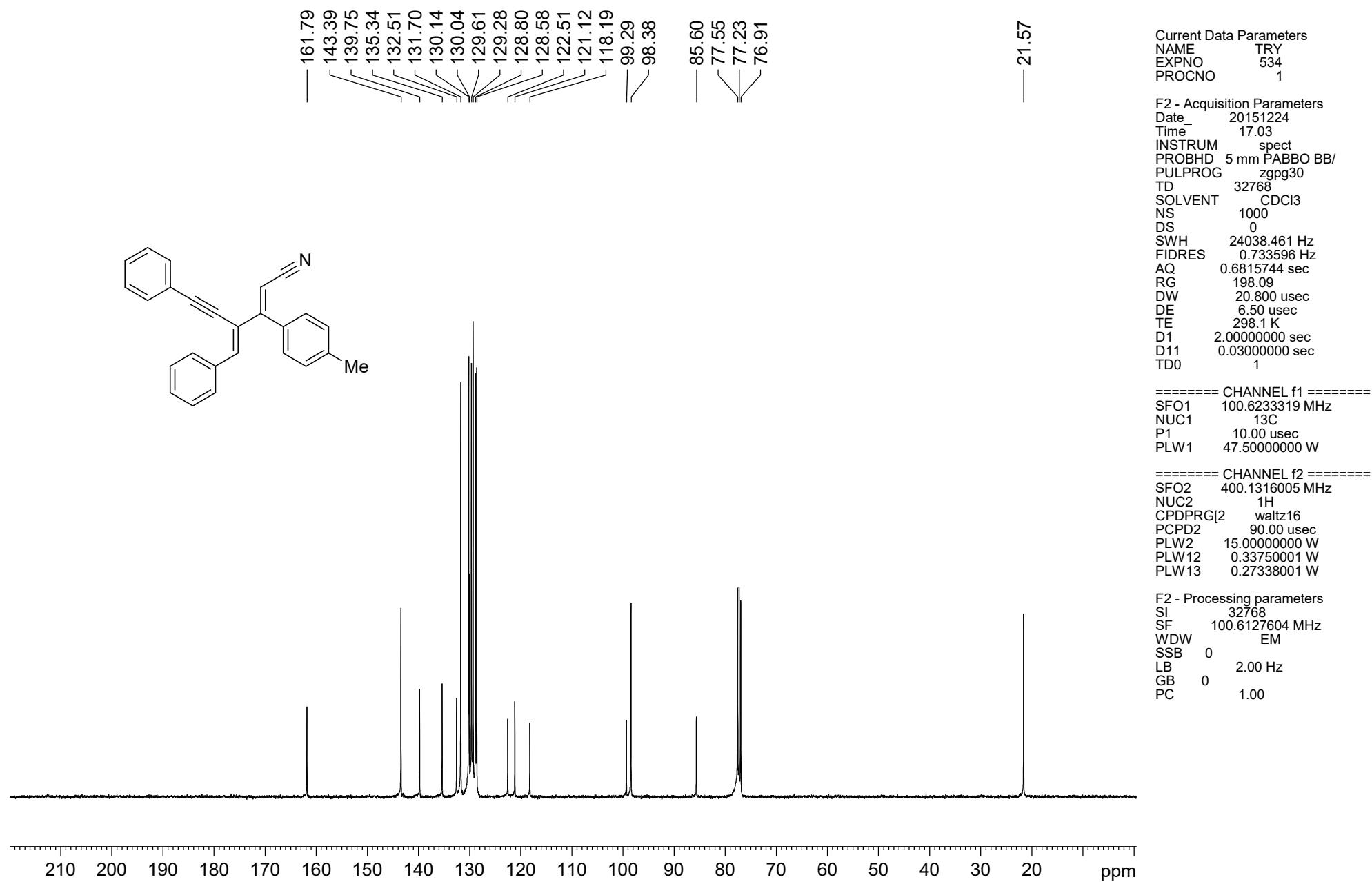
(2Z,4E)-4-benzylidene-3,6-diphenylhex-2-en-5-ynenitrile (6'a)



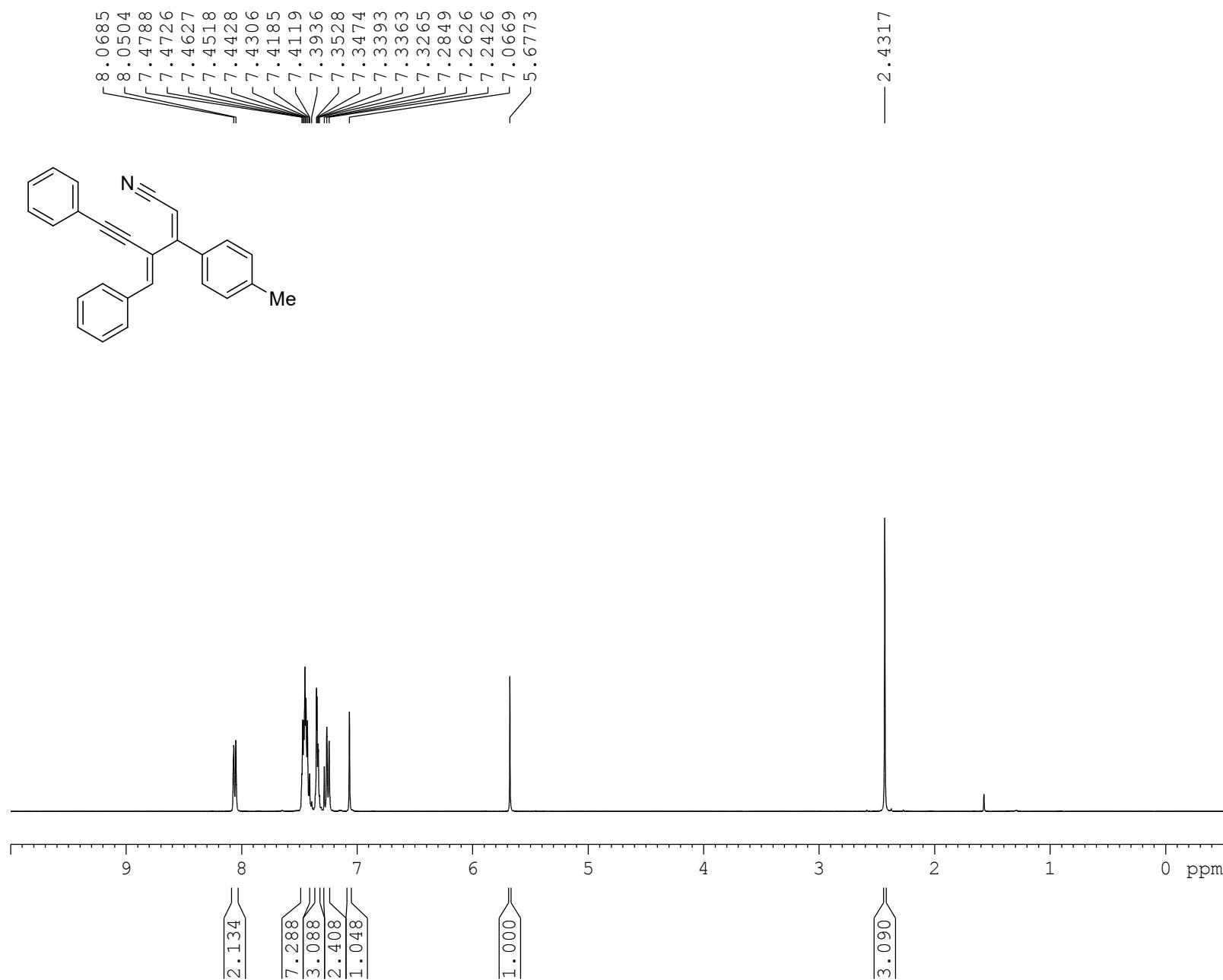
(2E, 4E)-4-benzylidene-6-phenyl-3-(p-tolyl)hex-2-en-5-ynenitrile (6b)



(2E, 4E)-4-benzylidene-6-phenyl-3-(p-tolyl)hex-2-en-5-ynenitrile (6b)



(2Z,4E)-4-benzylidene-6-phenyl-3-(p-tolyl)hex-2-en-5-ynenitrile (6'b)



Current Data Parameters  
 NAME TRY  
 EXPNO 607  
 PROCNO 1

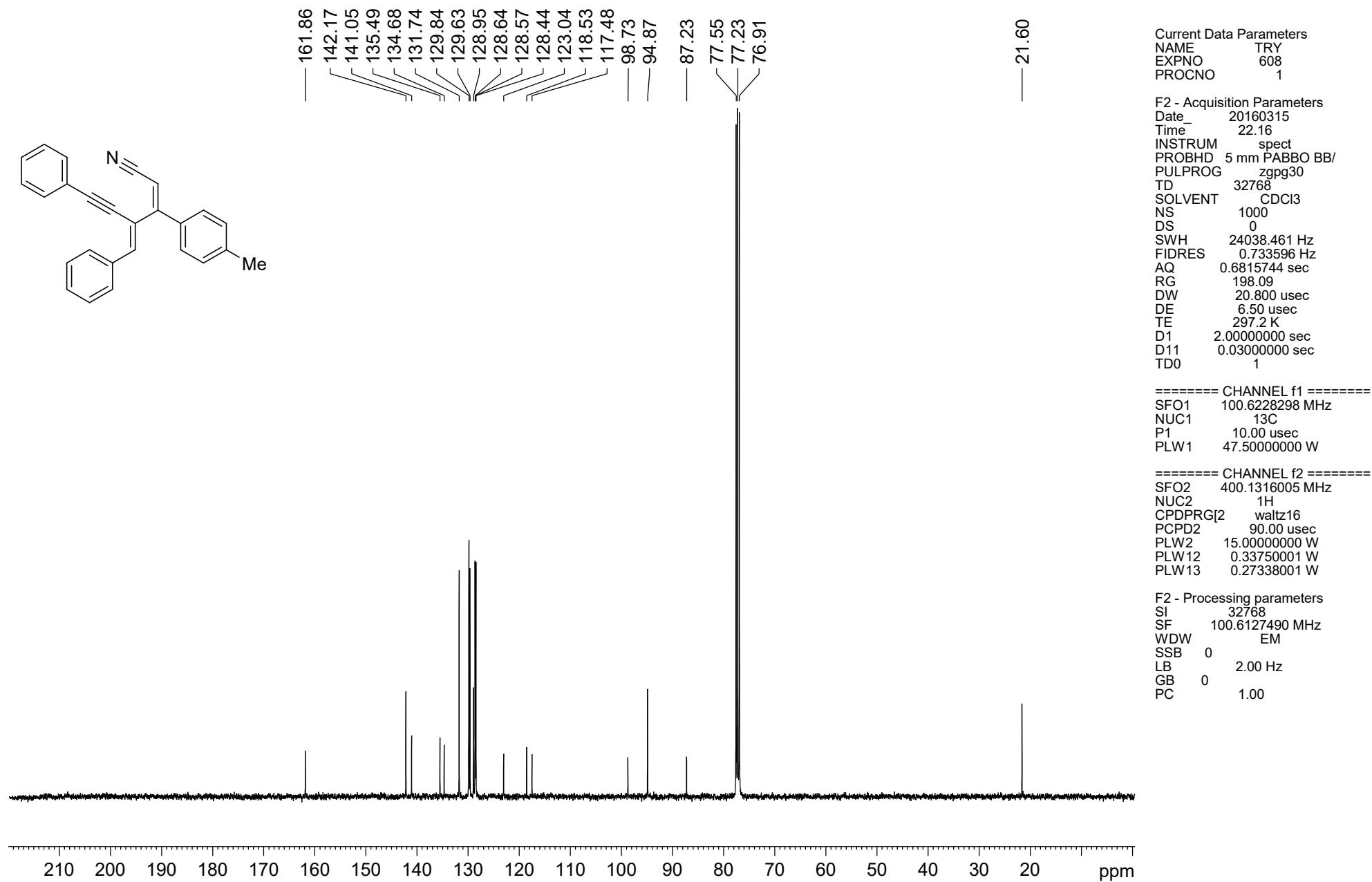
F2 - Acquisition Parameters  
 Date 20160315  
 Time 22.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 34  
 DS 0  
 SWH 7211.539 Hz  
 FIDRES 0.220079 Hz  
 AQ 2.2719147 sec  
 RG 113.31  
 DW 69.333 usec  
 DE 10.50 usec  
 TE 296.8 K  
 D1 2.0000000 sec  
 TDO 1

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

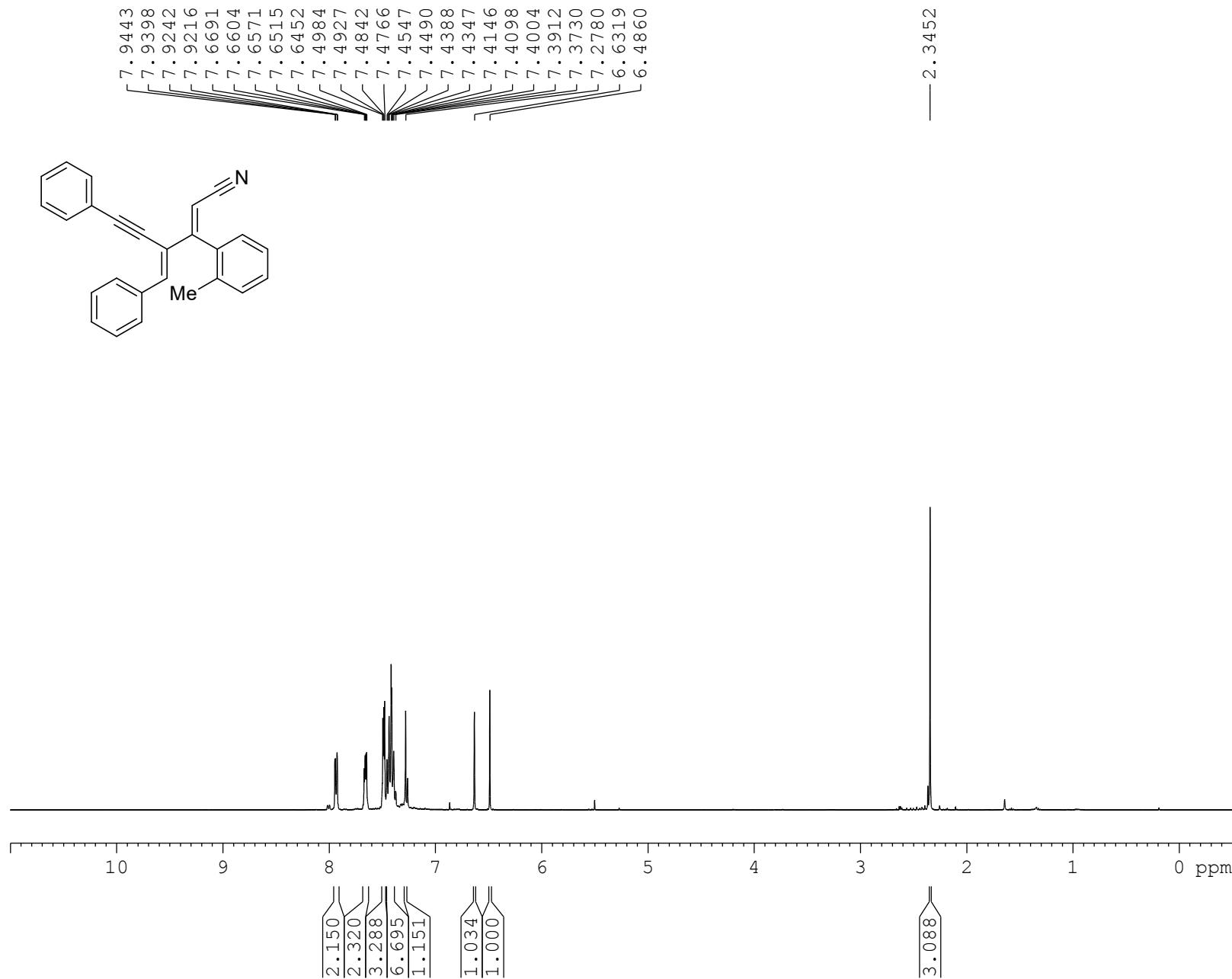
SFO1 400.1324008 MHz  
 NUC1 1H  
 P1 12.90 usec  
 PLW1 15.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2Z,4E)-4-benzylidene-6-phenyl-3-(p-tolyl)hex-2-en-5-ynenitrile (6'b)



(2E, 4E)-4-benzylidene-6-phenyl-3-(o-tolyl)hex-2-en-5-ynenitrile (6c)



Current Data Parameters  
 NAME TRY  
 EXPNO 614  
 PROCNO 1

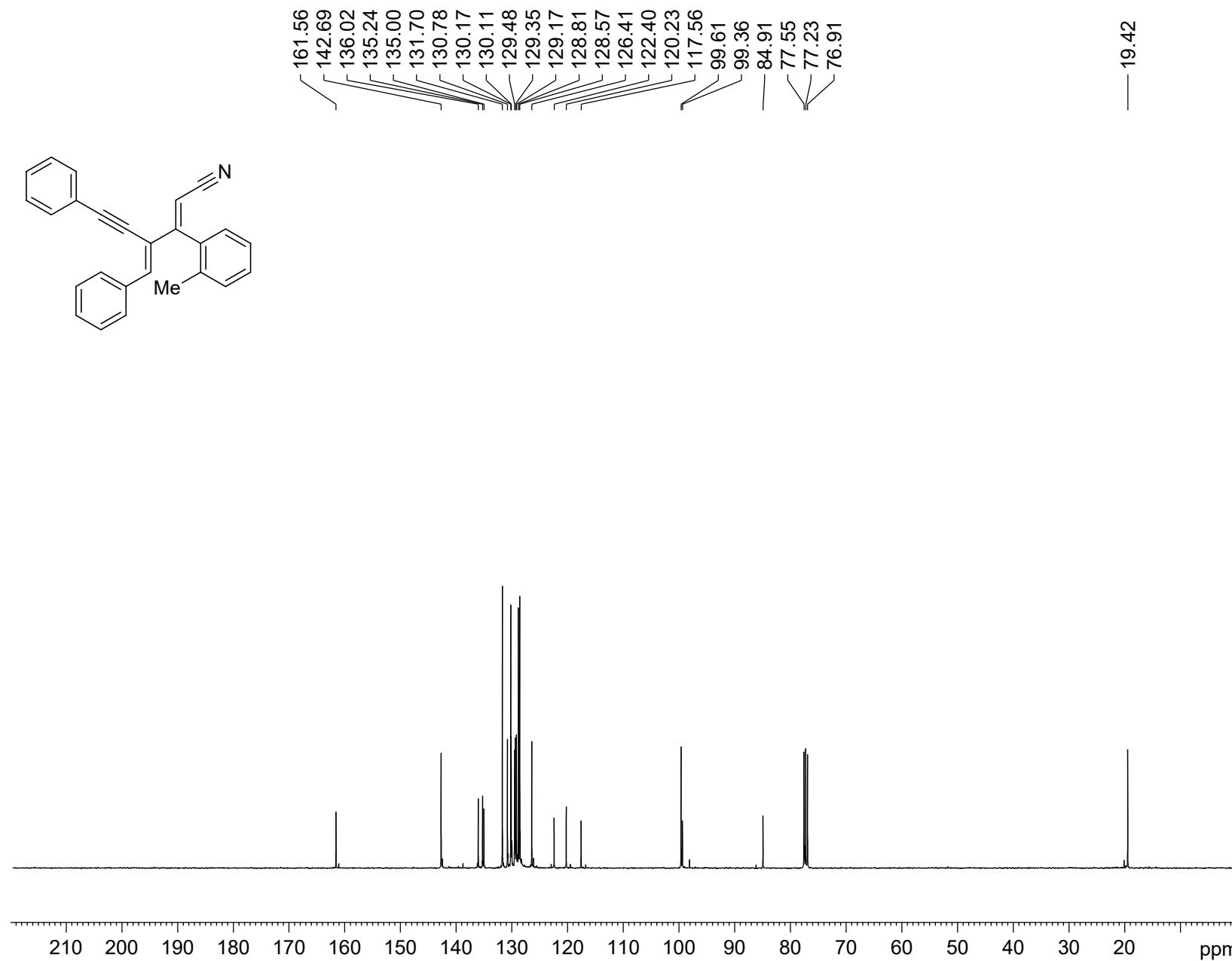
F2 - Acquisition Parameters  
 Date 20160315  
 Time 23.30  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 32  
 DS 0  
 SWH 7211.539 Hz  
 FIDRES 0.220079 Hz  
 AQ 2.2719147 sec  
 RG 29.06  
 DW 69.333 usec  
 DE 10.50 usec  
 TE 297.0 K  
 D1 2.0000000 sec  
 TDO 1

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

SFO1 400.1324008 MHz  
 NUC1 1H  
 P1 12.90 usec  
 PLW1 15.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 400.1300027 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2E, 4E)-4-benzylidene-6-phenyl-3-(o-tolyl)hex-2-en-5-ynenitrile (6c)



Current Data Parameters  
 NAME TRY  
 EXPNO 615  
 PROCNO 1

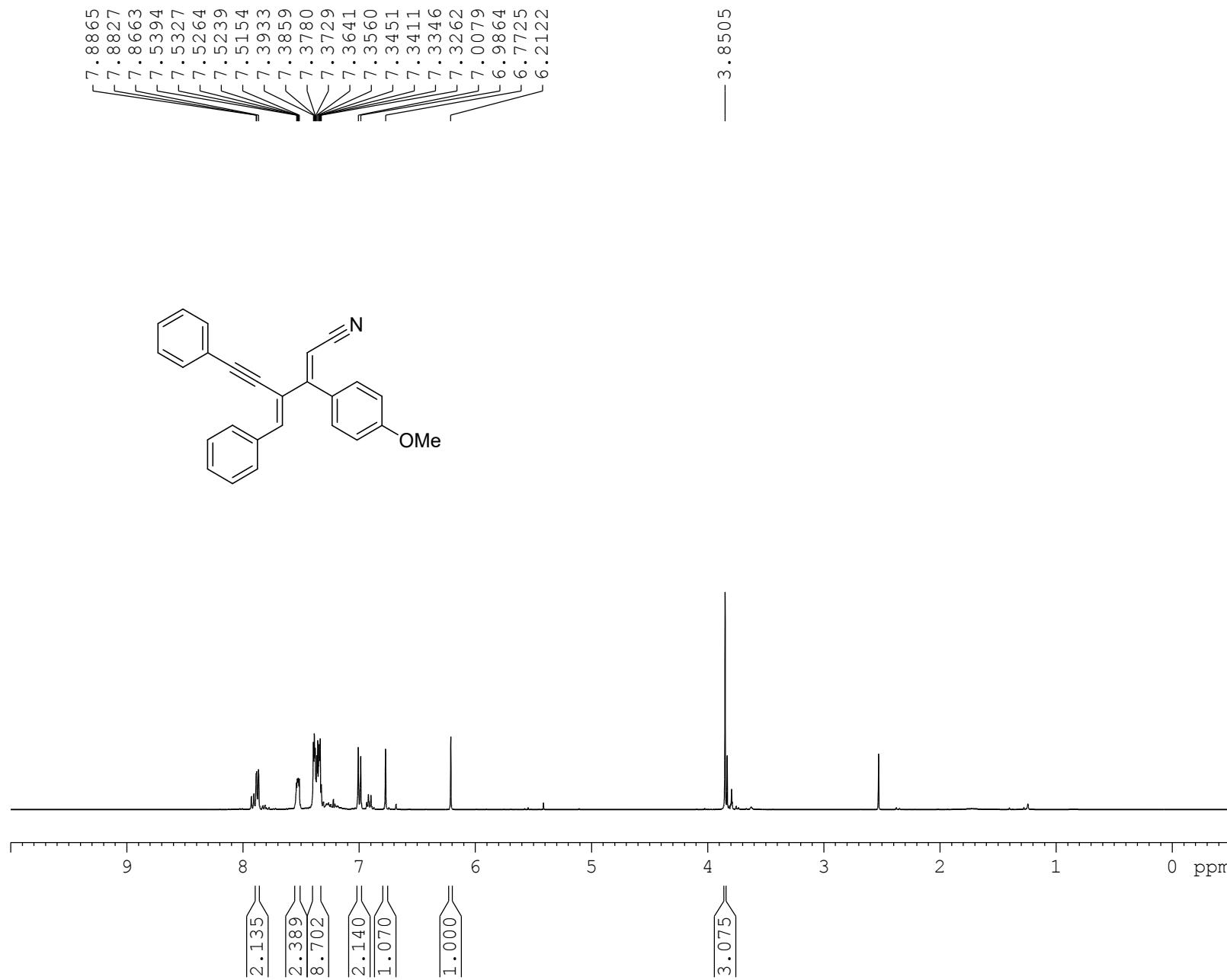
F2 - Acquisition Parameters  
 Date 20160315  
 Time 23.34  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 841  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 198.09  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 47.5000000 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.27338001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127659 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 1.00

