Supplementary information

Palladacycles of novel bisoxazoline chelating ligands based on the dimeric cyclobutadiene linked cobalt sandwich compound $[(\eta^5\text{-Cp})Co(\eta^4\text{-}C_4Ph_3)]_2$

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Table 1. Selected bond lengths and bond angles of compound **1**

Bond Lengths (Å)

Co(1)-C(1)	2.057(3)	Co(1)-C(6)	2.010(3)
O(1)-C(10)	1.211(5)	O(2)-C(10)	1.344(5)
O(2)-C(11)	1.450(5)	C(1)-C(2)	1.432(5)
C(1)-C(10)	1.459(6)	C(6)-C(7)	1.475(5)
C(7)-C(12)	1.477(5)	C(7)-C(8)	1.460(5)

Bond Angles (deg)

C(1)-Co(1)-C(9)	122.4(2)	O(1)-C(10)-C(1)	124.5(4)
O(1)-C(10)-O(2)	124.0(4)	C(10)-O(2)-C(11)	116.5(3)
C(1)-C(2)-C(3)	107.7(3)	C(6)-C(7)-C(8)	89.7(3)

Table 2. Selected bond lengths and bond angles of compound **3**

Bond Lengths (Å)

O(1)-C(10)	1.355(5)	O(1)-C(11)	1.464(4)
N(1)-C(10)	1.272(5)	N(1)-C(12)	1.481(5)
C(1)-C(10)	1.463(5)	C(1)-C(2)	1.424(5)

C(11)-C(12)	1.533(5)	C(12)-C(13)	1.526(5)
C(1)-Co(1)	2.100(4)	Co(1)-C(6)	2.023(4)
C(6)-C(7)	1.465(5)	C(6)-C(21)	1.443(3)

Bond Angles (deg)

O(1)-C(10)-N(1)	119.3(4)	O(1)-C(10)-C(1)	113.8(3)
C(10)-N(1)-C(12)	105.9(3)	C(10)-O(1)-C(11)	104.8(3)
N(1)-C(12)-C(13)	113.8(3)	C(1)-C(10)-N(1)	126.9(4)
C(5)-C(1)-C(10)	126.6(3)	C(14)-C(13)-C(15)	111.1(3)
C(1)-Co(1)-C(6)	117.5(2)	C(1)-C(2)-C(3)	107.6(3)
C(7)-C(6)-C(21)	134.3(3)	C(7)-C(6)-C(9)	90.1(3)

Table 3. Selected bond lengths and bond angles of compound **4**

Bond Lengths (Å)

Pd(1)-O(3)	2.098(2)	Pd(1)-N(1)	2.054(3)
Pd(1)-C(2)	1.977(3)	Pd(1)-N(2)	2.017(3)
C(1)-C(2)	1.436(5)	C(1)-C(10)	1.440(5)
N(1)-C(10)	1.288(5)	C(16)-C(20)	1.425(6)
N(2)-C(25)	1.293(5)	C(16)-C(25)	1.451(6)

C(10)-O(1)	1.322(5)	C(25)-O(2)	1.347(5)
O(1)-C(11)	1.469(5)	O(2)-C(26)	1.455(5)
N(1)-C(12)	1.468(5)	N(2)-C(27)	1.481(5)
O(3)-C(67)	1.233(4)	O(4)-C(67)	1.249(5)

Bond Angles (deg)

N(1)-Pd(1)-O(3)	98.8(1)	N(1)-Pd(1)-C(2)	80.3(2)
N(2)-Pd(1)-O(3)	89.6(1)	N(2)-Pd(1)-C(2)	91.5(1)
Pd(1)-C(2)-C(1)	114.0(3)	Pd(1)-N(1)-C(10)	115.2(3)
N(1)-C(10)-C(1)	117.0(3)	N(2)-C(25)-C(16)	128.7(4)
Pd(1)-C(2)-Co(1)	131.5(2)	C(25)-C(16)-Co(2)	128.6(3)

Table 4. Selected bond lengths and bond angles of compound **5**

Bond Lengths (Å)