(2E, 4E)-4-benzylidene-3-(4-methoxyphenyl)-6-phenylhex-2-en-5-ynenitrile (6d)



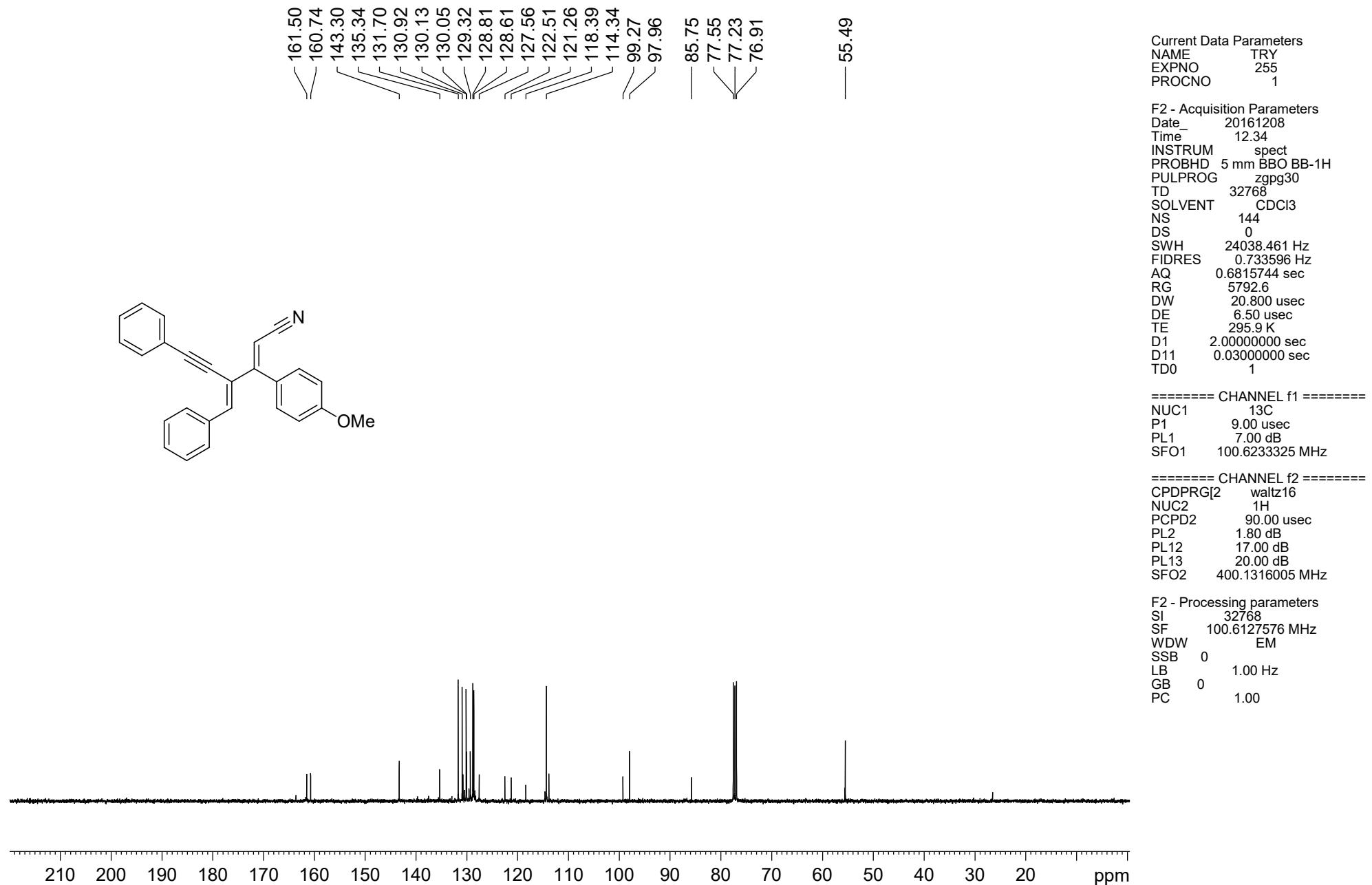
Current Data Parameters  
 NAME TRY  
 EXPNO 254  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20161208  
 Time 12.26  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 64  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 295.8 K  
 D1 2.0000000 sec  
 TDO 1

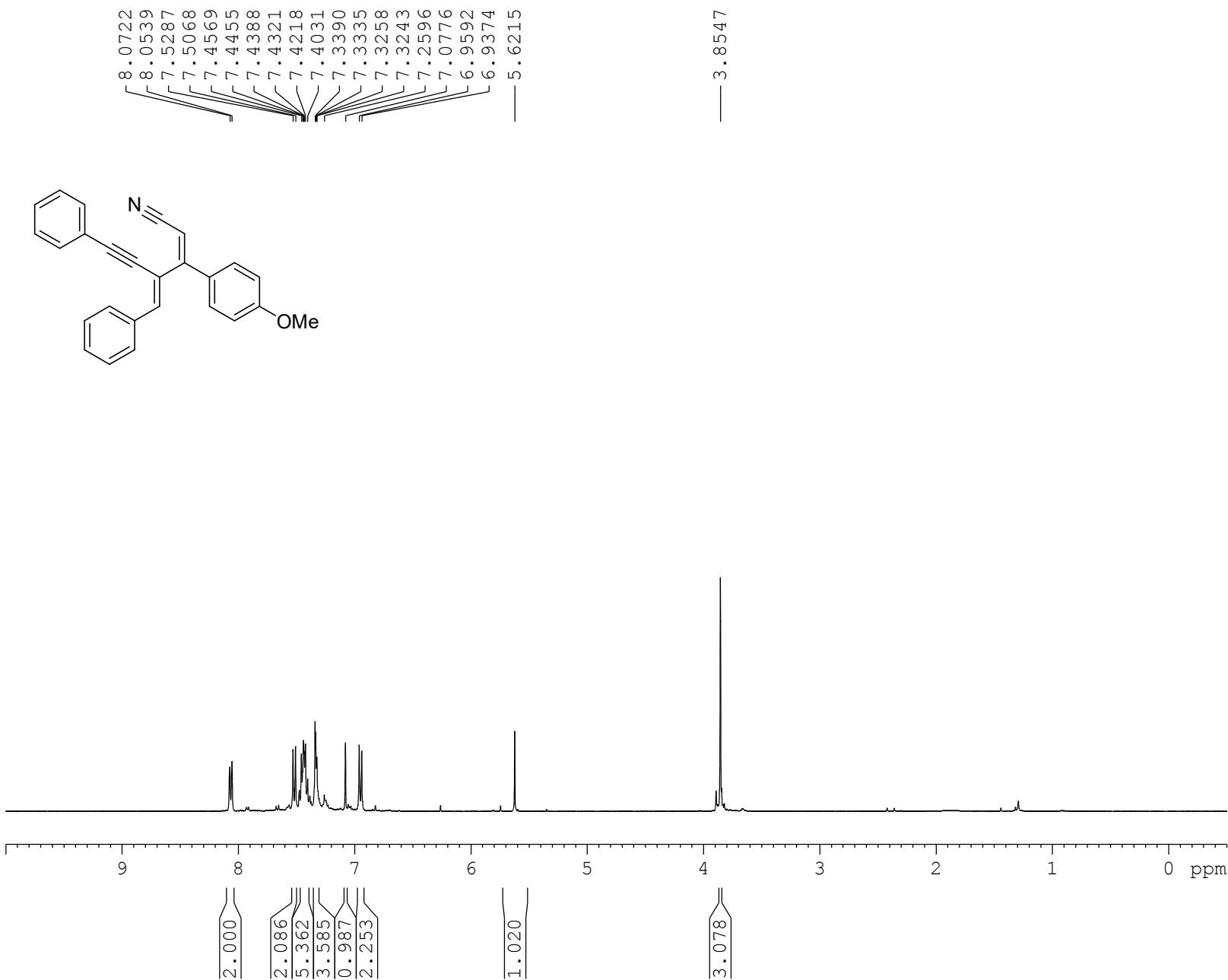
===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 P1 14.40 usec  
 PL1 1.80 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300246 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2E,4E)-4-benzylidene-3-(4-methoxyphenyl)-6-phenylhex-2-en-5-ynenitrile (6d)



*(2Z,4E)-4-benzylidene-3-(4-methoxyphenyl)-6-phenylhex-2-en-5-ynenitrile (6'd)*



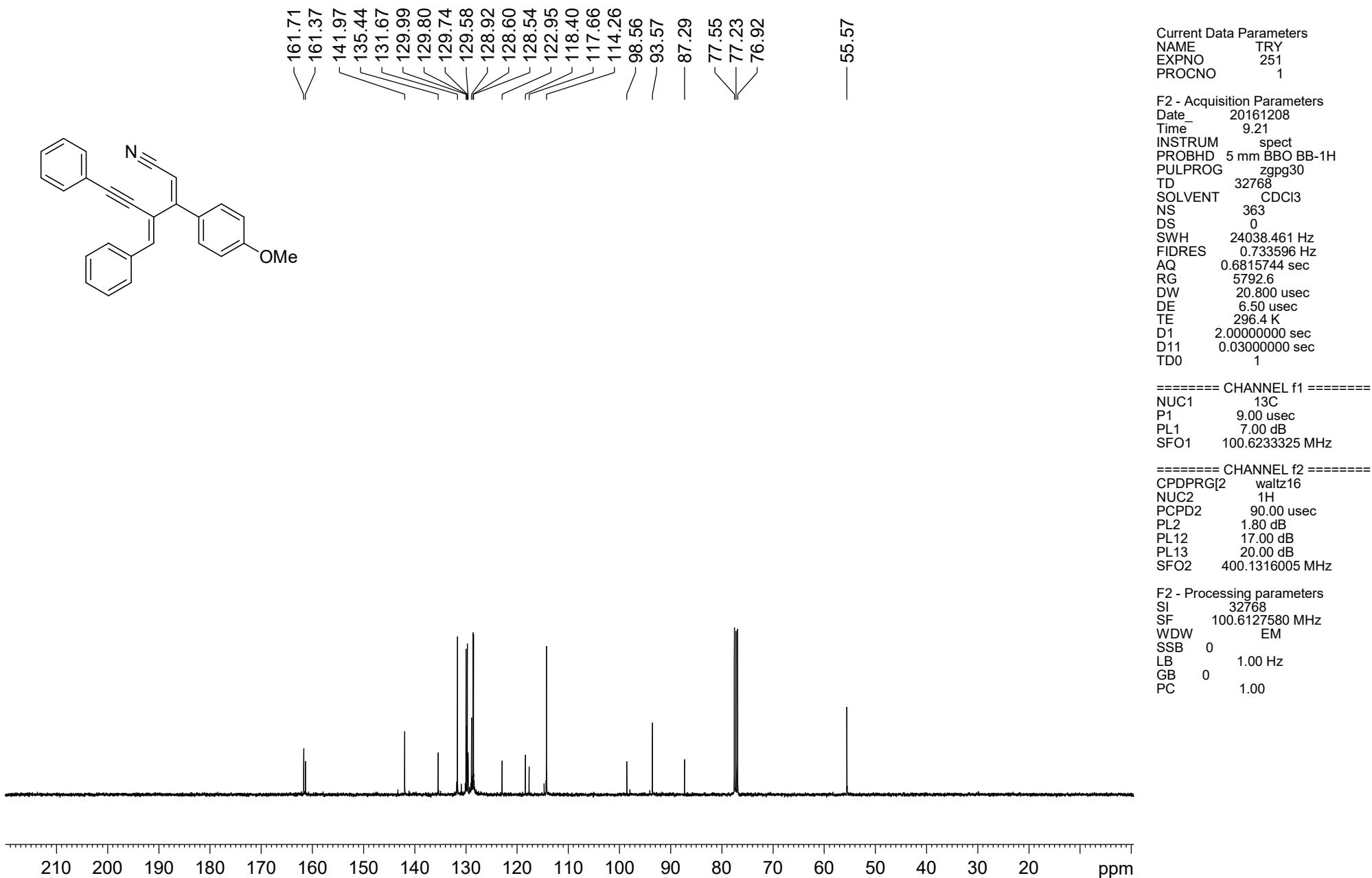
Current Data Parameters  
 NAME TRY  
 EXPNO 250  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20161208  
 Time 9.20  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 57  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 296.4 K  
 D1 2.0000000 sec  
 TDO 1

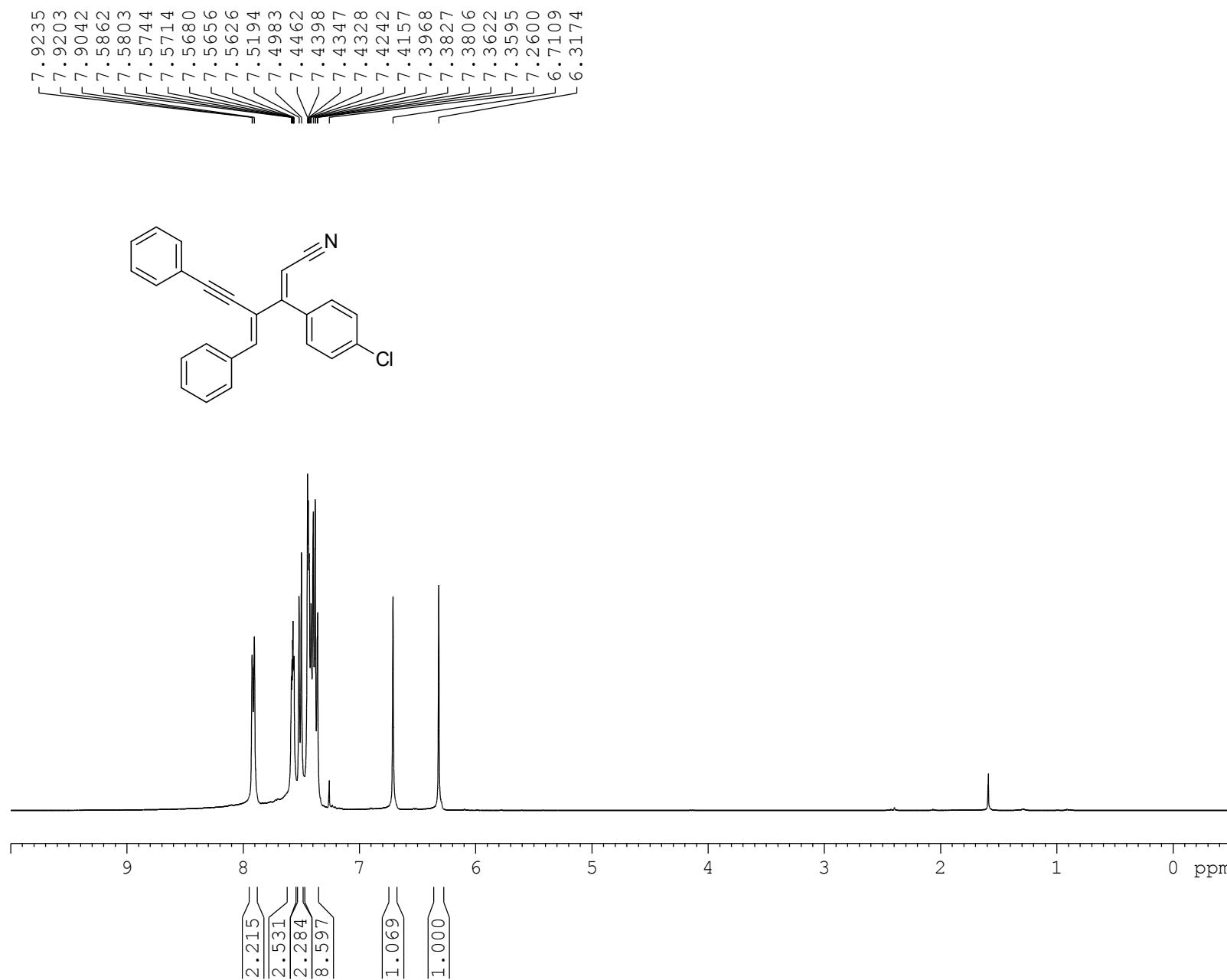
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.40 usec  
 PL1 1.80 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300091 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2Z,4E)-4-benzylidene-3-(4-methoxyphenyl)-6-phenylhex-2-en-5-ynenitrile (6'd)



(2E, 4E)-4-benzylidene-3-(4-chlorophenyl)-6-phenylhex-2-en-5-ynenitrile (6e)



Current Data Parameters  
NAME TRY  
EXPNO 529  
PROCNO 1

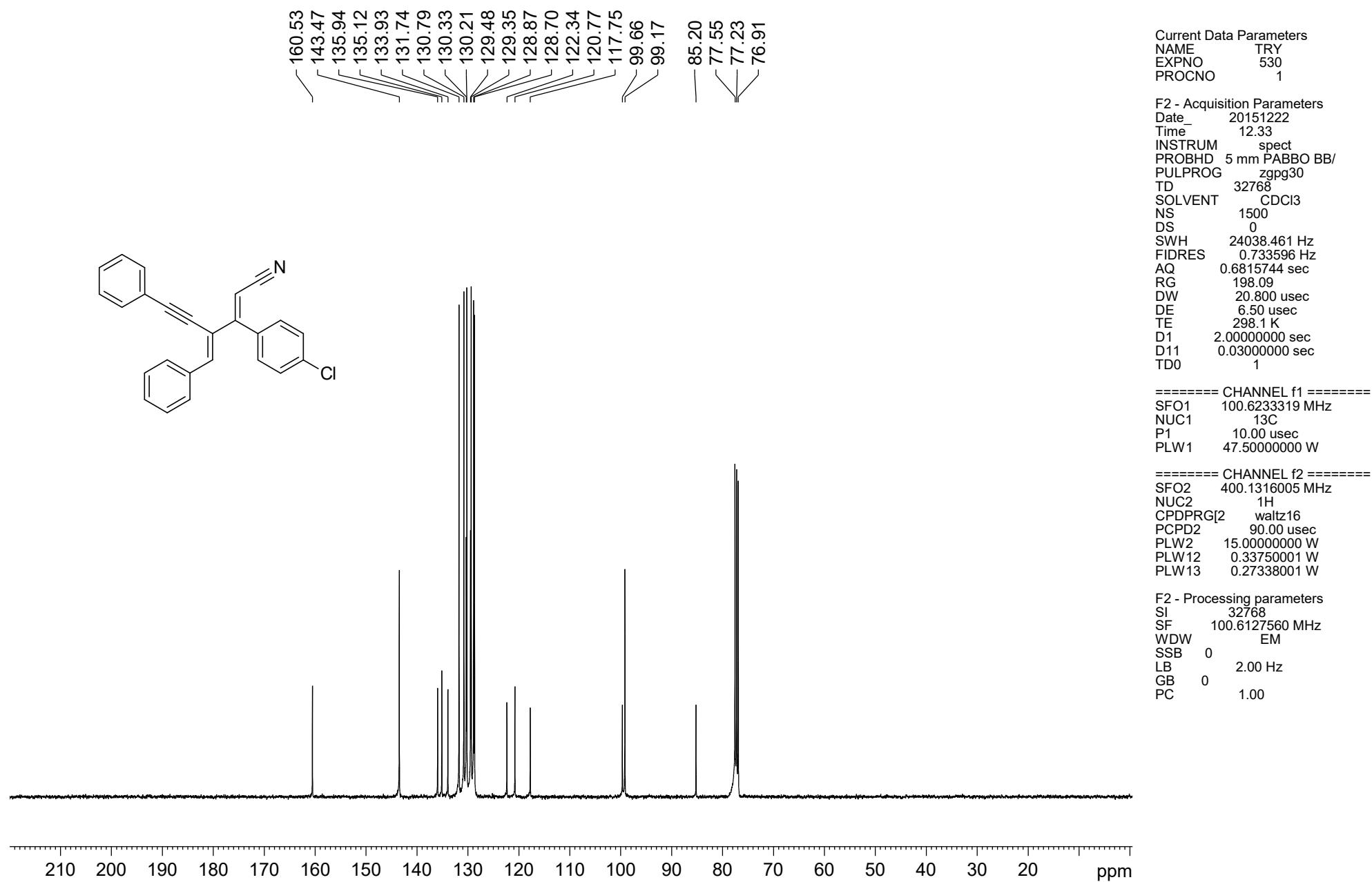
F2 - Acquisition Parameters  
Date 20151222  
Time 12.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 64  
DS 0  
SWH 7211.539 Hz  
FIDRES 0.220079 Hz  
AQ 2.2719147 sec  
RG 57.42  
DW 69.333 usec  
DE 10.50 usec  
TE 297.6 K  
D1 2.0000000 sec  
TDO 1

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

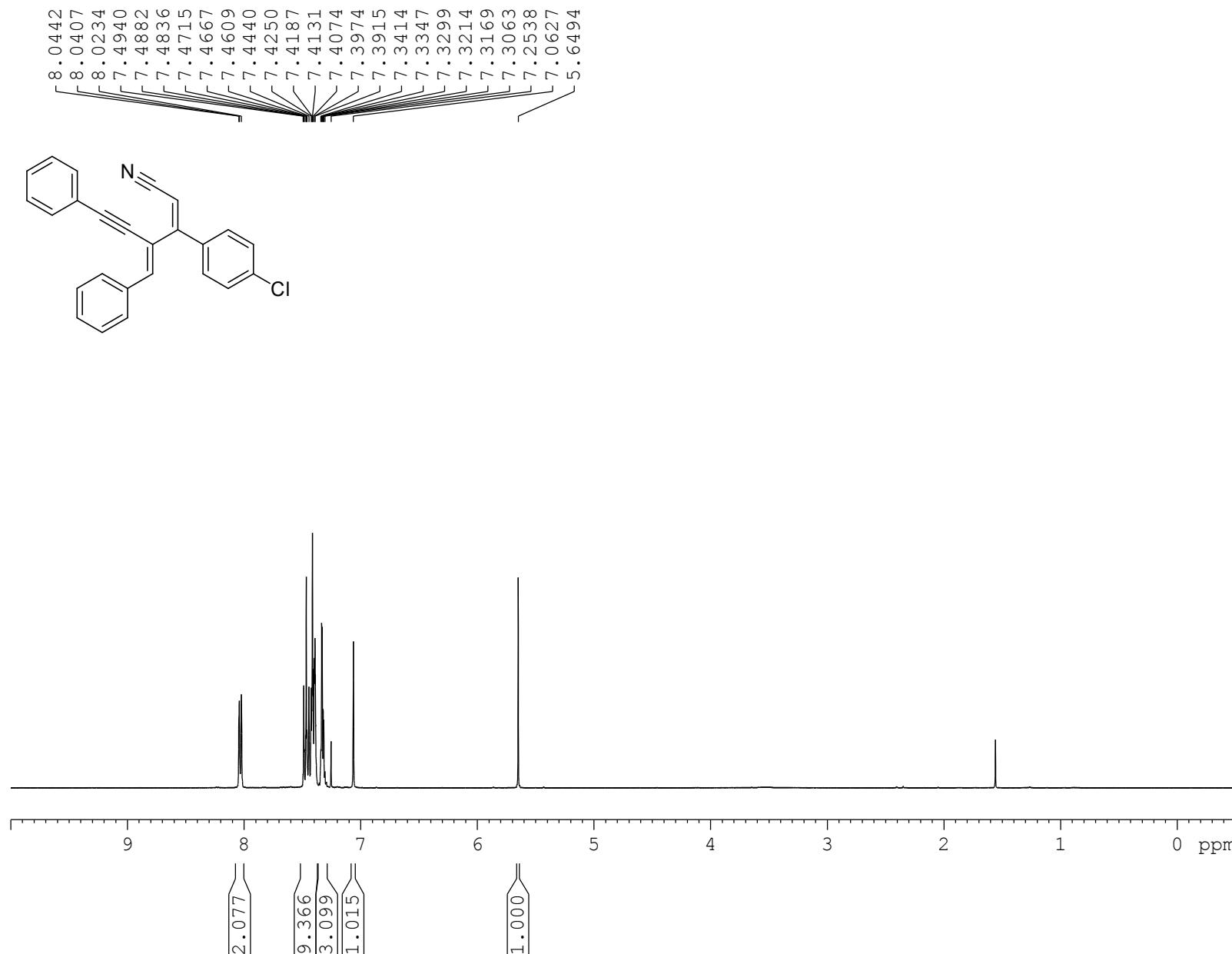
SFO1 400.1324008 MHz  
NUC1 1H  
P1 12.90 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1300097 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

(2E,4E)-4-benzylidene-3-(4-chlorophenyl)-6-phenylhex-2-en-5-ynenitrile (6e)



(2Z,4E)-4-benzylidene-3-(4-chlorophenyl)-6-phenylhex-2-en-5-ynenitrile (6'e)



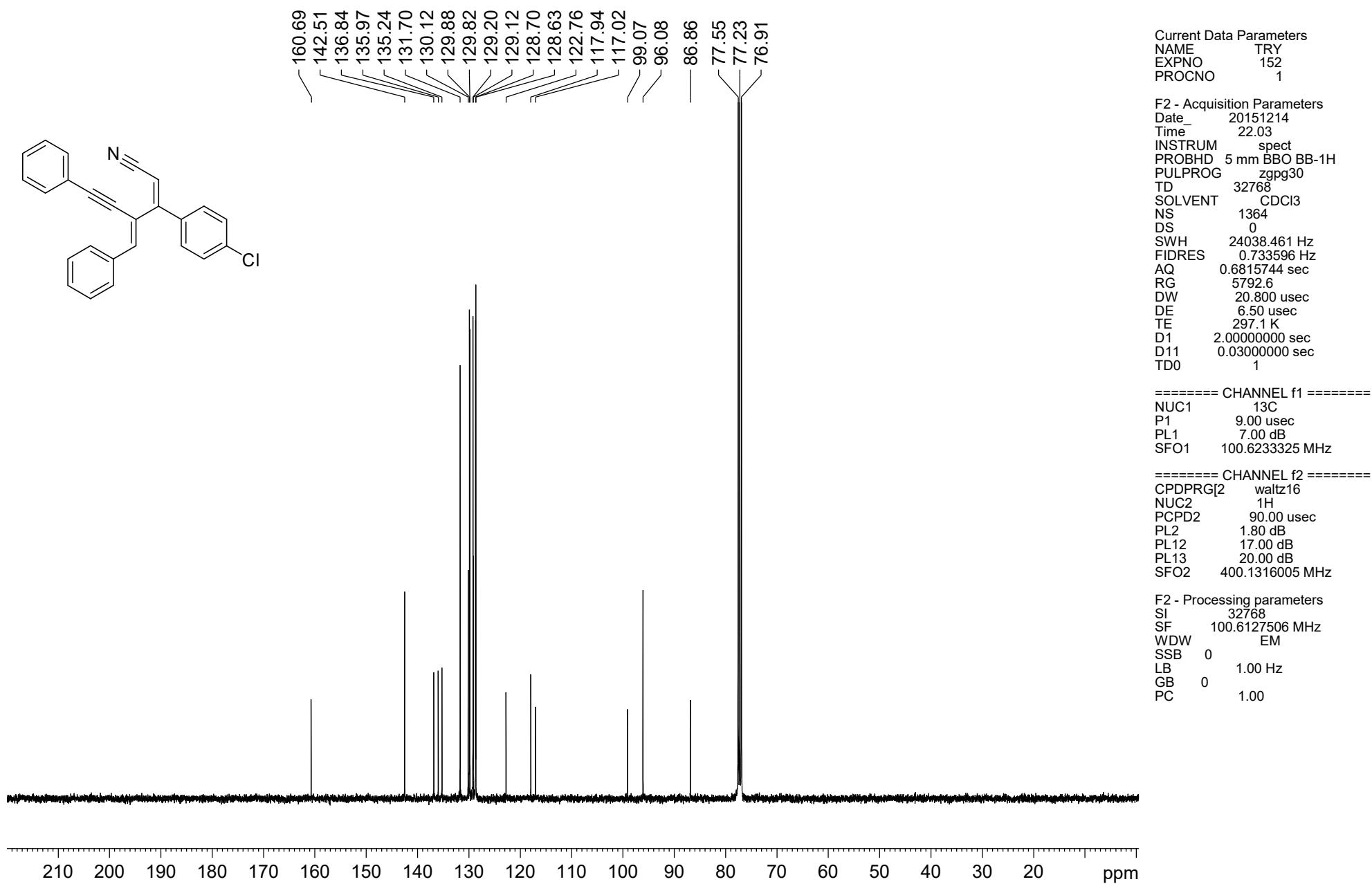
Current Data Parameters  
 NAME TRY  
 EXPNO 151  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20151214  
 Time 22.02  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 64  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 114  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 297.1 K  
 D1 2.0000000 sec  
 TDO 1

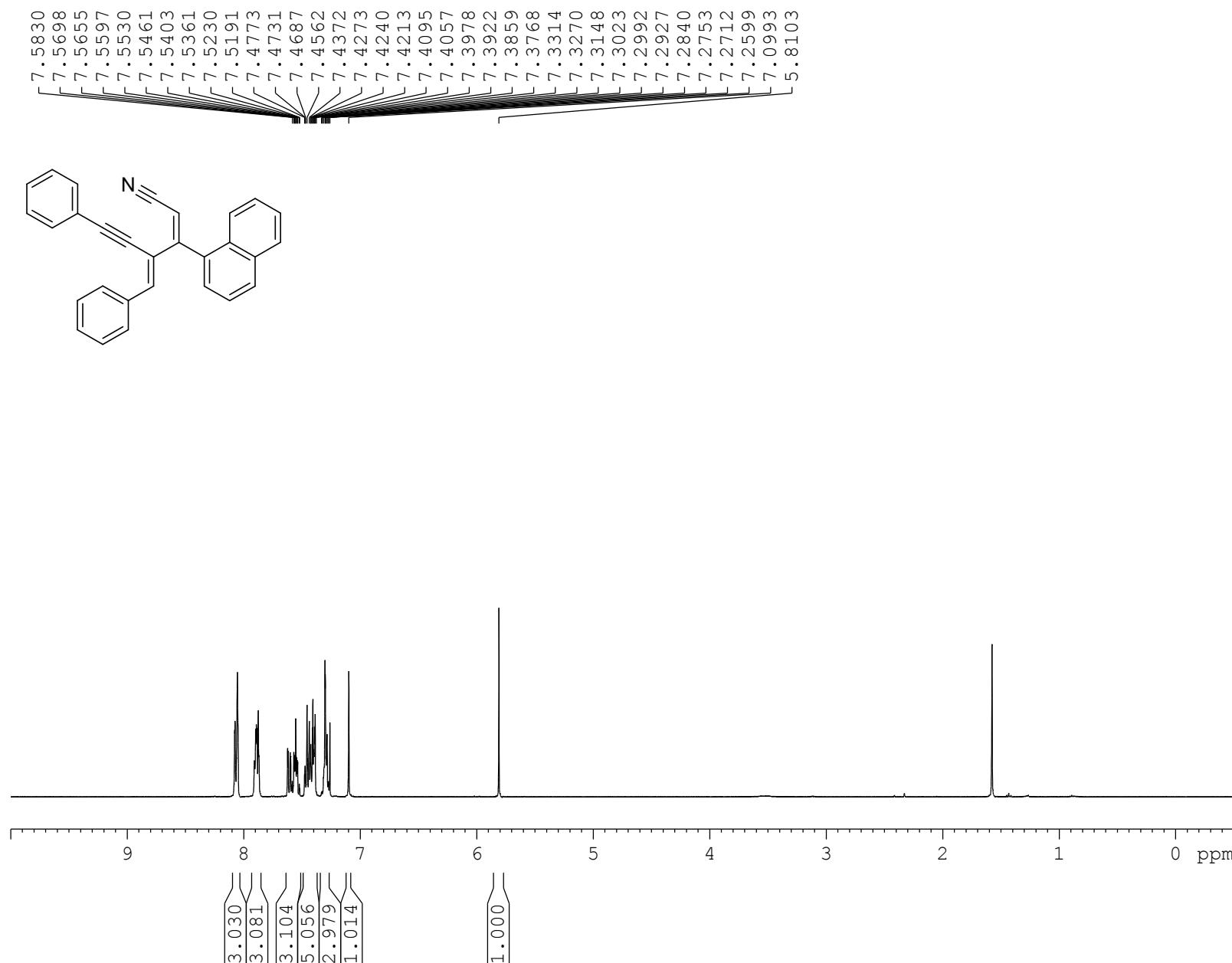
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.40 usec  
 PL1 1.80 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300118 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

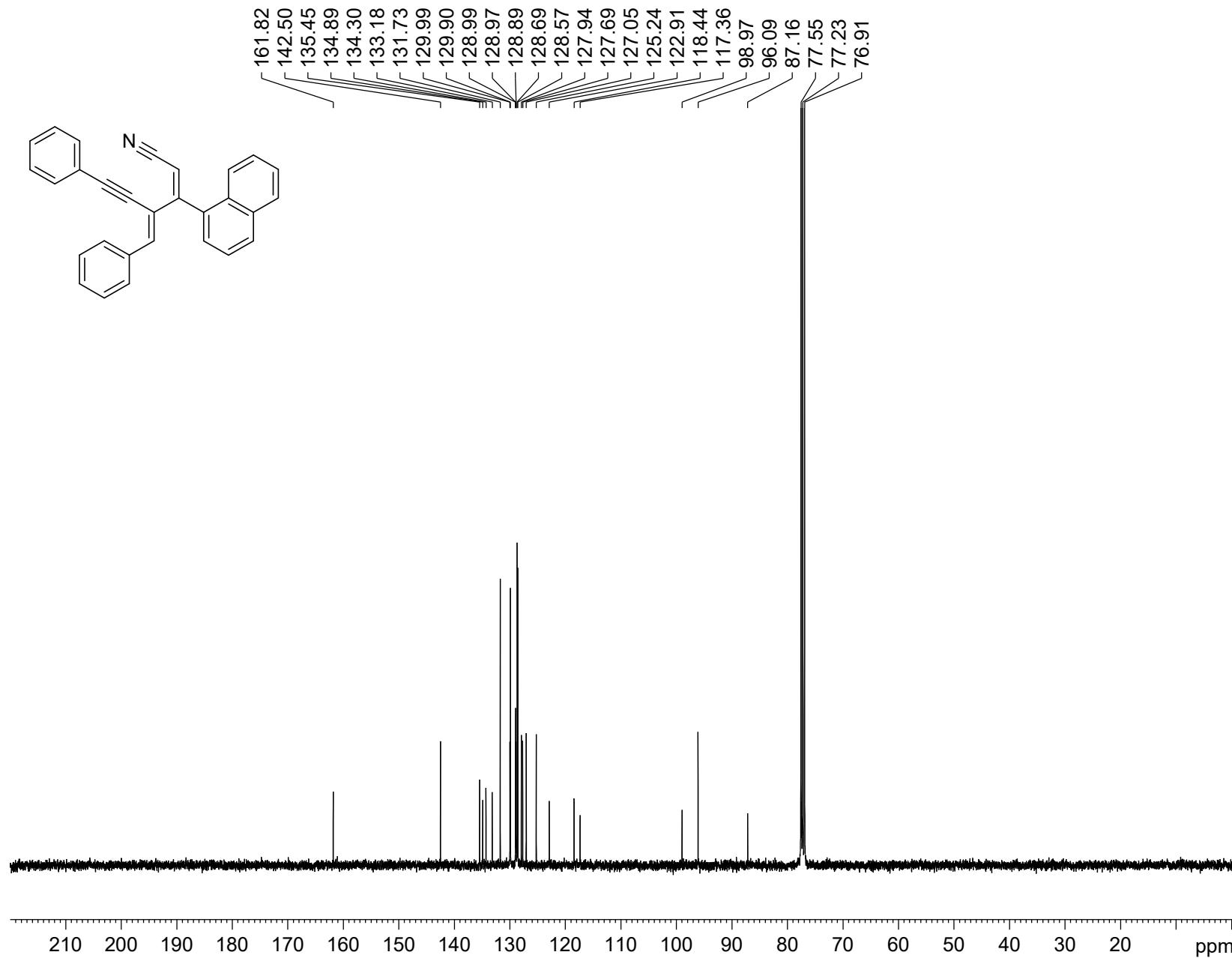
(2Z,4E)-4-benzylidene-3-(4-chlorophenyl)-6-phenylhex-2-en-5-yenenitrile (6'e)



(2Z,4E)-4-benzylidene-3-(naphthalen-1-yl)-6-phenylhex-2-en-5-ynenitrile (6'f)



(2Z,4E)-4-benzylidene-3-(naphthalen-1-yl)-6-phenylhex-2-en-5-ynenitrile (6'f)



Current Data Parameters  
 NAME TRY  
 EXPNO 223  
 PROCNO 1

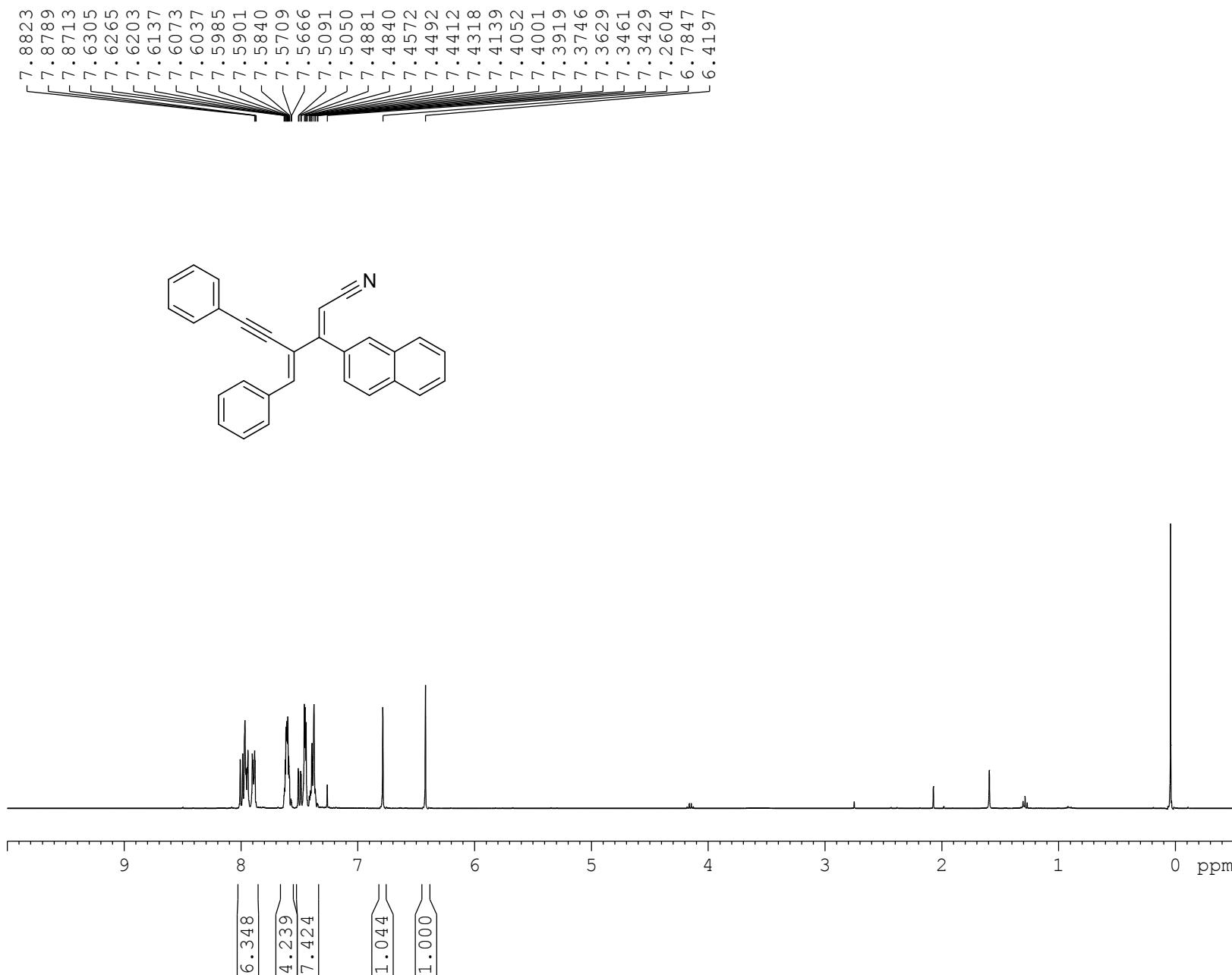
F2 - Acquisition Parameters  
 Date 20161201  
 Time 12.19  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 1000  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 8192  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 7.00 dB  
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 1.80 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127499 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

(2E,4E)-4-benzylidene-3-(naphthalen-2-yl)-6-phenylhex-2-en-5-ynenitrile (6g)



Current Data Parameters  
NAME TRY  
EXPNO 248  
PROCNO 1

```

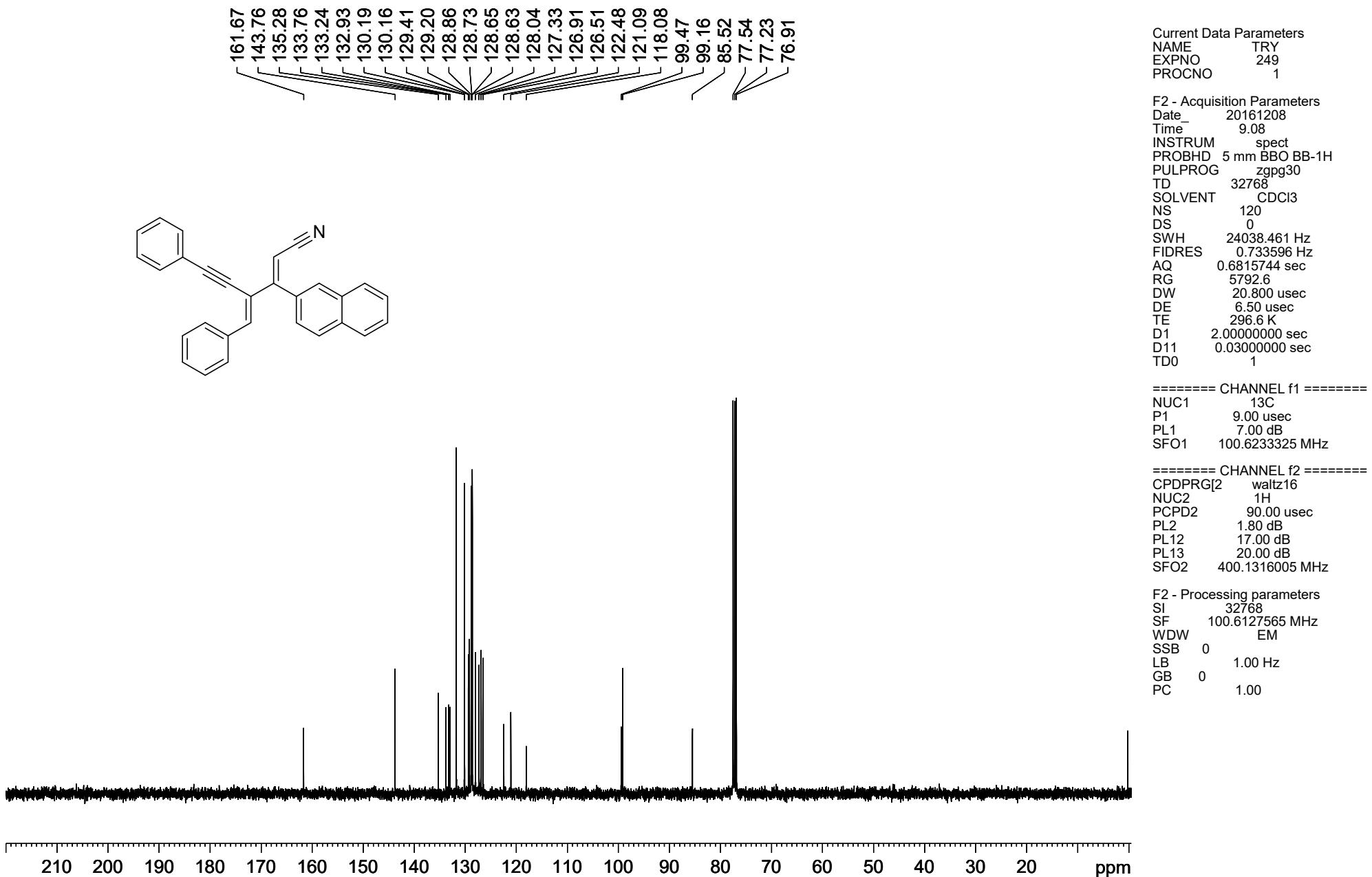
F2 - Acquisition Parameters
Date_   20161208
Time_   9.06
INSTRUM spect
PROBHD  5 mm BBO BB-1H
PULPROG zg30
TD      32768
SOLVENT CDCl3
NS      32
DS      0
SWH    7246.377 Hz
FIDRES 0.221142 Hz
AQ     2.2609921 sec
RG     71.8
DW     69.000 usec
DE     6.50 usec
TE     296.5 K
D1     2.00000000 sec
TD0    1