Pd(1)-Cl(1)	2.390(1)	Pd(1)-N(1)	2.054(5)
Pd(1)-C(2)	1.978(5)	Pd(1)-N(2)	2.002(5)
C(1)-C(2)	1.418(9)	C(1)-C(10)	1.417(8)
N(1)-C(10)	1.285(7)	C(16)-C(20)	1.437(8)
N(2)-C(25)	1.272(7)	C(16)-C(25)	1.460(8)

C(10)-O(1)	1.344(7)	C(25)-O(2)	1.352(7)
O(1)-C(11)	1.447(7)	O(2)-C(26)	1.461(6)
N(1)-C(12)	1.484(7)	N(2)-C(27)	1.508(7)

Bond Angles (deg)

N(1)-Pd(1)-Cl(1)	96.9(1)	N(1)-Pd(1)-C(2)	80.2(3)
N(2)-Pd(1)-Cl(1)	93.0(1)	N(2)-Pd(1)-C(2)	90.0(2)
Pd(1)-C(2)-C(1)	114.4(5)	Pd(1)-N(1)-C(10)	113.5(4)
N(1)-C(10)-C(1)	119.2(6)	N(2)-C(25)-C(16)	128.6(6)
Pd(1)-C(2)-Co(1)	130.7(3)	C(25)-C(16)-Co(2)	128.3(4)

Table 5. Selected bond lengths and bond angles of compound **6**

Bond Lengths (Å)

O(1)-C(10)	1.318(4)	O(1)-C(11)	1.458(5)
N(1)-C(10)	1.275(4)	N(1)-C(12)	1.440(5)
C(1)-C(10)	1.463(5)	C(1)-C(2)	1.407(5)
C(11)-C(12)	1.514(6)	C(1)-Co(1)	2.105(3)
Co(1)-C(6)	2.032(3)	C(6)-C(7)	1.466(4)

Bond Angles (deg)

O(1)-C(10)-N(1)	119.6(4)	O(1)-C(10)-C(1)	118.9(4)
C(10)-N(1)-C(12)	106.1(3)	C(10)-O(1)-C(11)	105.0(3)
N(1)-C(12)-C(11)	105.1(3)	C(1)-C(10)-N(1)	121.5(4)
C(5)-C(1)-C(10)	127.1(3)	C(1)-Co(1)-C(6)	117.7(1)
C(1)-C(2)-C(3)	108.0(3)	C(7)-C(6)-C(9)	90.0(2)

Table 6. Selected bond lengths and bond angles of compound **7**

Bond Lengths (Å)

Co(1)-C(1)	2.083(3)	Co(1)-C(6)	2.016(3)
C(1)-C(2)	1.407(5)	C(2)-C(3)	1.405(5)
C(6)-C(7)	1.466(4)	C(7)-C(8)	1.465(4)
C(7)-C(10)	1.471(4)	C(8)-C(16)	1.456(5)

Bond Angles (deg)

C(1)-Co(1)-C(6)	112.9(1)	C(1)-C(2)-C(3)	108.8(3)
C(6)-C(7)-C(8)	90.6(2)	C(6)-C(7)-C(10)	134.7(3)
Co(1)-C(7)-C(10)	129.9(2)	C(7)-C(8)-C(9)	89.7(2)