```

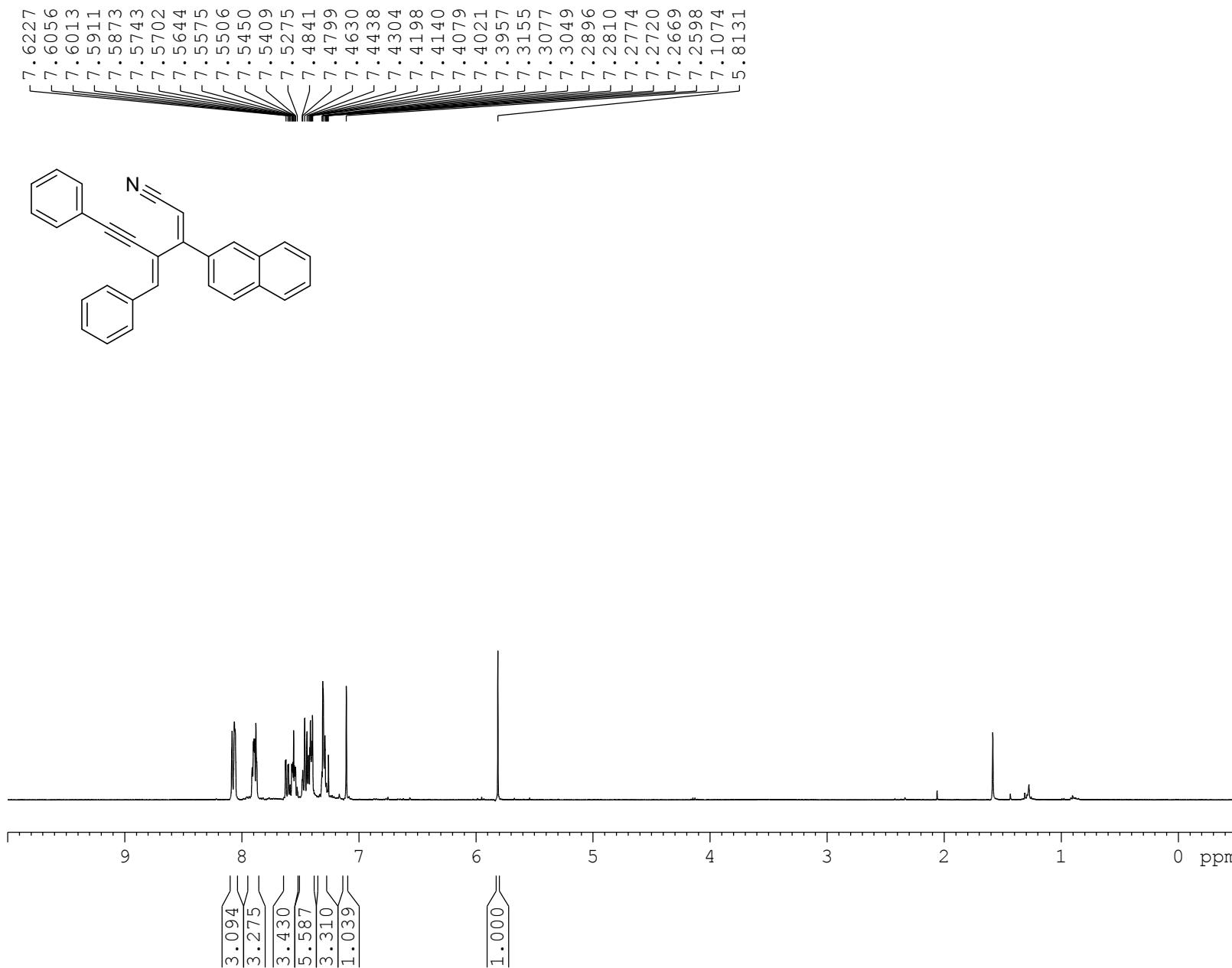
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.40 usec  
PL1 1.80 dB  
SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300091 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2E, 4E)-4-benzylidene-3-(naphthalen-2-yl)-6-phenylhex-2-en-5-ynenitrile (6g)



(2Z,4E)-4-benzylidene-3-(naphthalen-2-yl)-6-phenylhex-2-en-5-ynenitrile (6'g)



Current Data Parameters  
NAME TRY  
EXPNO 234  
PROCNO 1

```

F2 - Acquisition Parameters
Date_   20161207
Time_   8.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD      32768
SOLVENT CDCl3
NS      32
DS      0
SWH    7246.377 Hz
FIDRES 0.221142 Hz
AQ     2.2609921 sec
RG     114
DW     69.000 usec
DE     6.50 usec
TE     296.6 K
D1     2.0000000 sec
TD0          1

```

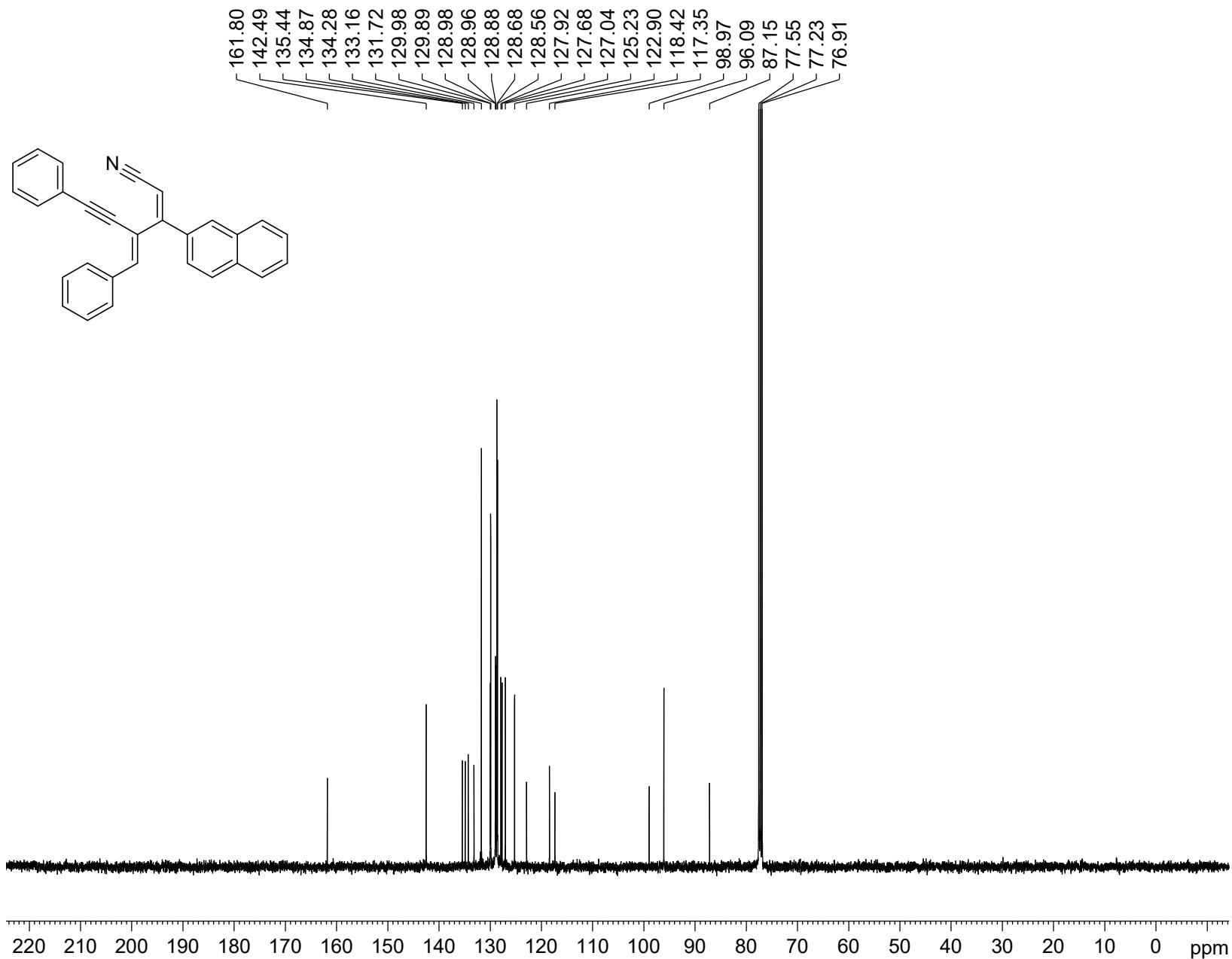
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.40 usec  
PL1 1.80 dB  
SFO1 400.1324008 MHz

```

F2 - Processing parameters
SI           16384
SF          400.1300096 MHz
WDW           EM
SSB            0
LB            0 Hz
GB            0
PC           1.00

```

(2Z,4E)-4-benzylidene-3-(naphthalen-2-yl)-6-phenylhex-2-en-5-ynenitrile (6'g)



Current Data Parameters  
NAME TRY  
EXPNO 235  
PROCNO 1

```

F2 - Acquisition Parameters
Date   20161207
Time   8.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD      32768
SOLVENT CDCl3
NS      788
DS      0
SWH    24038.461 Hz
FIDRES 0.733596 Hz
AQ     0.6815744 sec
RG     8192
DW     20.800 usec
DE     6.50 usec
TE     296.5 K
D1     2.0000000 sec
D11    0.03000000 sec
TD0          1

```

===== CHANNEL f1 ======  
NUC1 13C  
P1 9.00 usec  
PL1 7.00 dB  
SFO1 100.6233325 MHz

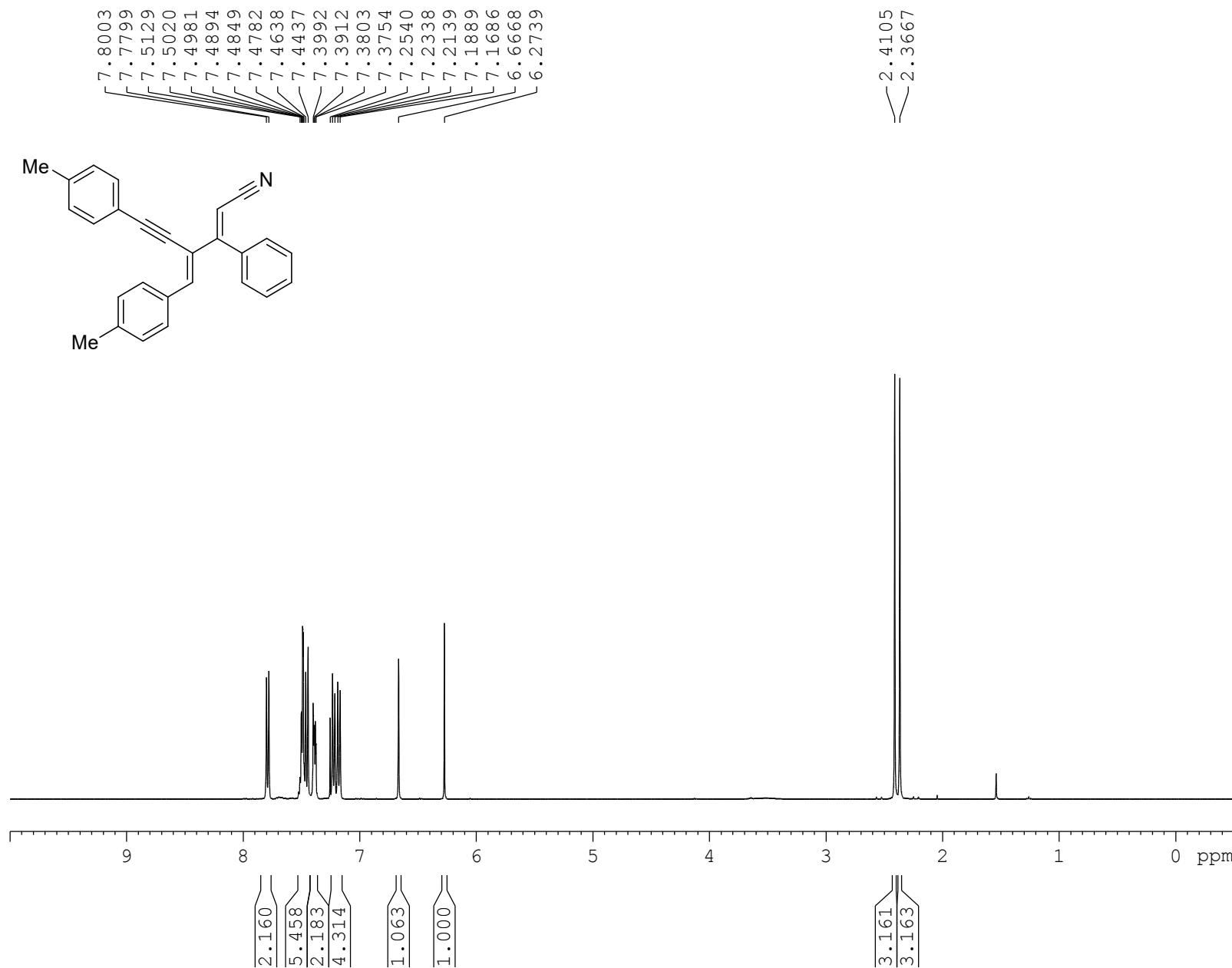
```
===== CHANNEL f2 ======  
CPDPRG[2]      walt16  
NUC2          1H  
PCPD2        90.00 usec  
PL2           1.80 dB  
PL12          17.00 dB  
PL13          20.00 dB  
SEQ2        400.1316005 MHz
```

```

F2 - Processing parameters
SI      32768
SF      100.6127521 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB      0
PC      1.00

```

(2E, 4E)-4-(4-methylbenzylidene)-3-phenyl-6-(p-tolyl)hex-2-en-5-ynenitrile (6h)



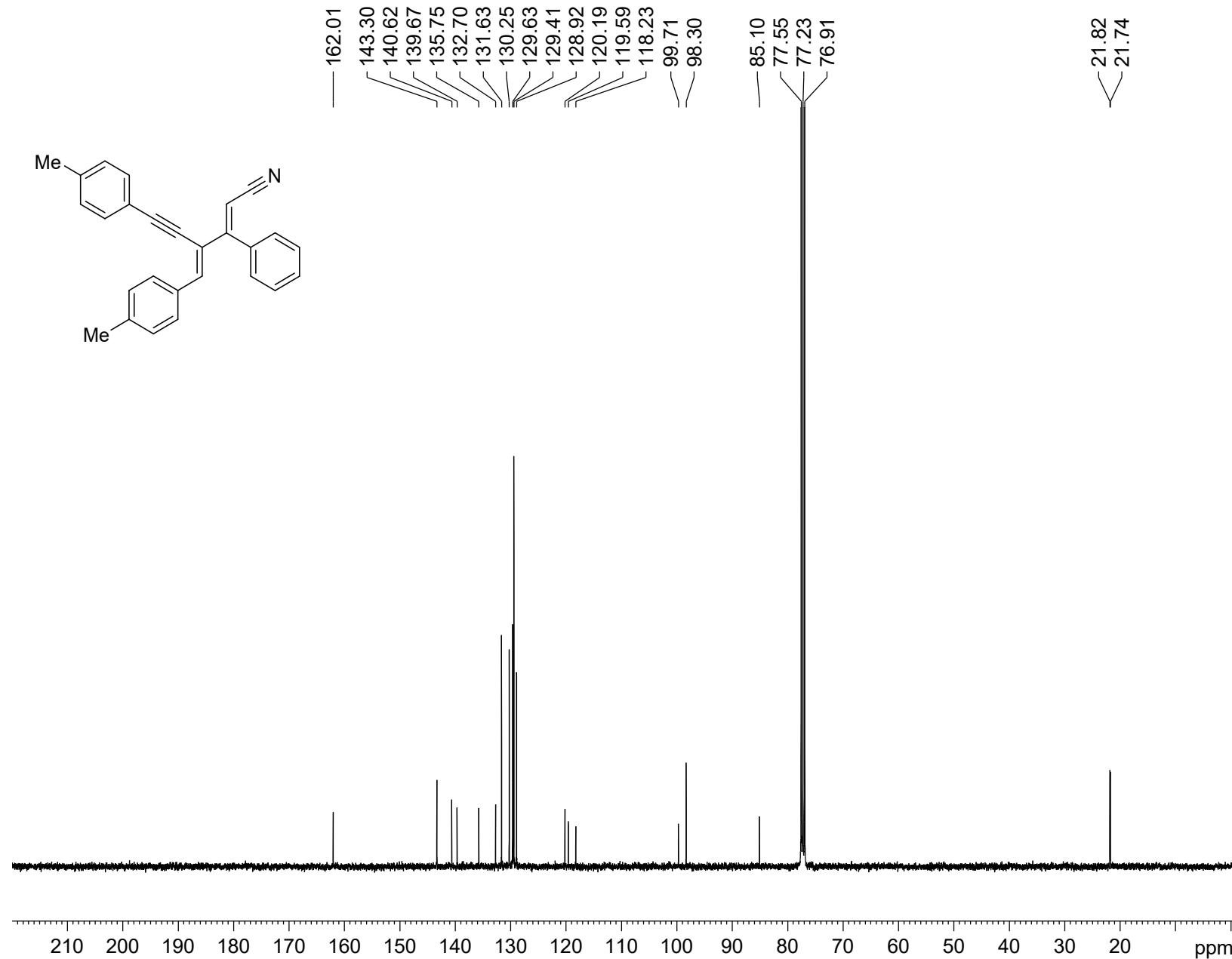
Current Data Parameters  
 NAME TRY  
 EXPNO 143  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20151208  
 Time 18.09  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 64  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 181  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 2.0000000 sec  
 TDO 1

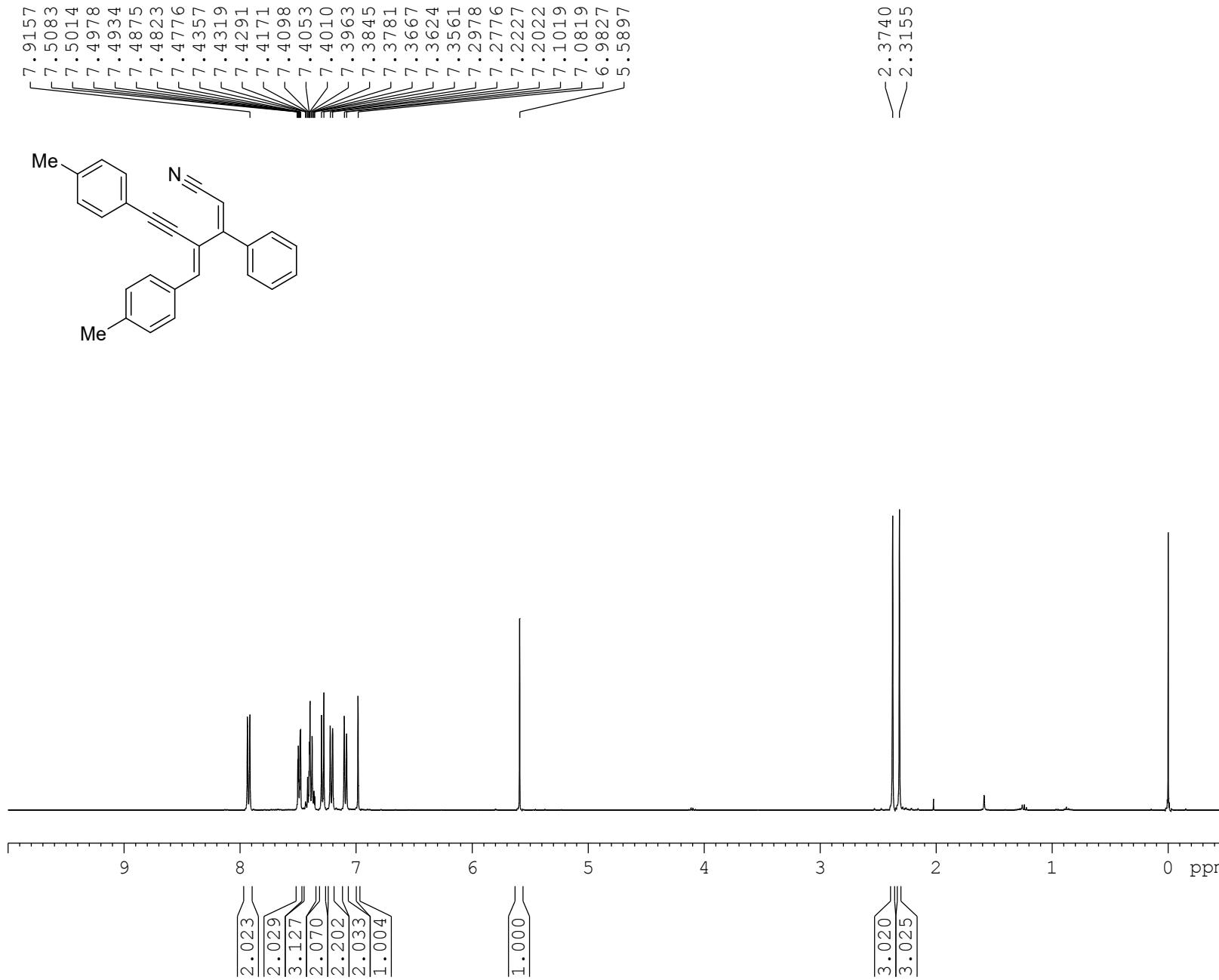
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.40 usec  
 PL1 1.80 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300118 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2E,4E)-4-(4-methylbenzylidene)-3-phenyl-6-(p-tolyl)hex-2-en-5-yenenitrile (6h)



(2Z,4E)-4-(4-methylbenzylidene)-3-phenyl-6-(p-tolyl)hex-2-en-5-yenitrile (6'h)



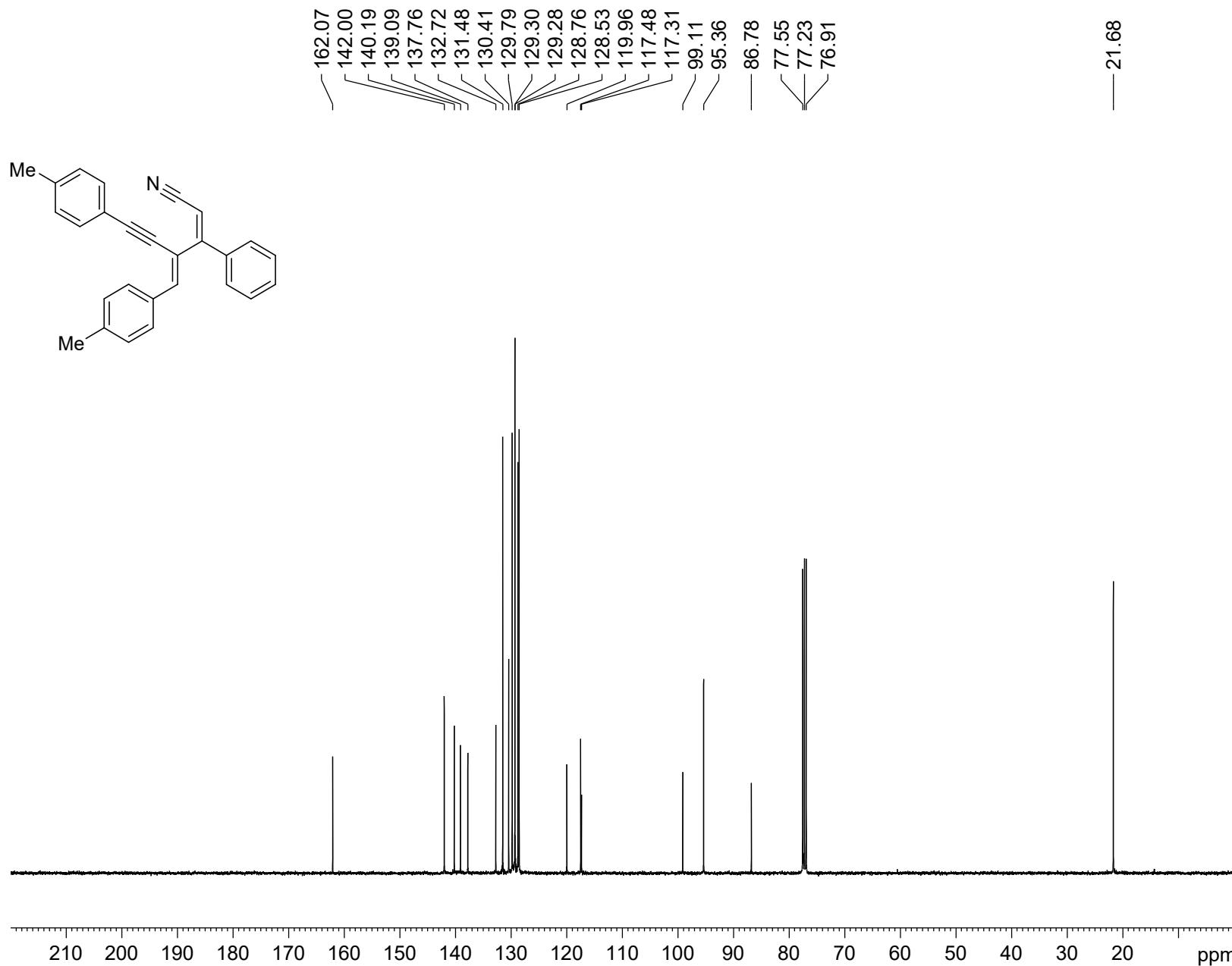
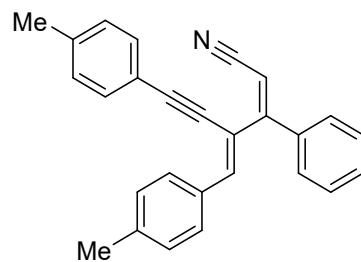
Current Data Parameters  
 NAME TRY  
 EXPNO 230  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20161207  
 Time 7.08  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 35.9  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 2.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.40 usec  
 PL1 1.80 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300335 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

(2Z,4E)-4-(4-methylbenzylidene)-3-phenyl-6-(p-tolyl)hex-2-en-5-ynenitrile (6'h)



Current Data Parameters  
NAME TRY  
EXPNO 231  
PROCNO 1

```

F2 - Acquisition Parameters
Date_      20161207
Time       7.11
INSTRUM   spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        32768
SOLVENT   CDCl3
NS         760
DS          0
SWH       24038.461 Hz
FIDRES   0.733596 Hz
AQ        0.6815744 sec
RG        8192
DW        20.800 usec
DE        6.50 usec
TE        296.5 K
D1        2.0000000 sec
D11       0.03000000 sec
TD0           1

```

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PL1 7.00 dB  
SFO1 100.6233325 MHz

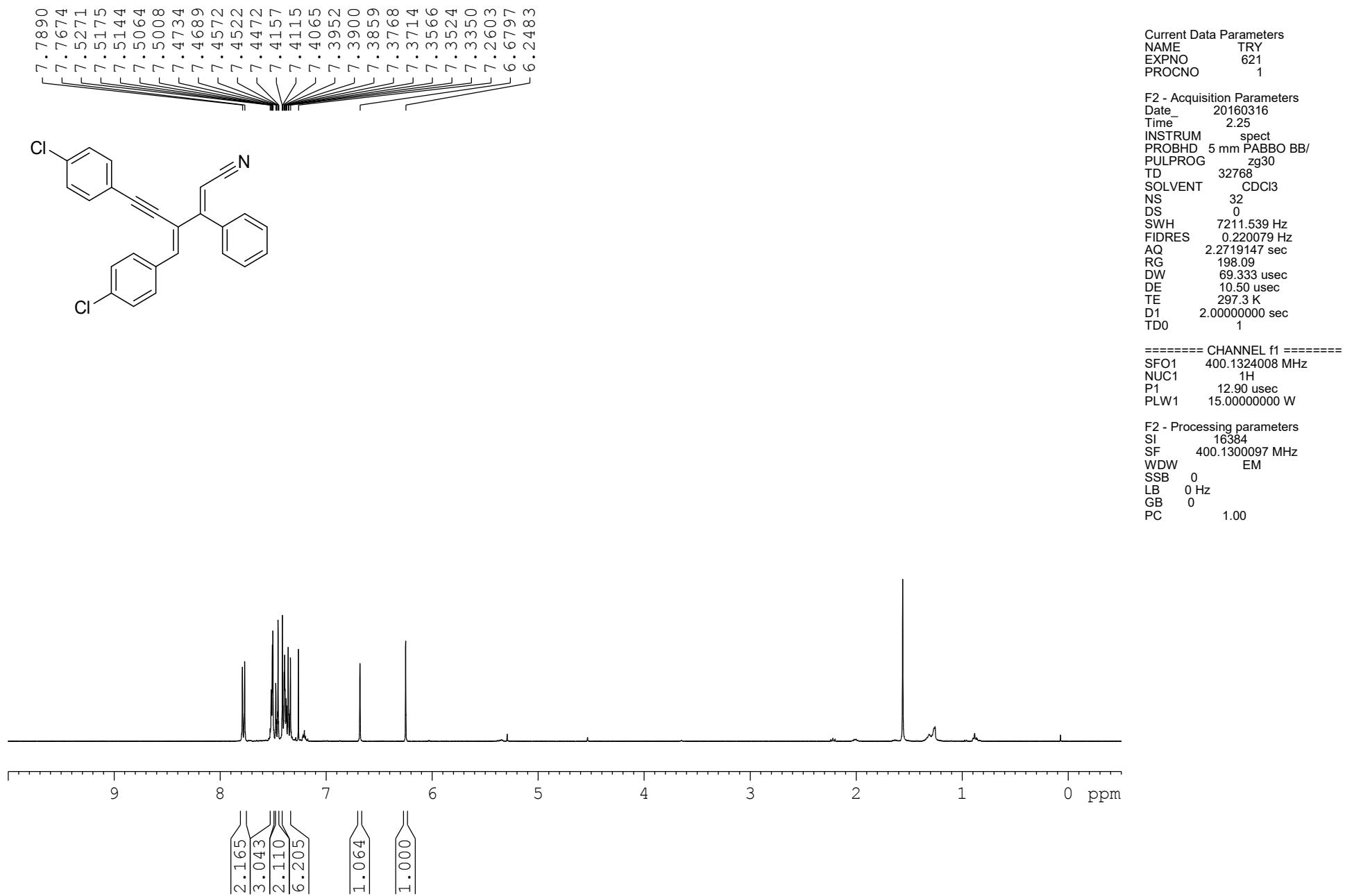
```
===== CHANNEL f2 ======  
CPDPRG[2]    waltz16  
NUC2         1H  
PCPD2        90.00 usec  
PL2          1.80 dB  
PL12         17.00 dB  
PL13         20.00 dB  
SEQ2        400_1316005 MHz
```

```

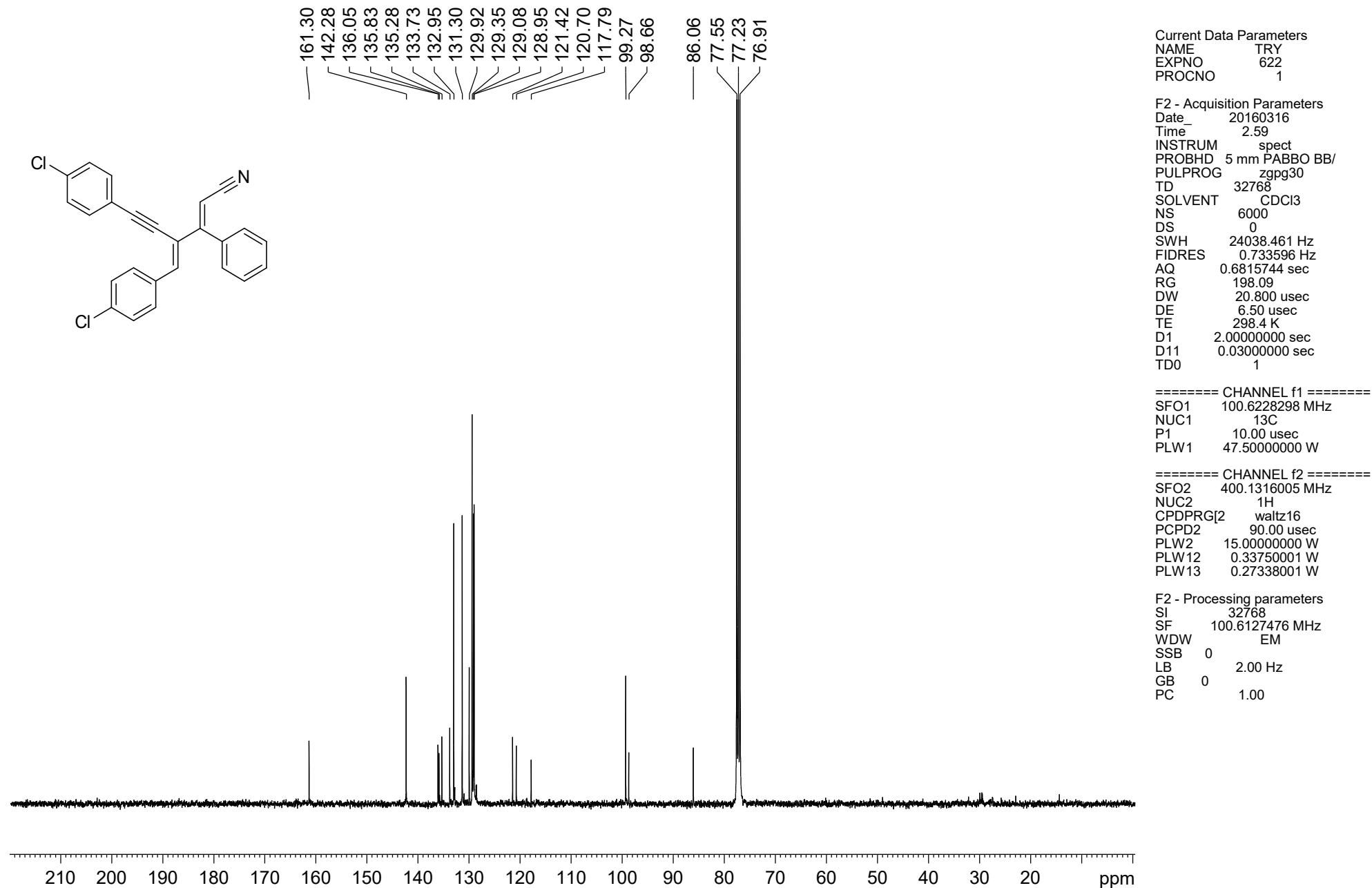
F2 - Processing parameters
SI      32768
SF      100.6127624 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB      0
PC      1.00

```

(2E, 4E)-4-(4-chlorobenzylidene)-6-(4-chlorophenyl)-3-phenylhex-2-en-5-ynenitrile (6i)

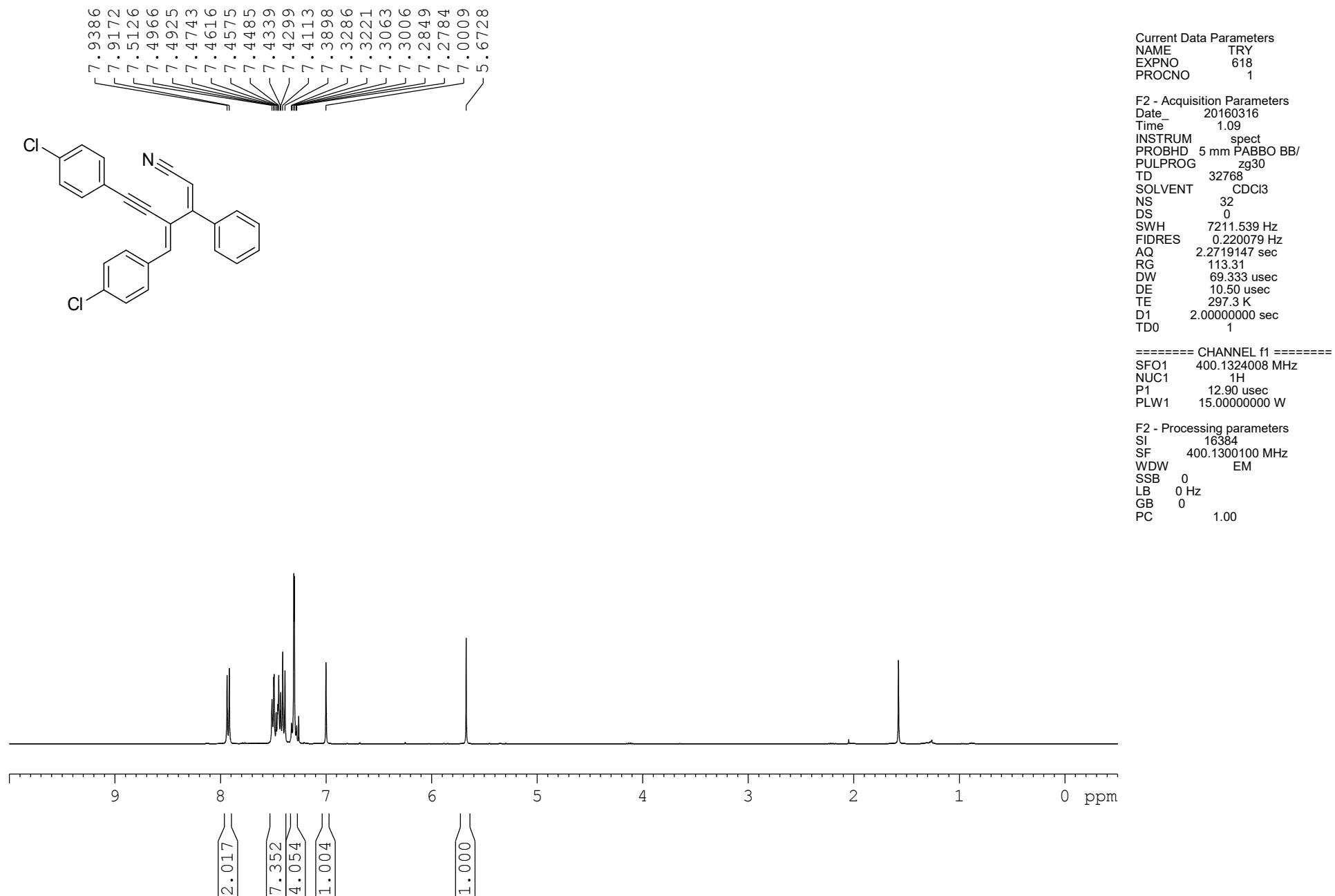


(2E,4E)-4-(4-chlorobenzylidene)-6-(4-chlorophenyl)-3-phenylhex-2-en-5-ynenitrile (6i)

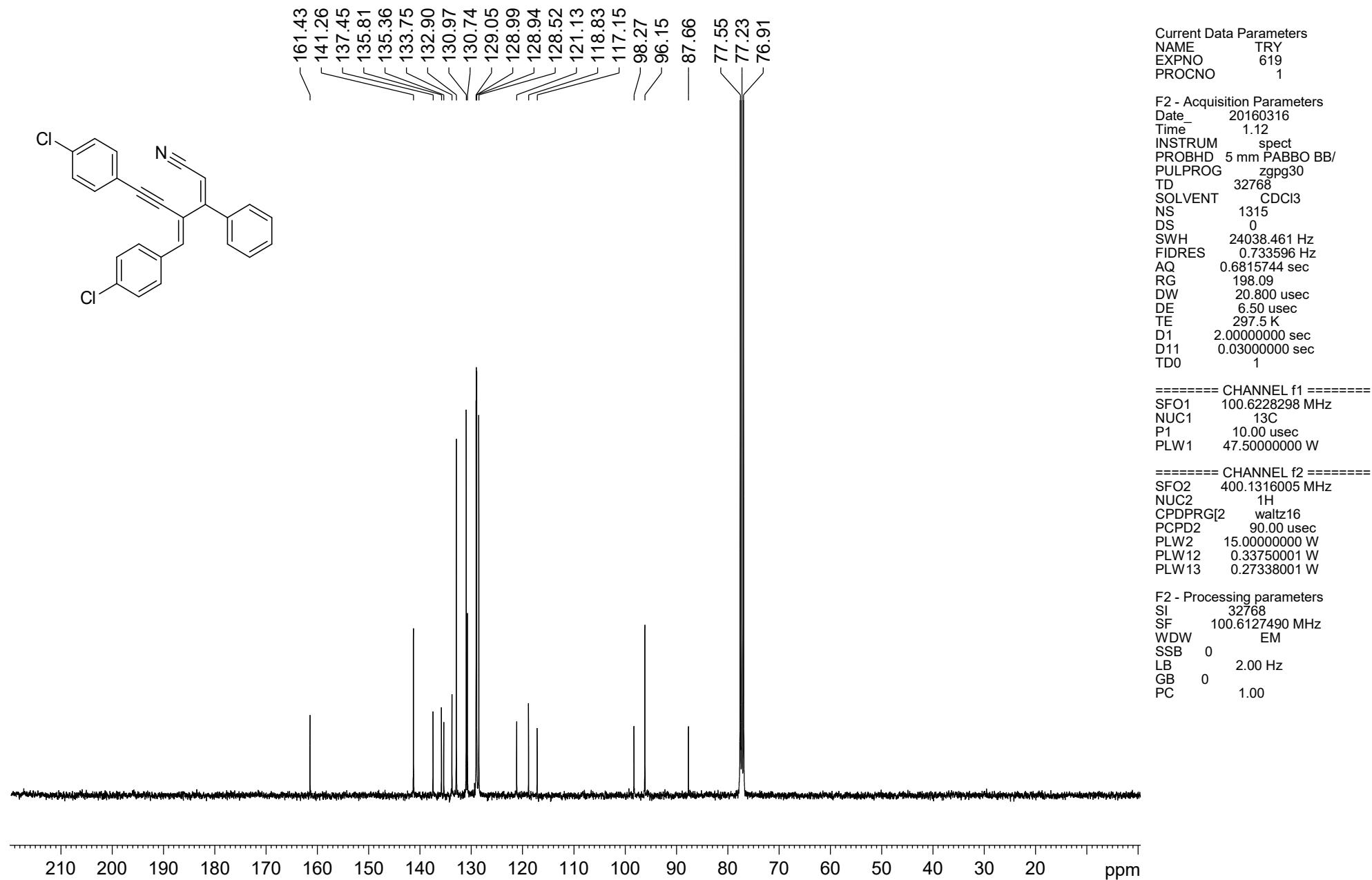


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

*(2Z,4E)-4-(4-chlorobenzylidene)-6-(4-chlorophenyl)-3-phenylhex-2-en-5-ynenitrile (6'i)*

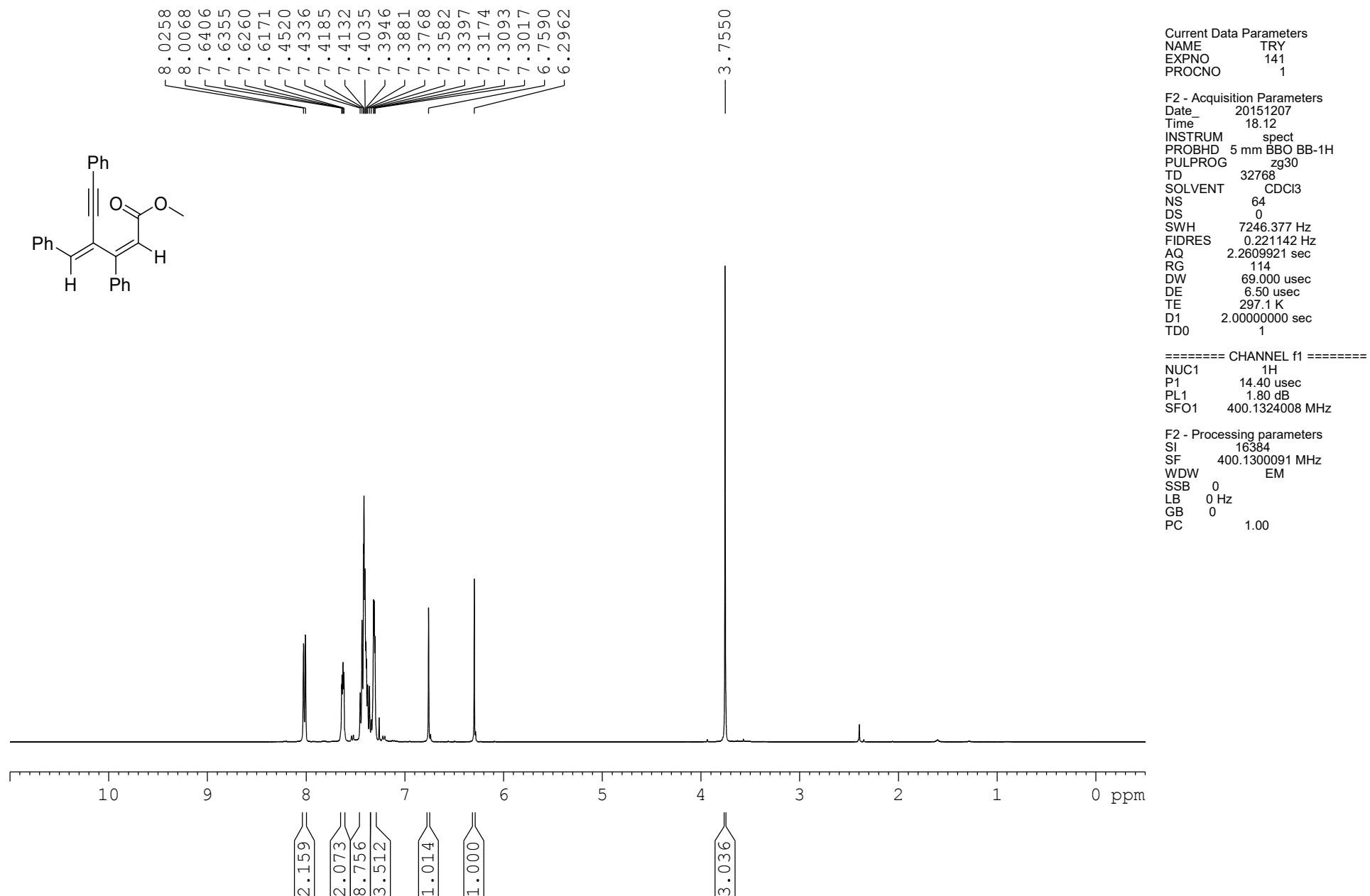


(2Z,4E)-4-(4-chlorobenzylidene)-6-(4-chlorophenyl)-3-phenylhex-2-en-5-ynenitrile (6'i)