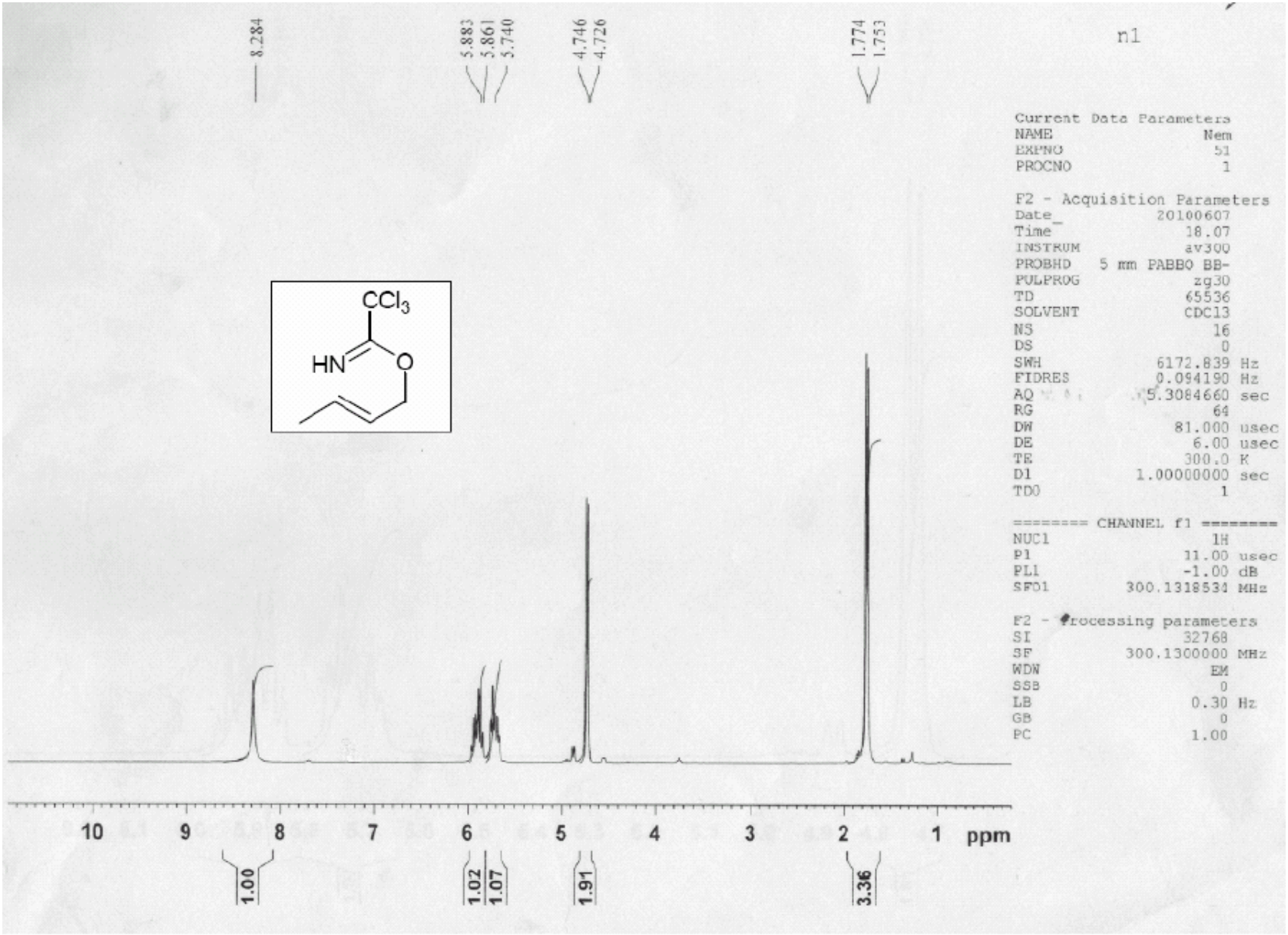
Table 7. Selected bond lengths and bond angles of compound **8**

Bond Lengths (Å)

Co(1)-C(1)	2.068(5)	Co(1)-C(6)	1.993(4)
Co(2)-C(10)	2.069(6)	Co(2)-C(15)	1.984(4)
Co(3)-C(19)	2.052(5)	Co(3)-C(24)	1.990(4)
C(1)-C(2)	1.418(8)	C(6)-C(7)	1.481(6)
C(10)-C(11)	1.393(9)	C(15)-C(16)	1.463(6)
C(6)-C(15)	1.462(6)	C(8)-C(24)	1.449(6)

Bond Angles (deg)