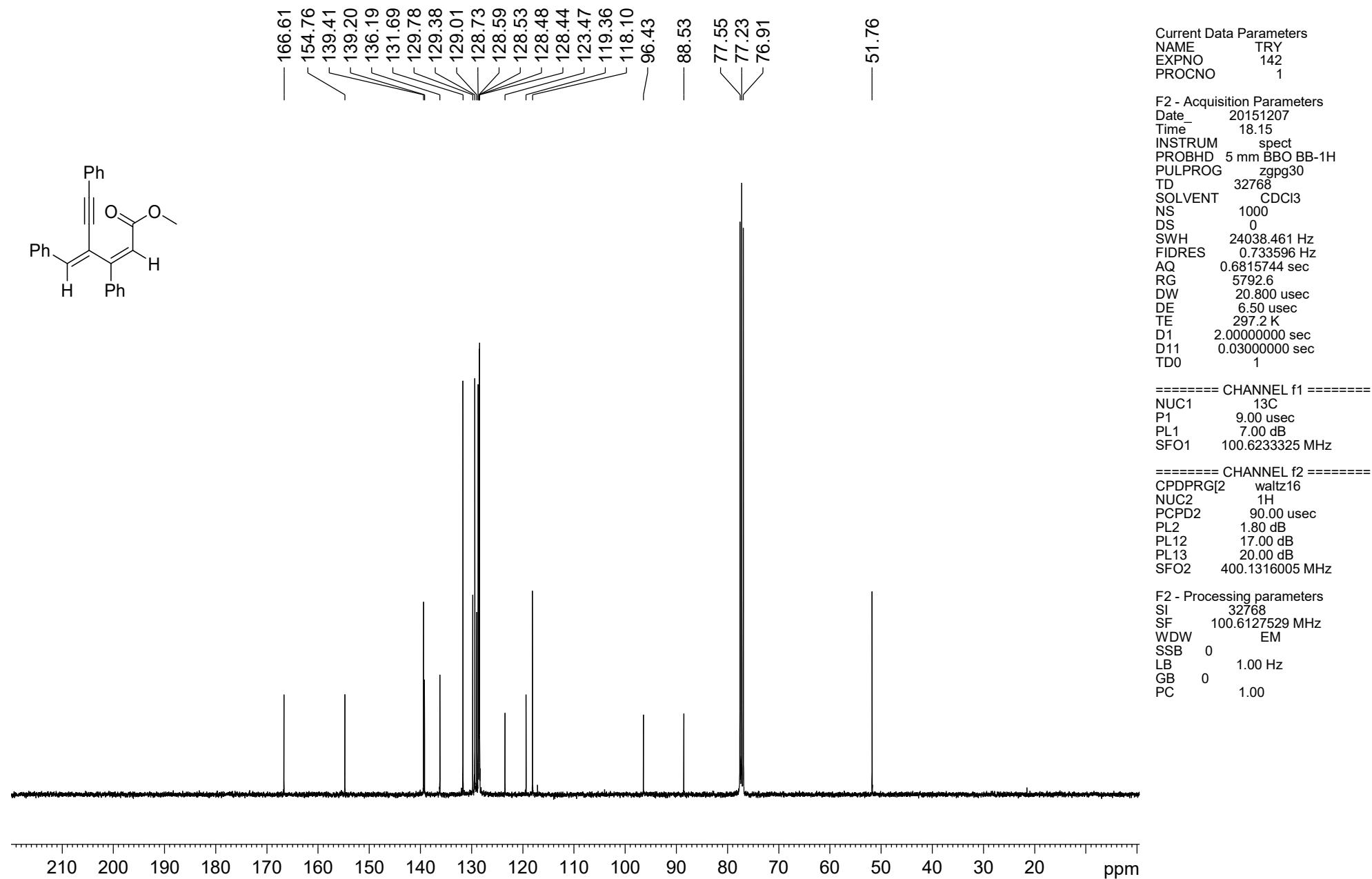


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

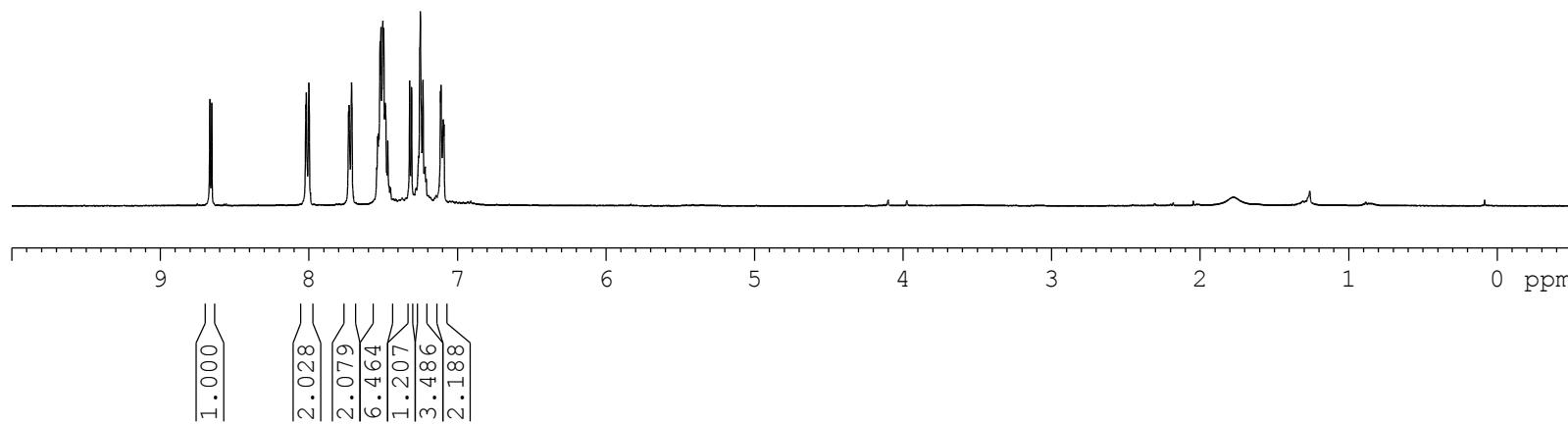
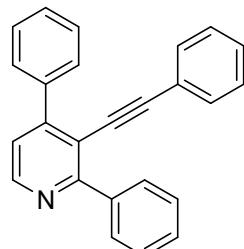
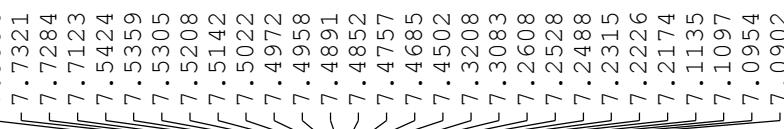
(2Z,4E)-methyl 4-benzylidene-3,6-diphenylhex-2-en-5-ynoate (8)



(2Z,4E)-methyl 4-benzylidene-3,6-diphenylhex-2-en-5-ynoate (8)



2,4-diphenyl-3-(phenylethynyl)pyridine (10a)



Current Data Parameters  
NAME TRY  
EXPNO 174  
PROCNO 1

```

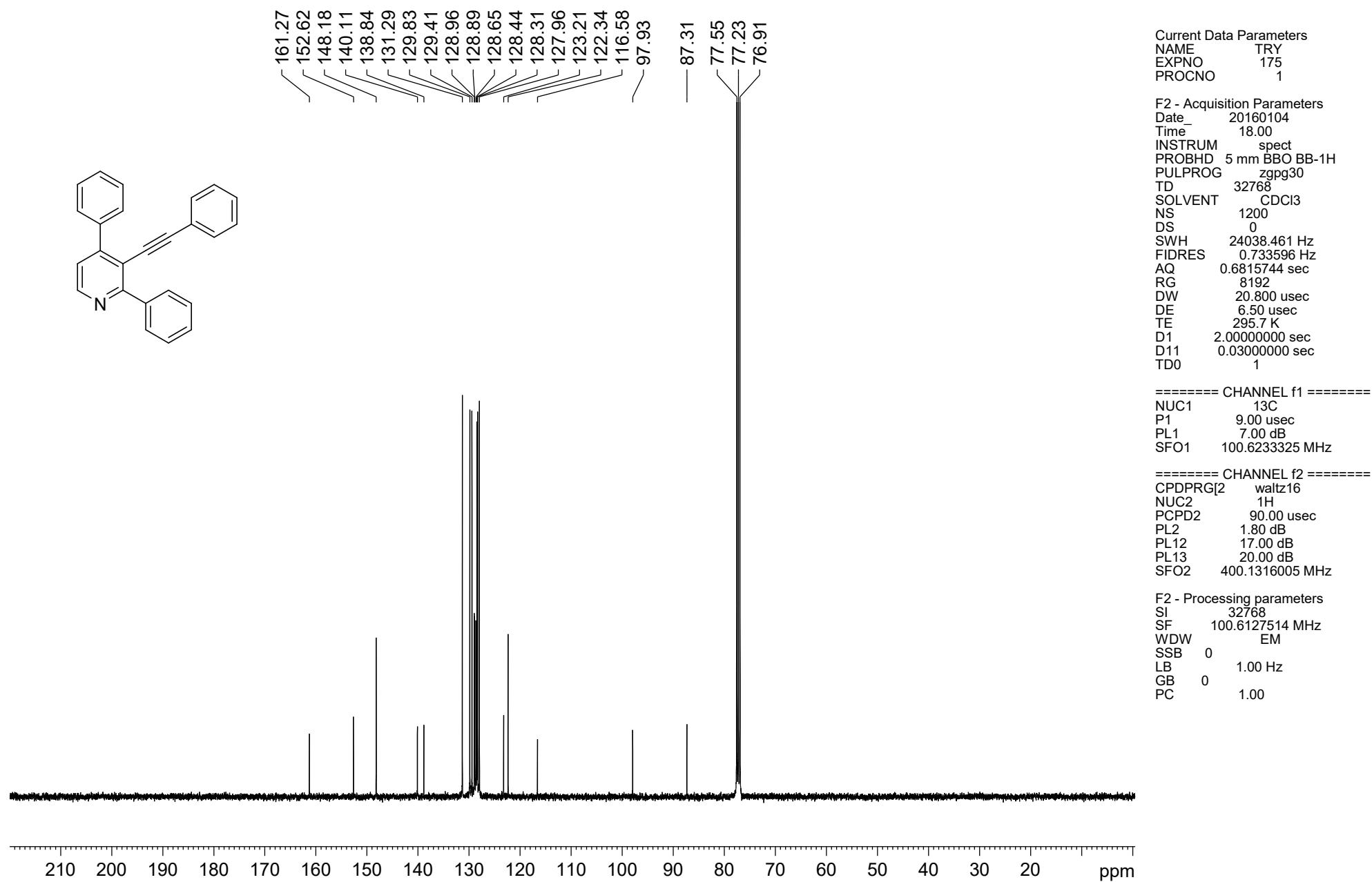
F2 - Acquisition Parameters
Date_   20160104
Time_   17.55
INSTRUM spect
PROBHD  5 mm BBO BB-1H
PULPROG zg30
TD      32768
SOLVENT CDCl3
NS      64
DS      0
SWH    7246.377 Hz
FIDRES 0.221142 Hz
AQ     2.2609921 sec
RG     114
DW     69.000 usec
DE     6.50 usec
TE     295.7 K
D1     2.0000000 sec
TD0          1

```

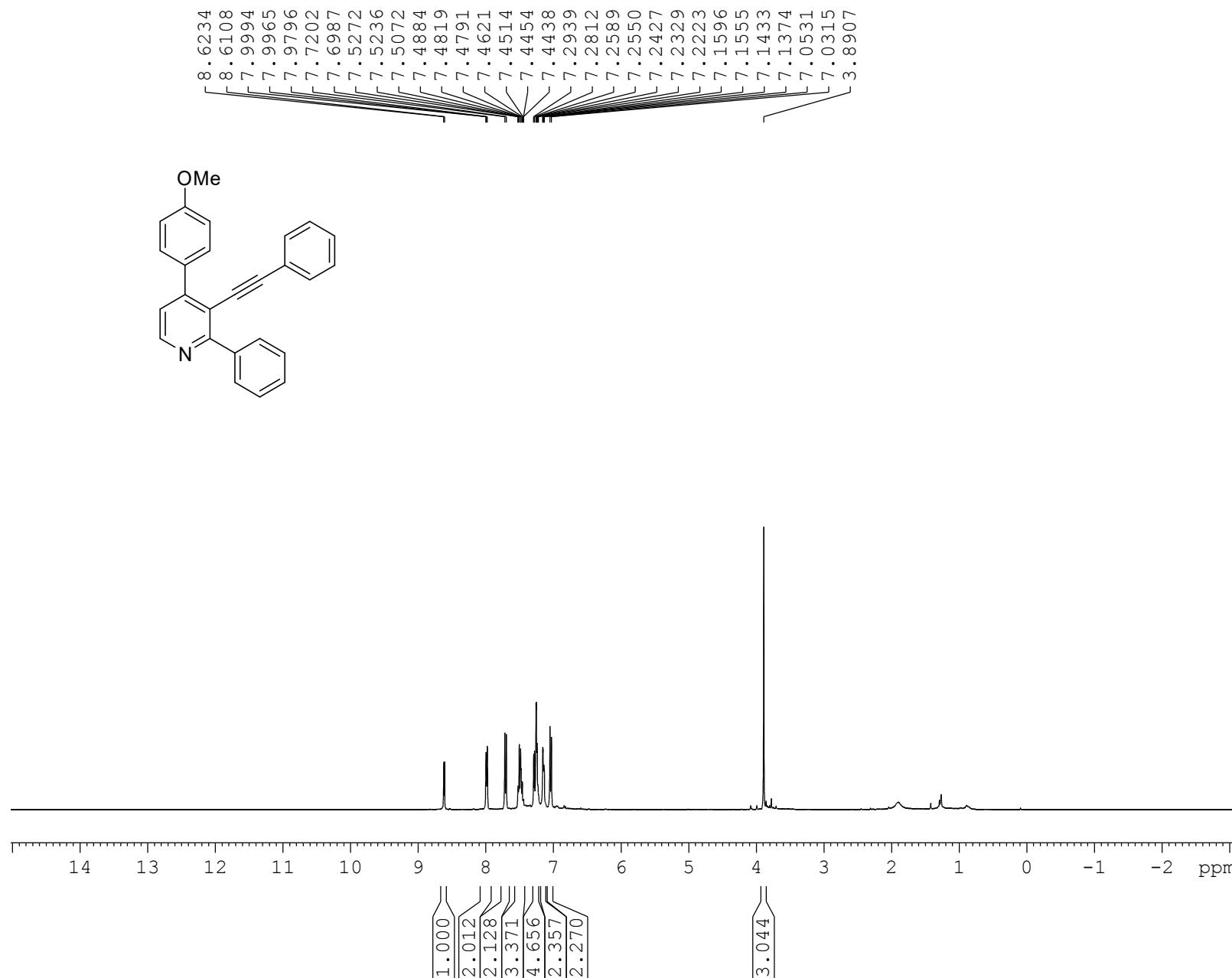
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.40 usec  
PL1 1.80 dB  
SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300118 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

2,4-diphenyl-3-(phenylethyynyl)pyridine (10a)



4-(4-methoxyphenyl)-2-phenyl-3-(phenylethyynyl)pyridine (10b) a



Current Data Parameters  
 NAME TRY  
 EXPNO 169  
 PROCNO 1

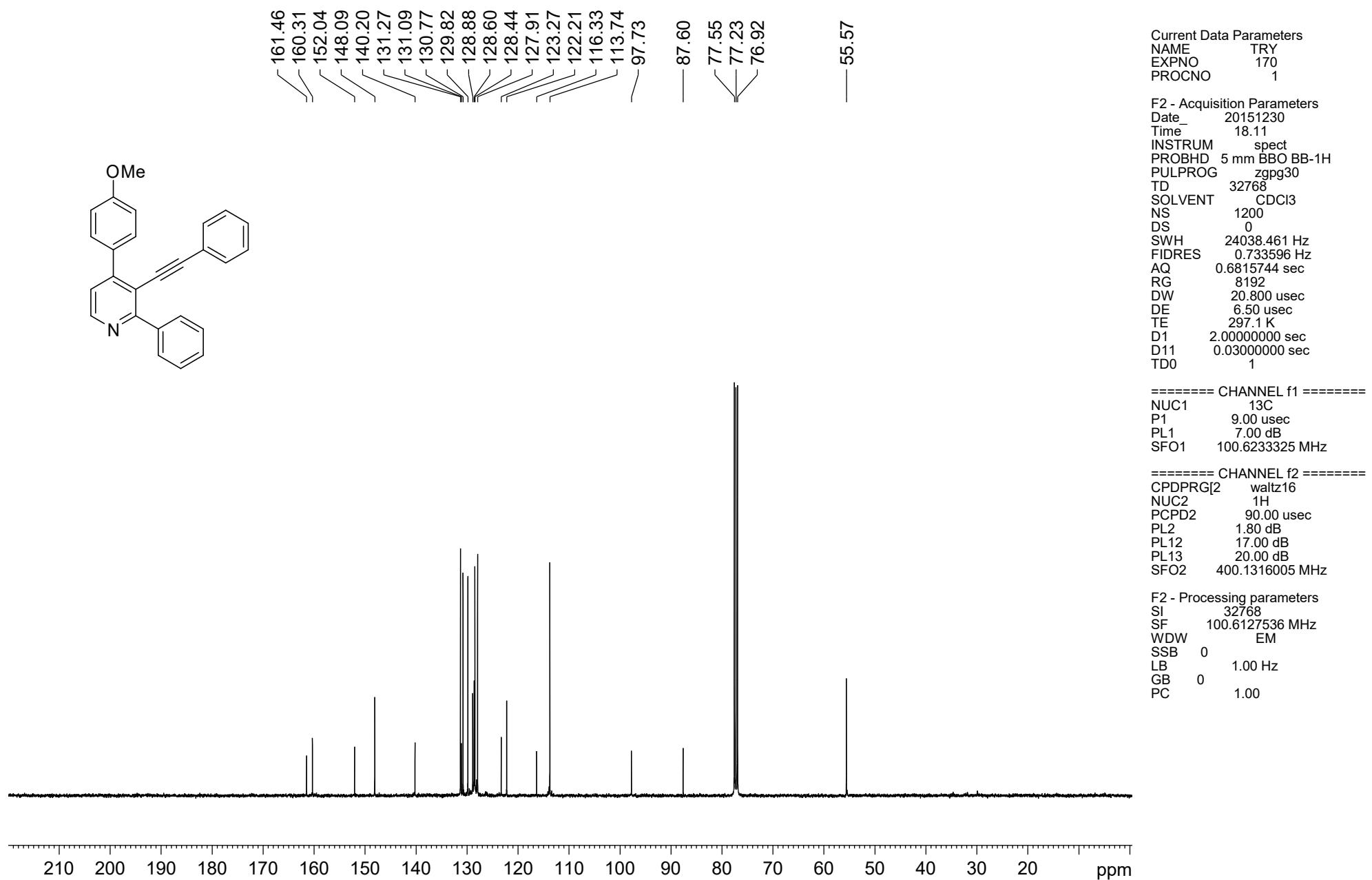
F2 - Acquisition Parameters  
 Date 20151230  
 Time 18.08  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 32  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2609921 sec  
 RG 64  
 DW 69.000 usec  
 DE 6.50 usec  
 TE 297.1 K  
 D1 2.0000000 sec  
 TDO 1

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

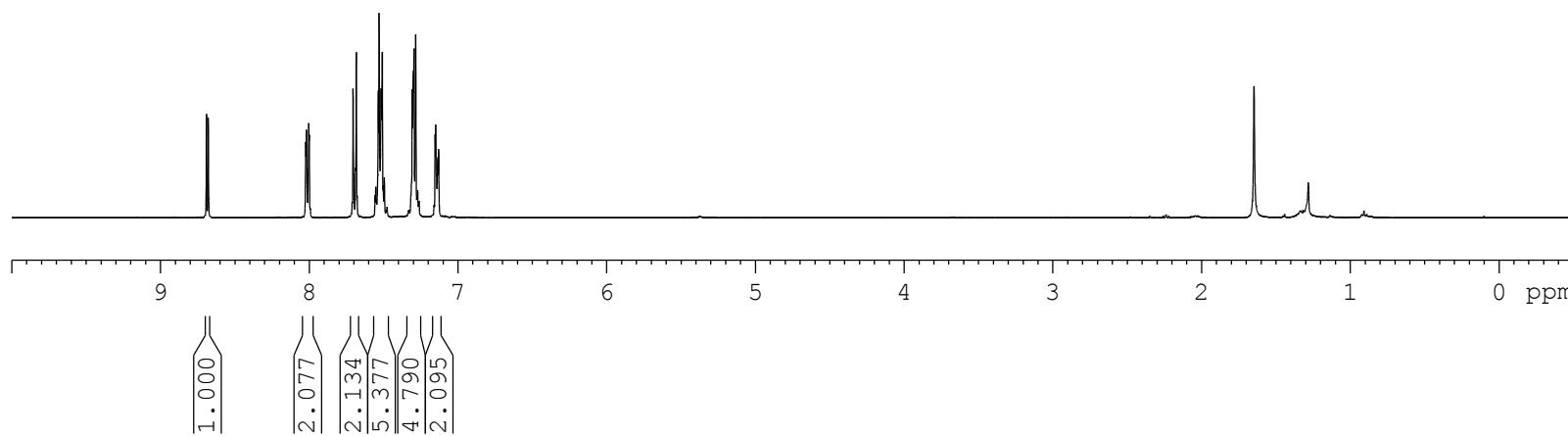
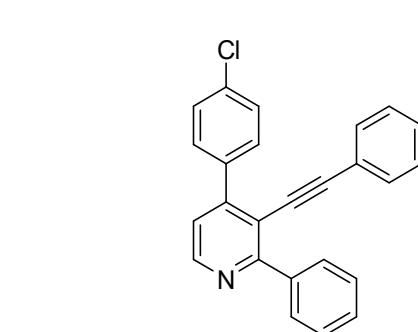
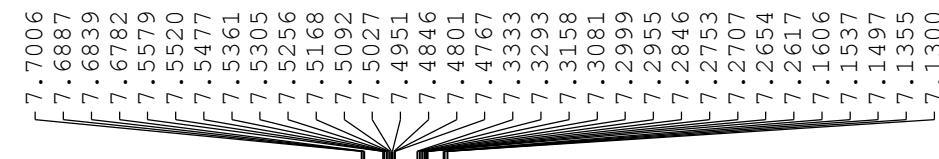
NUC1 <sup>1</sup>H  
 P1 14.40 usec  
 PL1 1.80 dB  
 SFO1 400.1324008 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300118 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

4-(4-methoxyphenyl)-2-phenyl-3-(phenylethynyl)pyridine (10b) a



4-(4-chlorophenyl)-2-phenyl-3-(phenylethyynyl)pyridine (10c)



Current Data Parameters  
NAME TRY  
EXPNO 600  
PROCNO 1

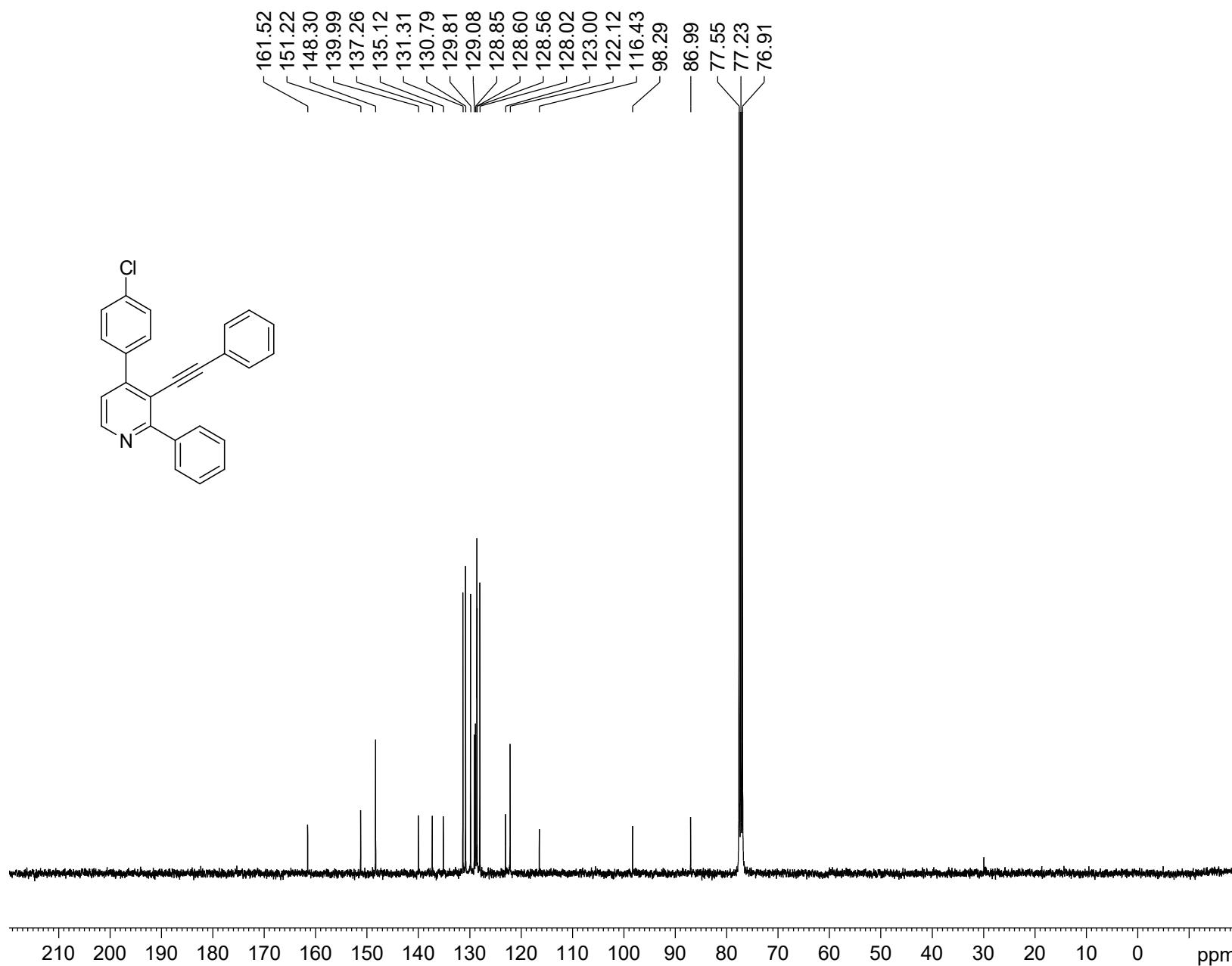
F2 - Acquisition Parameters  
Date 20160313  
Time 13.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 64  
DS 0  
SWH 7211.539 Hz  
FIDRES 0.220079 Hz  
AQ 2.2719147 sec  
RG 128.9  
DW 69.333 usec  
DE 10.50 usec  
TE 296.8 K  
D1 2.0000000 sec  
TDO 1

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

SFO1 400.1324008 MHz  
NUC1 1H  
P1 12.90 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

4-(4-chlorophenyl)-2-phenyl-3-(phenylethynyl)pyridine (10c)



Current Data Parameters  
 NAME TRY  
 EXPNO 601  
 PROCNO 1

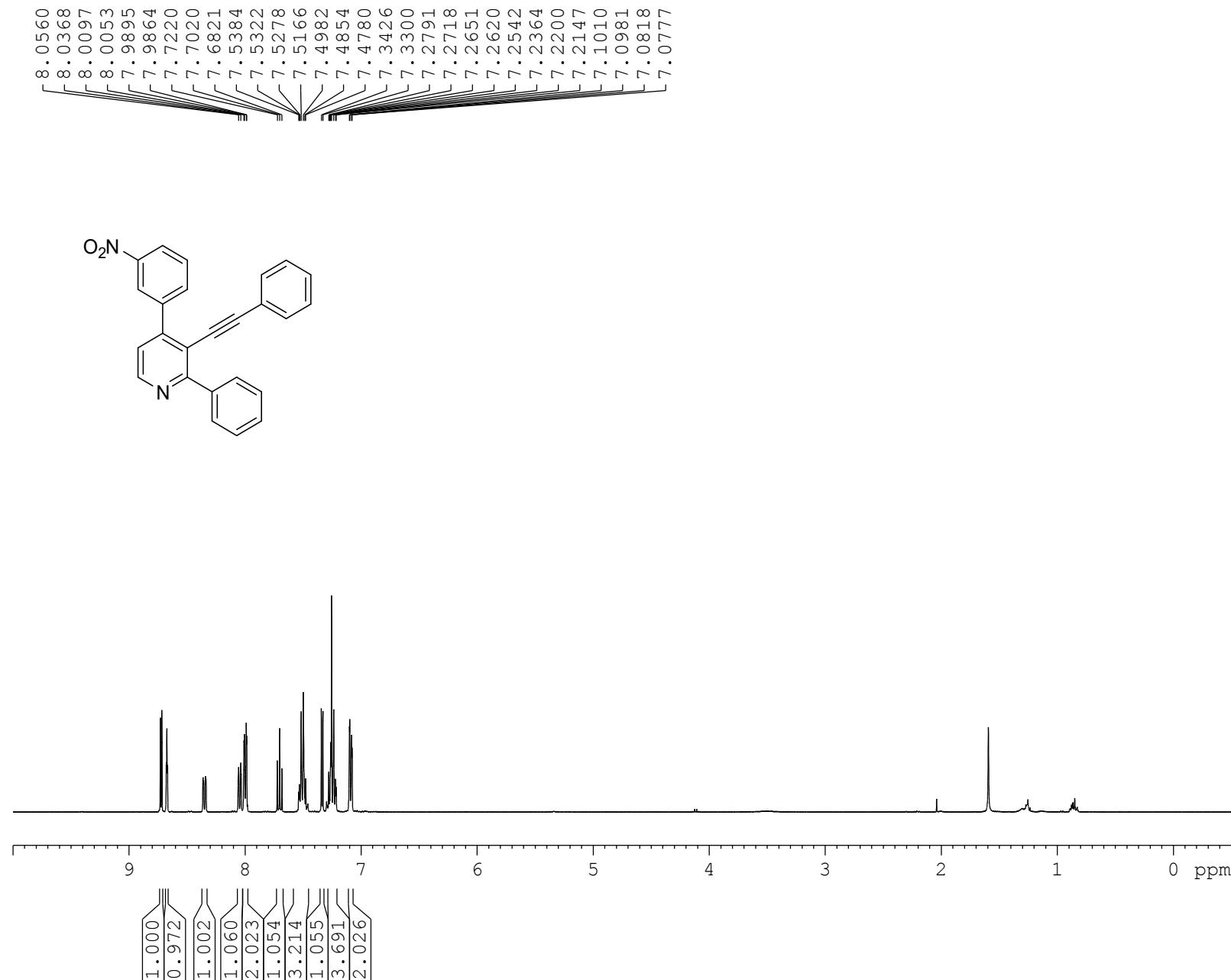
F2 - Acquisition Parameters  
 Date 20160313  
 Time 13.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 1500  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 198.09  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.1 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 ======  
 SFO1 100.6228298 MHz  
 NUC1 <sup>13</sup>C  
 P1 10.00 usec  
 PLW1 47.5000000 W

===== CHANNEL f2 ======  
 SFO2 400.1316005 MHz  
 NUC2 <sup>1</sup>H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.27338001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127482 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 1.00

4-(3-nitrophenyl)-2-phenyl-3-(phenylethynyl)pyridine (10d) 1



Current Data Parameters  
NAME TRY  
EXPNO 163  
PROCNO 1

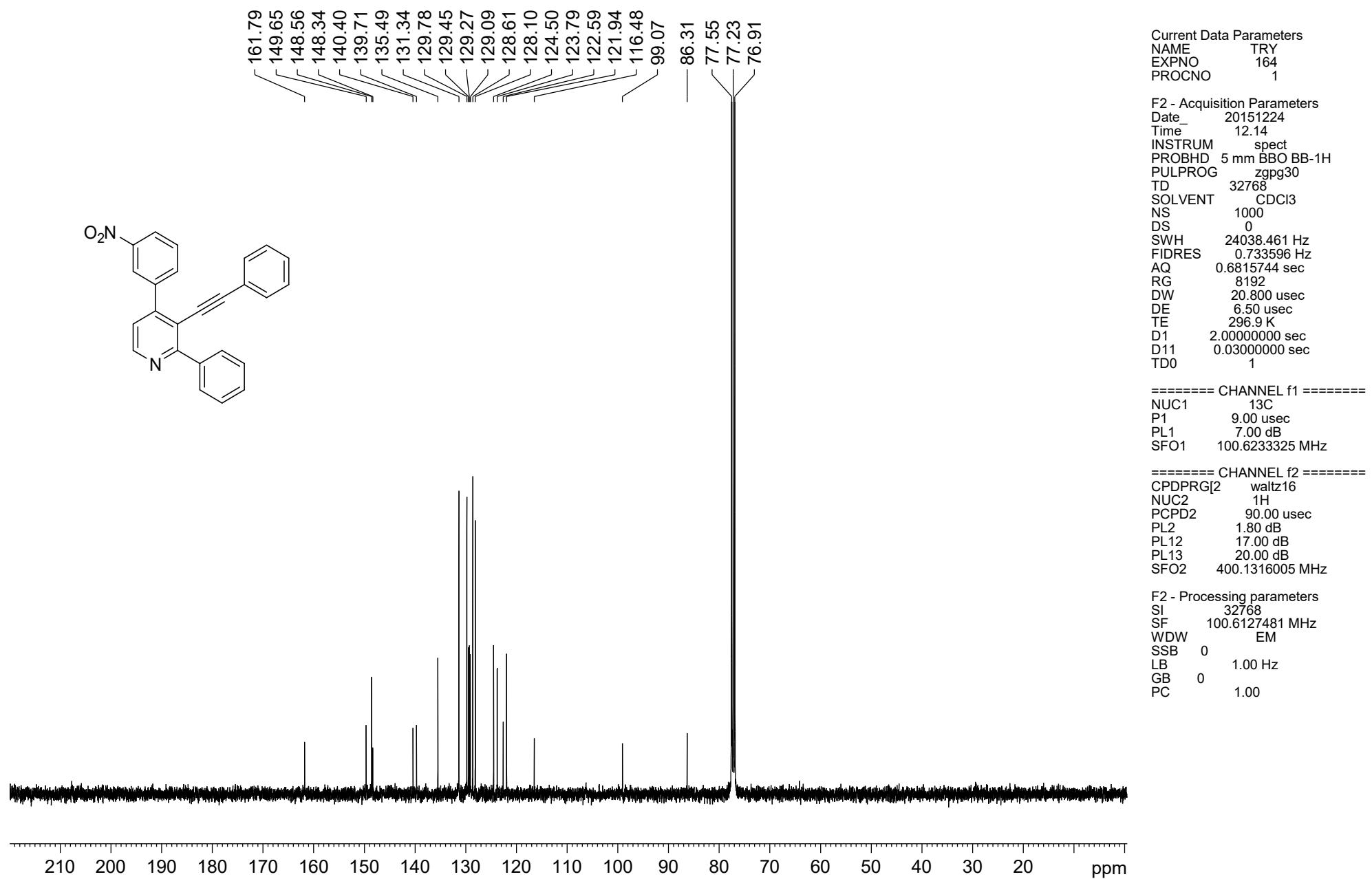
F2 - Acquisition Parameters  
Date 20151224  
Time 12.10  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 64  
DS 0  
SWH 7246.377 Hz  
FIDRES 0.221142 Hz  
AQ 2.2609921 sec  
RG 228.1  
DW 69.000 usec  
DE 6.50 usec  
TE 296.9 K  
D1 2.0000000 sec  
TDO 1

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

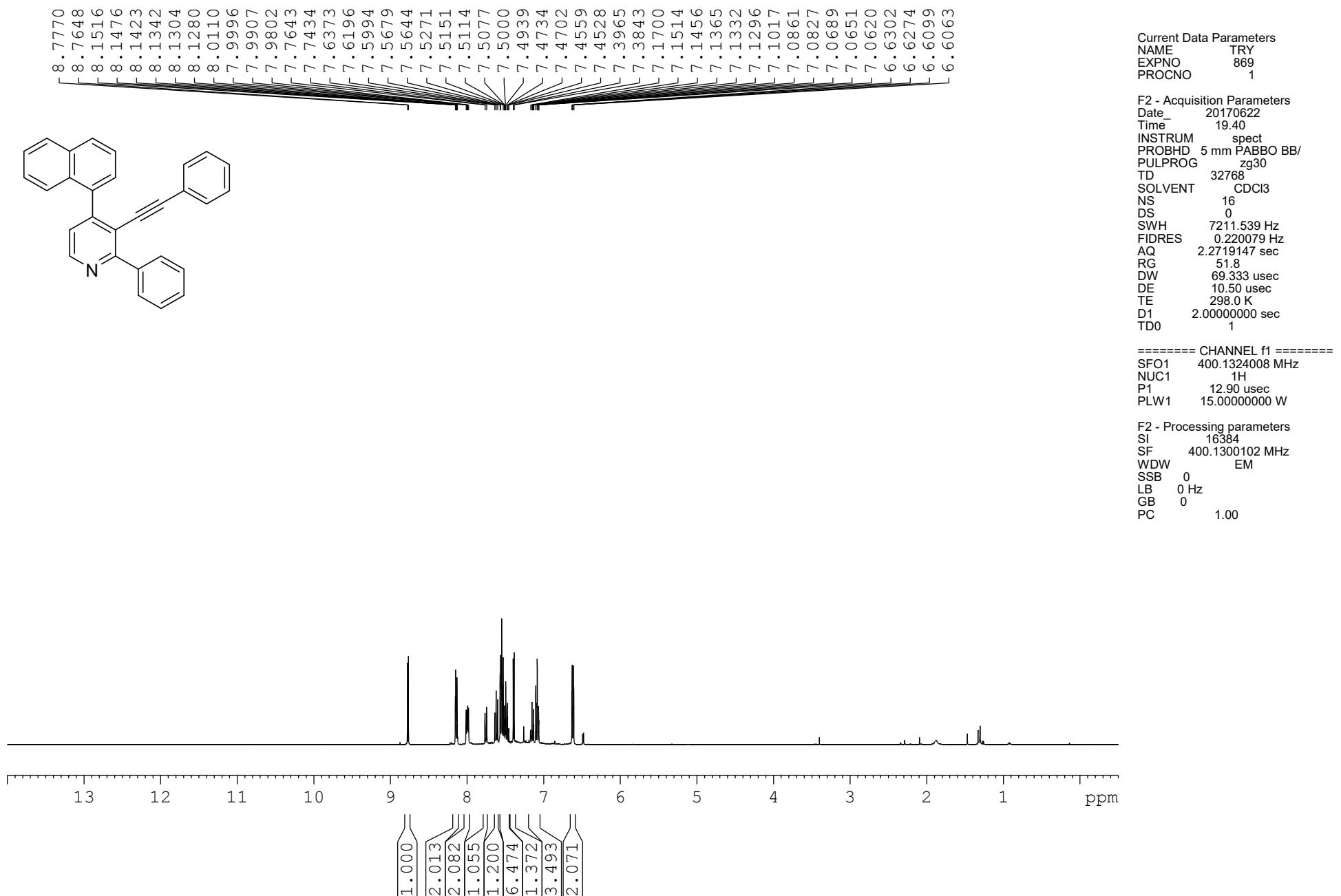
NUC1 1H  
P1 14.40 usec  
PL1 1.80 dB  
SFO1 400.1324008 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1300118 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

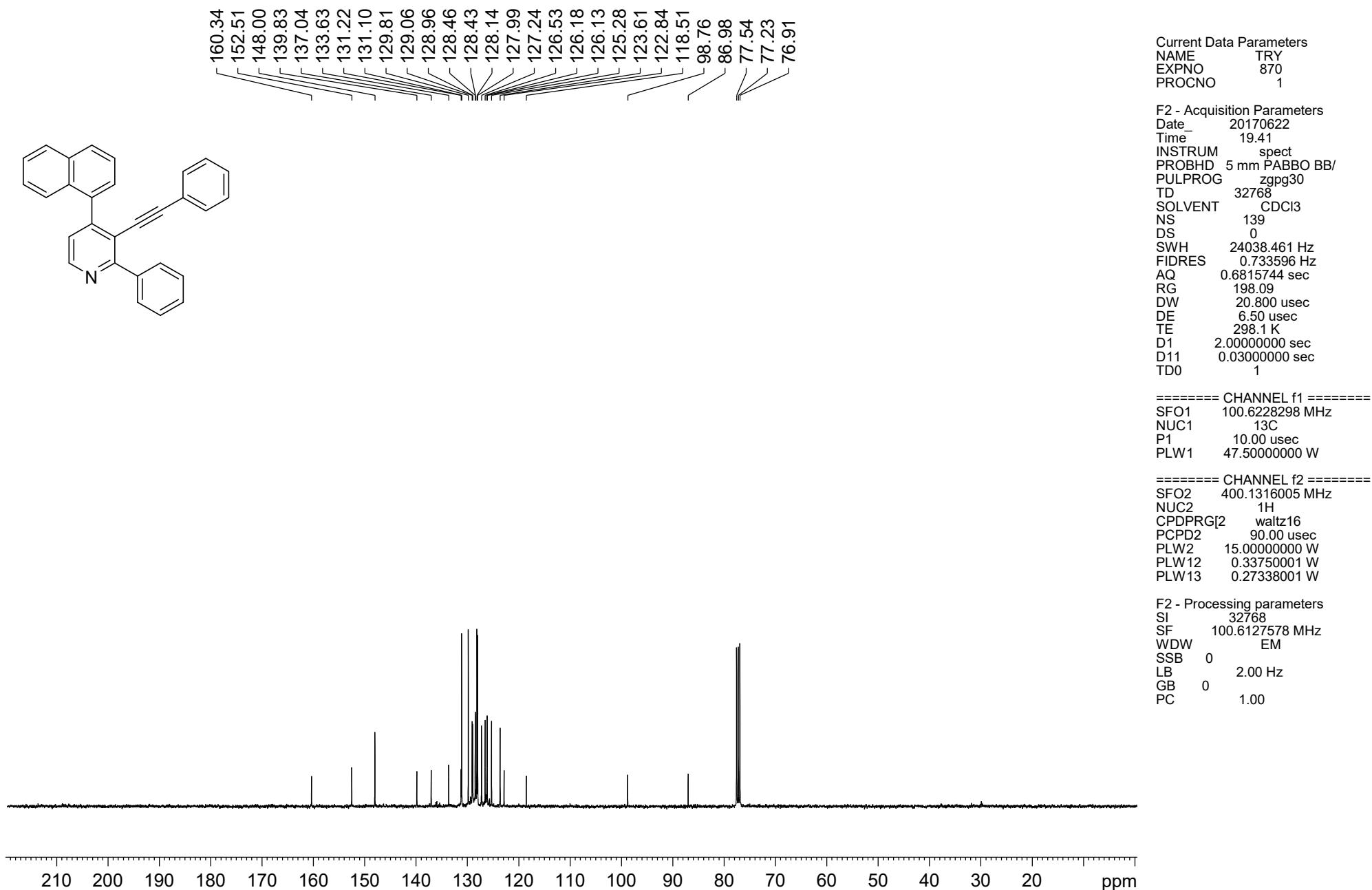
4-(3-nitrophenyl)-2-phenyl-3-(phenylethyynyl)pyridine (10d)



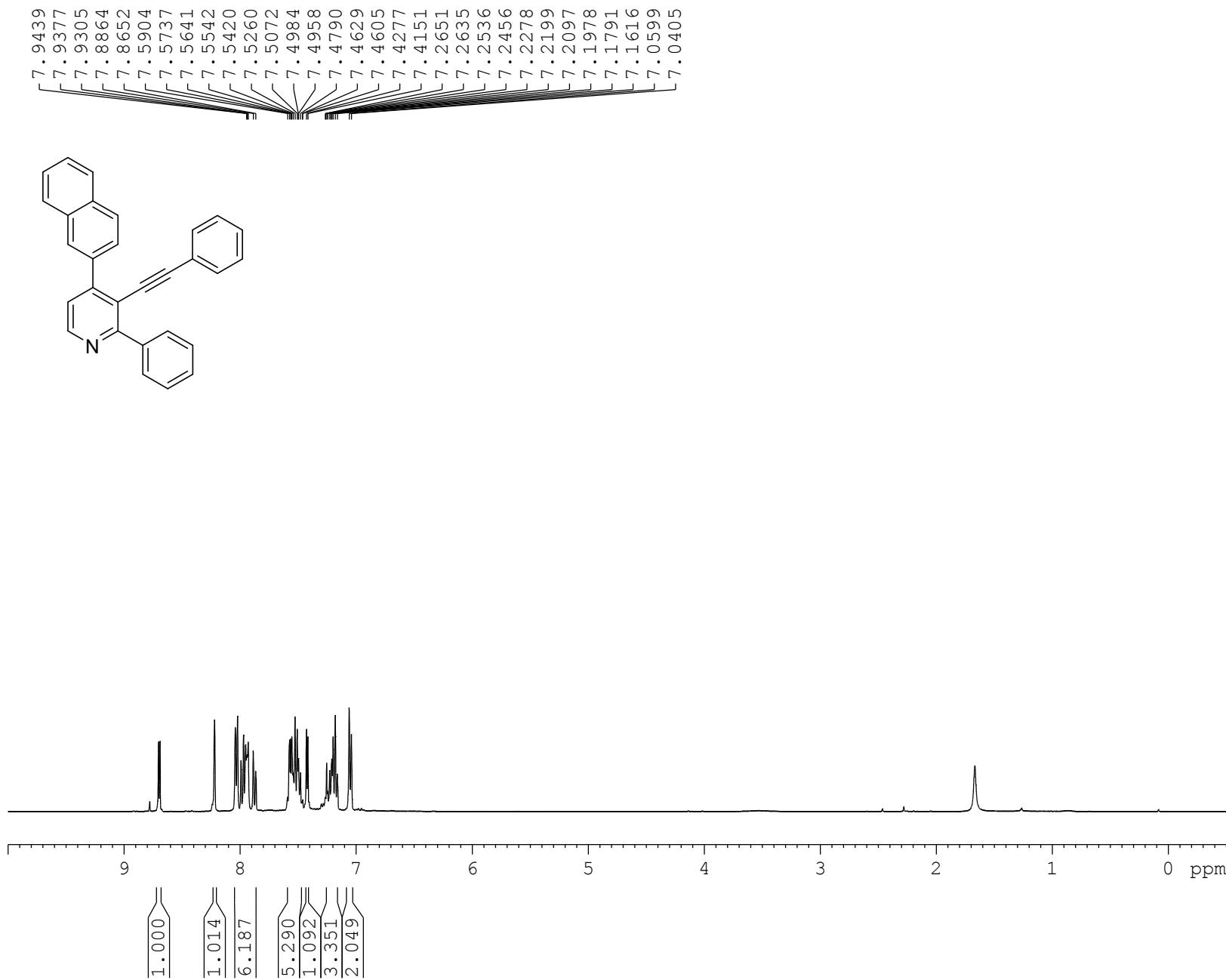
4-(naphthalen-1-yl)-2-phenyl-3-(phenylethyynyl)pyridine (10e)



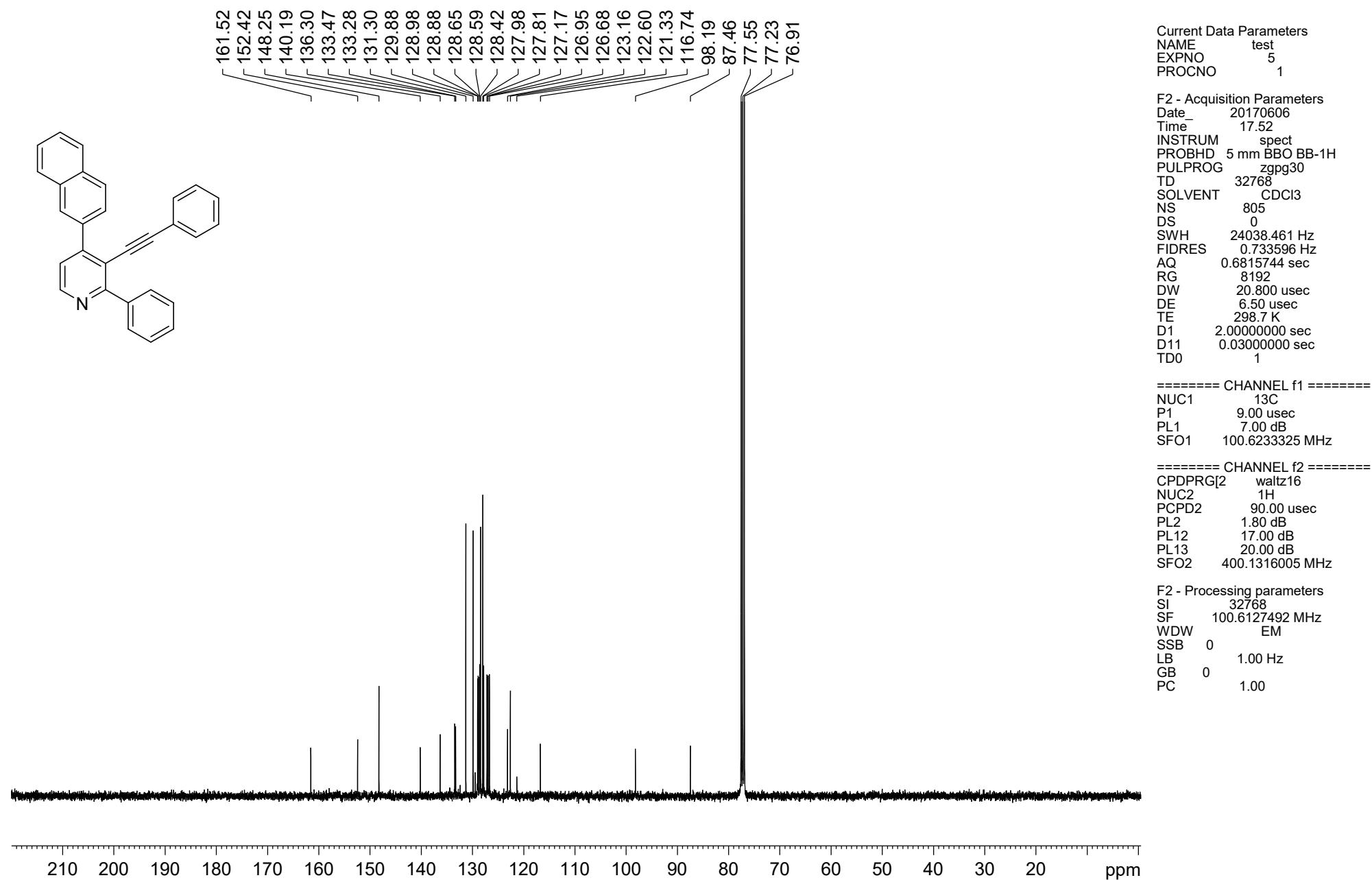
4-(naphthalen-1-yl)-2-phenyl-3-(phenylethynyl)pyridine (10e)



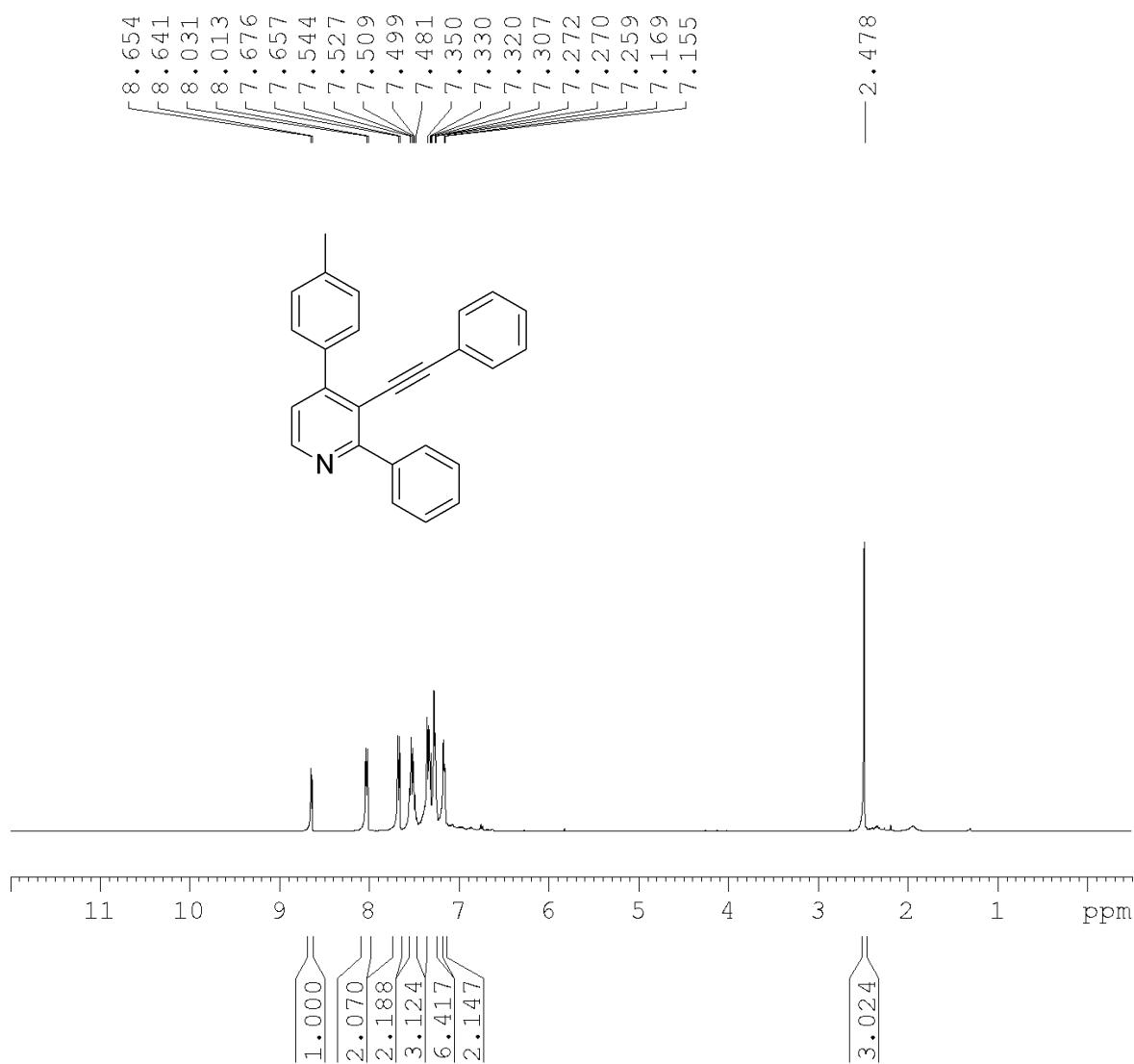
4-(naphthalen-2-yl)-2-phenyl-3-(phenylethynyl)pyridine (10f)



4-(naphthalen-2-yl)-2-phenyl-3-(phenylethyynyl)pyridine (10f)



2-phenyl-3-(phenylethyynyl)-4-(p-tolyl)pyridine (10g)



Current Data Parameters

NAME	vl
EXPNO	26
PROCNO	1

F2 - Acquisition Parameters

Date_	20170819
Time	18.10
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	64
DS	0
SWH	7246.377 Hz
FIDRES	0.221142 Hz
AQ	2.2609921 sec
RG	45.3
DW	69.000 usec
DE	6.50 usec
TE	297.8 K
D1	2.00000000 sec
TDO	1

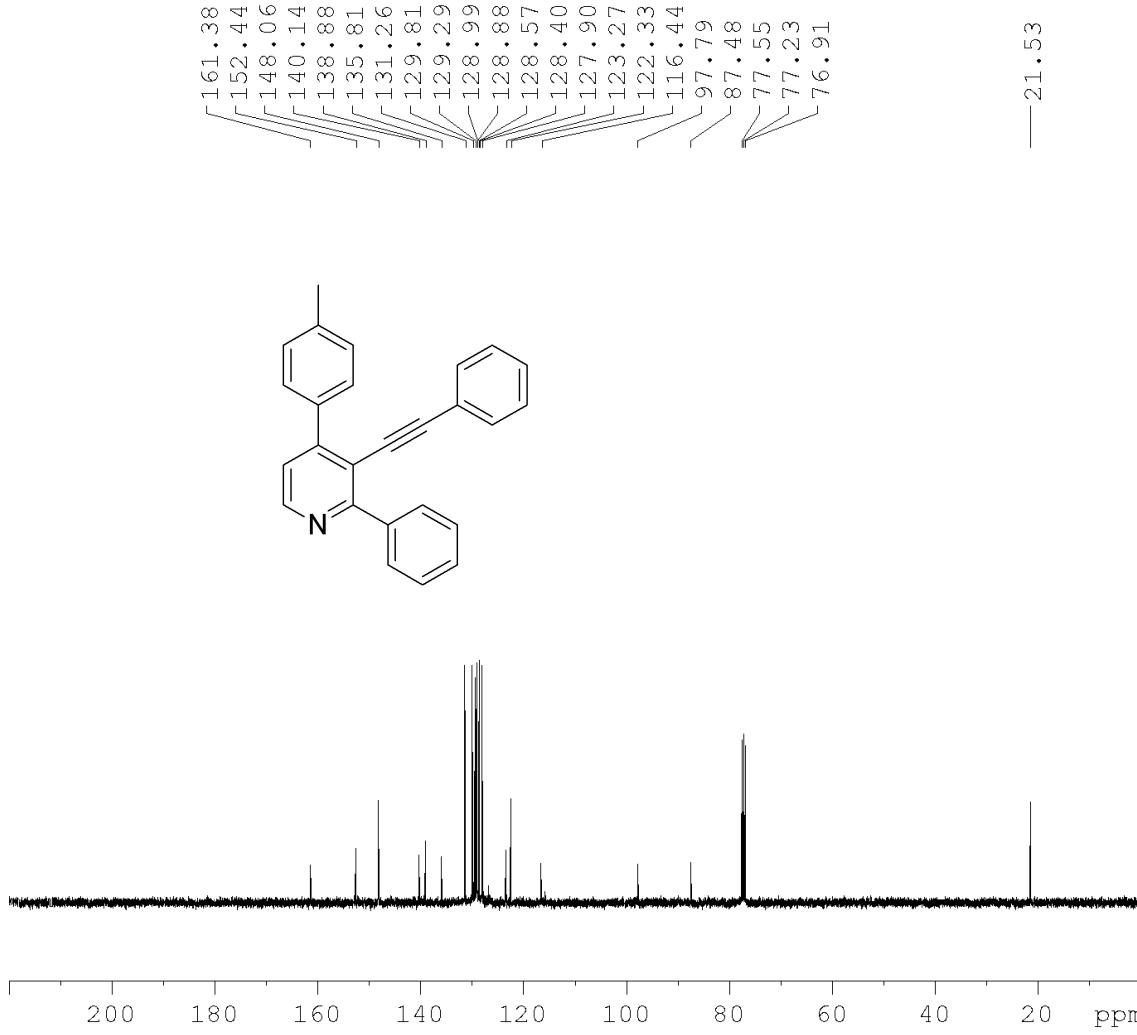
===== CHANNEL f1 =====

NUC1	1H
P1	15.00 usec
PL1	0 dB
SFO1	400.1324008 MHz

F2 - Processing parameters

SI	16384
SF	400.1300118 MHz
WDW	EM
SSB	0
LB	0 Hz
GB	0
PC	1.00

2-phenyl-3-(phenylethynyl)-4-(p-tolyl)pyridine (10g)



Current Data Parameters

NAME vl  
EXPNO 27  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170819  
Time 18.43  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zqpg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 81  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 5792.6  
DW 20.800 use  
DE 6.50 use  
TE 298.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

NUC1 <sup>13</sup>C  
P1 10.45 use  
PL1 7.00 dB  
SFO1 100.6233325 MHz

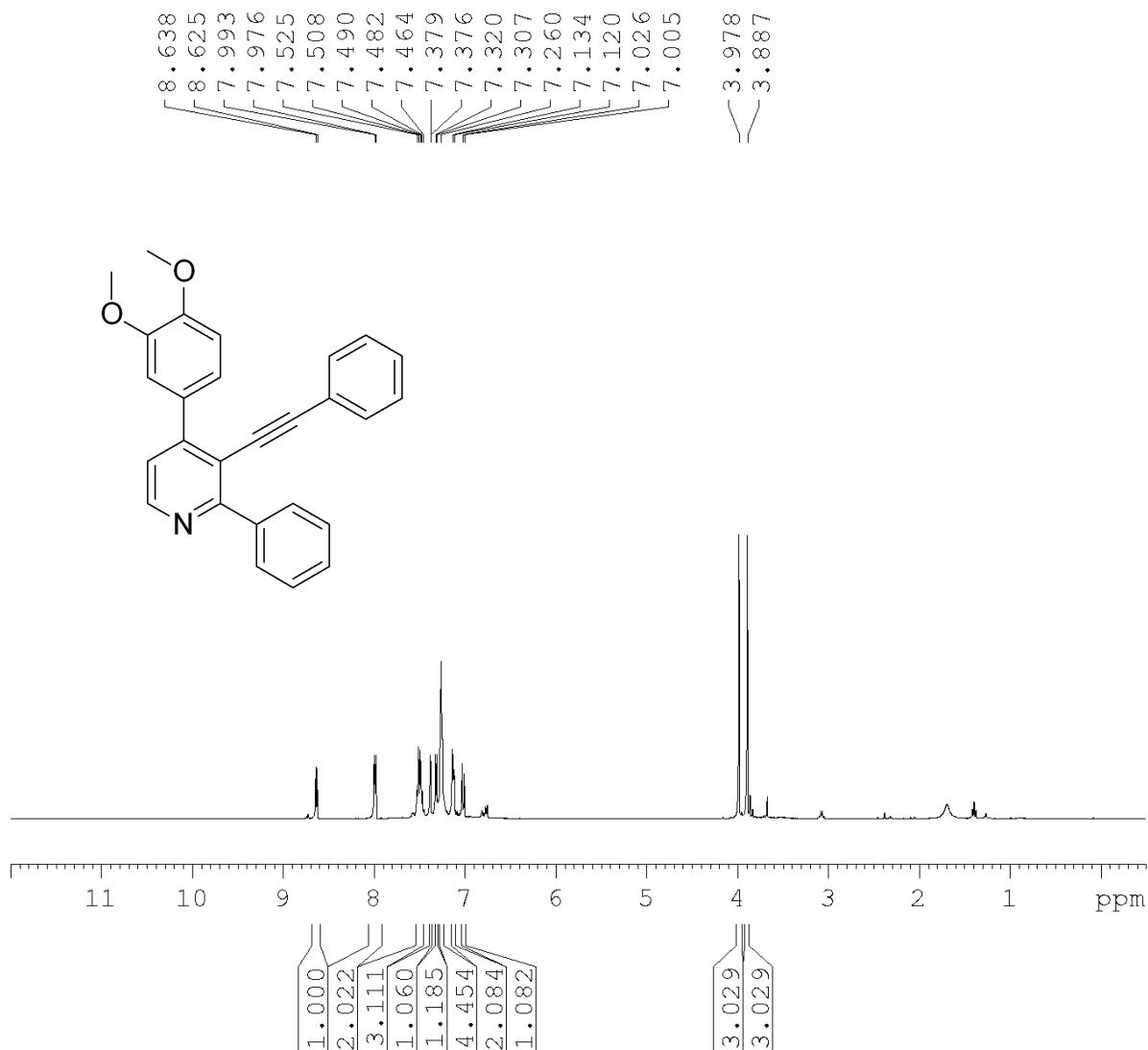
===== CHANNEL f2 =====

CPDPRG[2] waltz16  
NUC2 <sup>1</sup>H  
PCPD2 90.00 use  
PL2 0 dB  
PL12 15.00 dB  
PL13 20.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127580 MHz

4-(3,4-dimethoxyphenyl)-2-phenyl-3-(phenylethynyl)pyridine (10h)



Current Data Parameters

NAME vl  
EXPNO 34  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170828  
Time 19.33  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 64  
DS 0  
SWH 7246.377 Hz  
FIDRES 0.221142 Hz  
AQ 2.2609921 sec  
RG 114  
DW 69.000 usec  
DE 6.50 usec  
TE 297.9 K  
D1 2.00000000 sec  
TDO 1

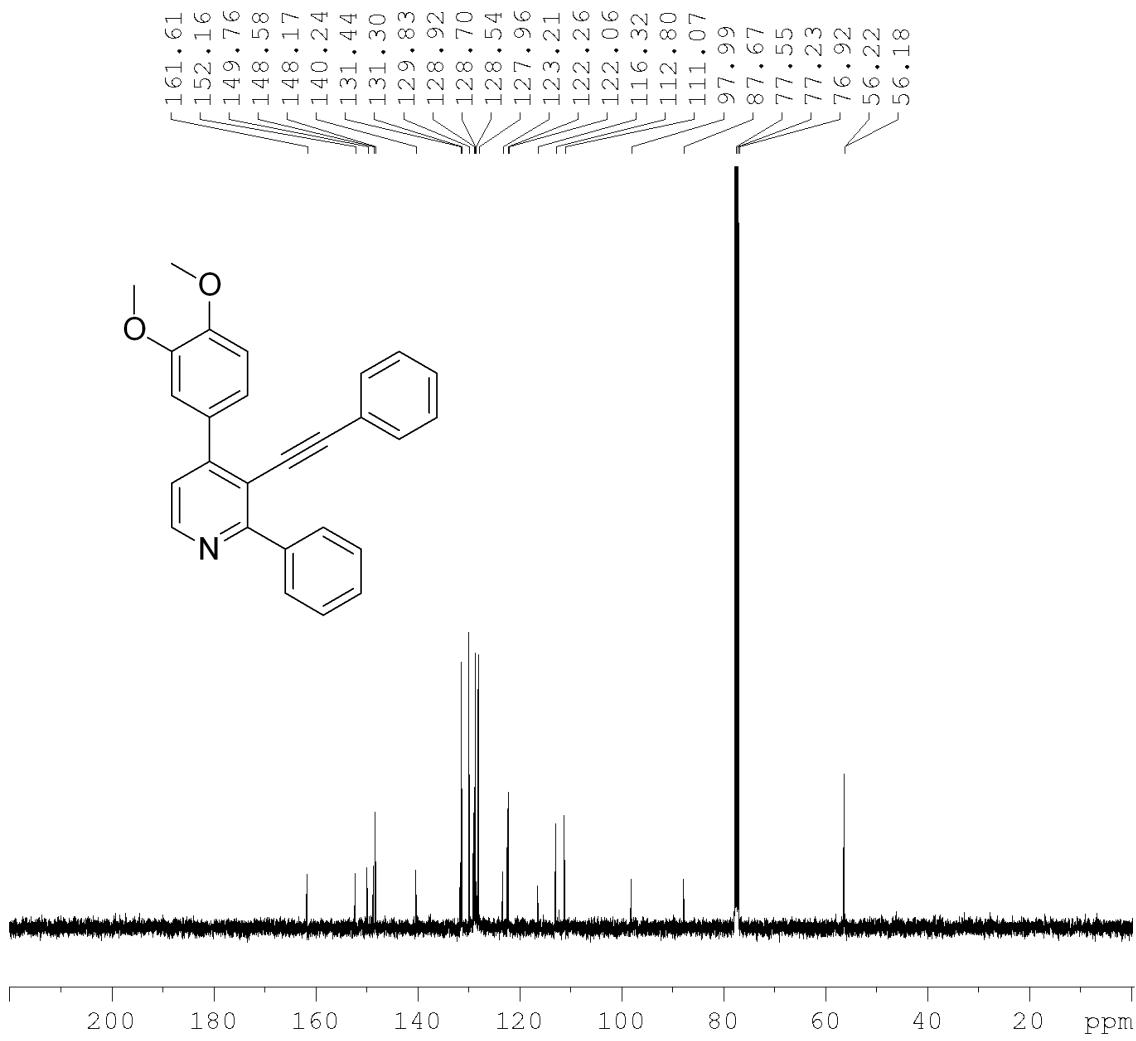
===== CHANNEL f1 =====

NUC1 1H  
P1 15.00 usec  
PL1 0 dB  
SFO1 400.1324008 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300091 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

4-(3,4-dimethoxyphenyl)-2-phenyl-3-(phenylethynyl)pyridine (10h)



Current Data Parameters

NAME	vl
EXPNO	35
PROCNO	1

F2 - Acquisition Parameters

Date_	20170828
Time	19.41
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl <sub>3</sub>
NS	524
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6815744 sec
RG	5792.6
DW	20.800 use
DE	6.50 use
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

NUC1	<sup>13</sup> C
P1	10.45 use
PL1	7.00 dB
SFO1	100.6233325 MHz

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

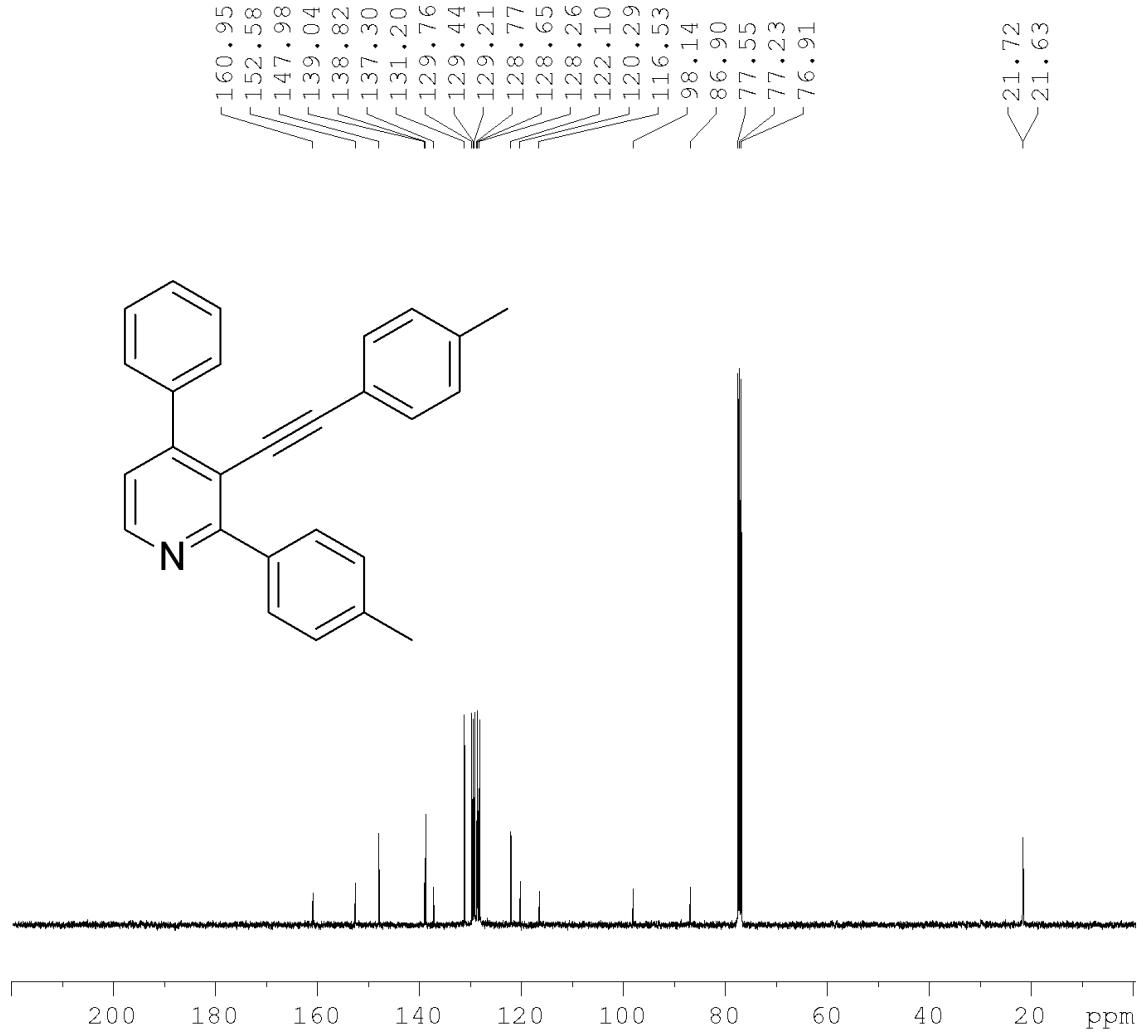
CPDPRG[2]	waltz16
NUC2	<sup>1</sup> H
PCPD2	90.00 use
PL2	0 dB
PL12	15.00 dB
PL13	20.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127492 MHz



4-phenyl-2-(p-tolyl)-3-(p-tolylethynyl)pyridine (10i)



Current Data Parameters

NAME vl  
EXPNO 896  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170819  
Time 15.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zpgg30  
TD 32768  
SOLVENT CDCl3  
NS 647  
DS 0  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 198.09  
DW 20.800 use  
DE 6.50 use  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

SFO1 100.6228298 MHz  
NUC1 13C  
P1 10.00 use  
PLW1 47.50000000 W

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

SFO2 400.1316005 MHz  
NUC2 1H  
CPDPG[2] waltz16  
PCPD2 90.00 use  
PLW2 15.00000000 W  
PLW12 0.33750001 W  
PLW13 0.27338001 W

F2 - Processing parameters

SI 32768  
SF 100.6127494 MHz