C(3)-Co(1)-C(7)	111.9(2)	C(13)-Co(2)-C(17)	108.4(3)
C(19)-Co(3)-C(24)	112.7(2)	C(1)-C(2)-C(3)	107.8(5)
C(6)-C(7)-C(8)	89.7(3)	C(11)-C(12)-C(13)	107.9(6)
C(15)-C(16)-C(17)	90.4(3)	C(19)-C(20)-C(21)	108.5(6)
C(24)-C(25)-C(26)	89.8(4)	C(6)-C(15)-C(16)	130.9(4)
C(7)-C(6)-C(15)	131.9(4)	C(8)-C(24)-C(27)	130.8(4)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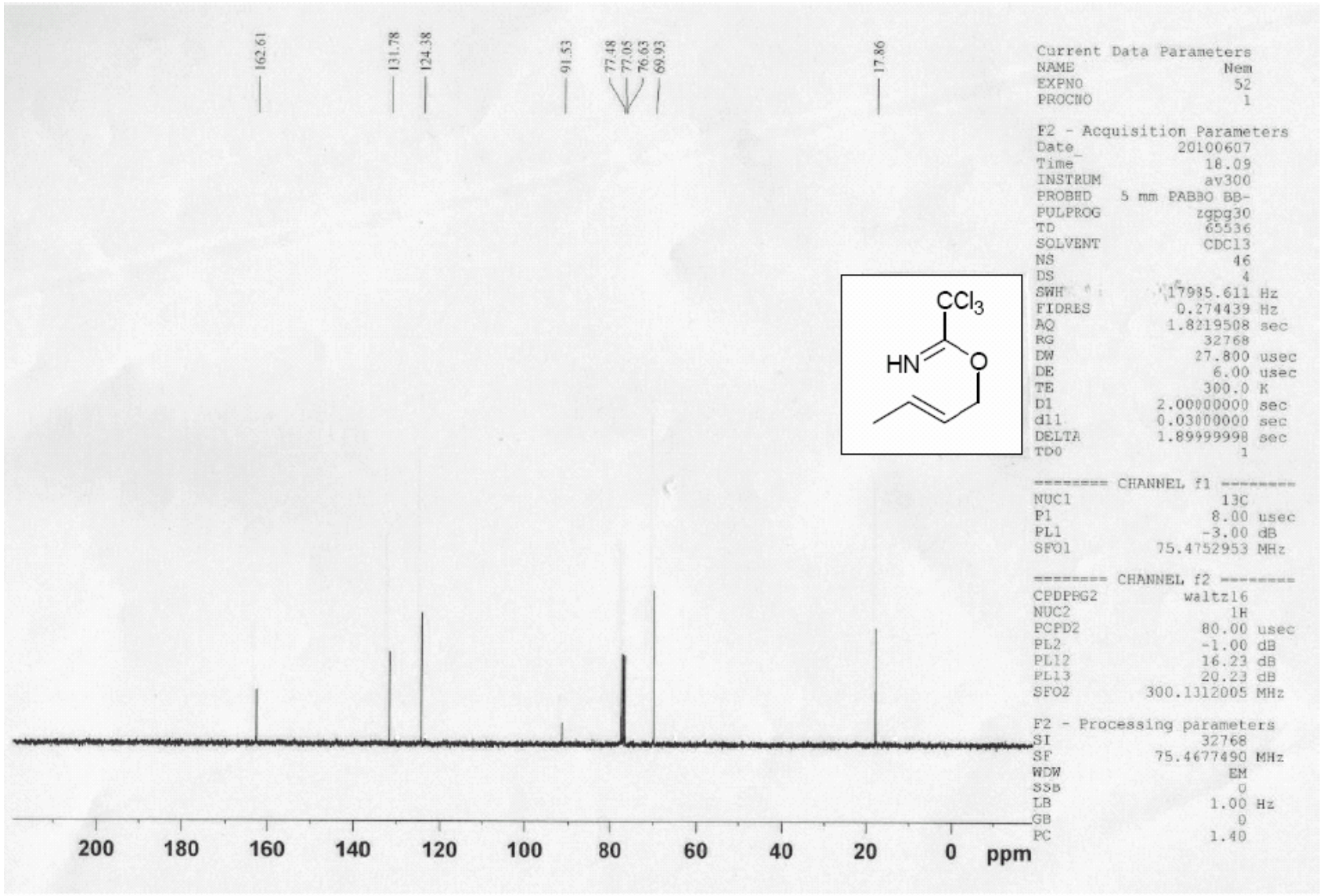
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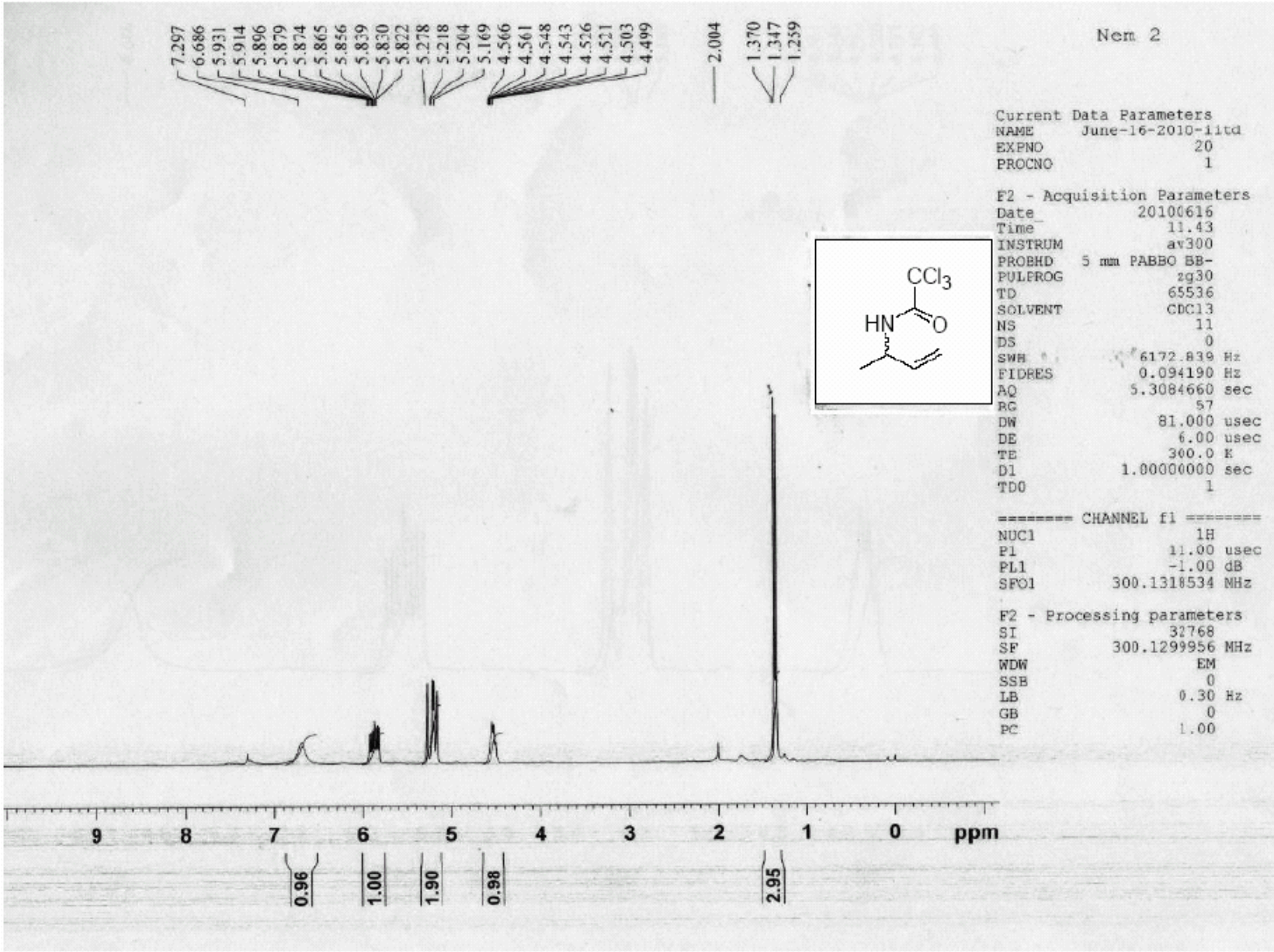
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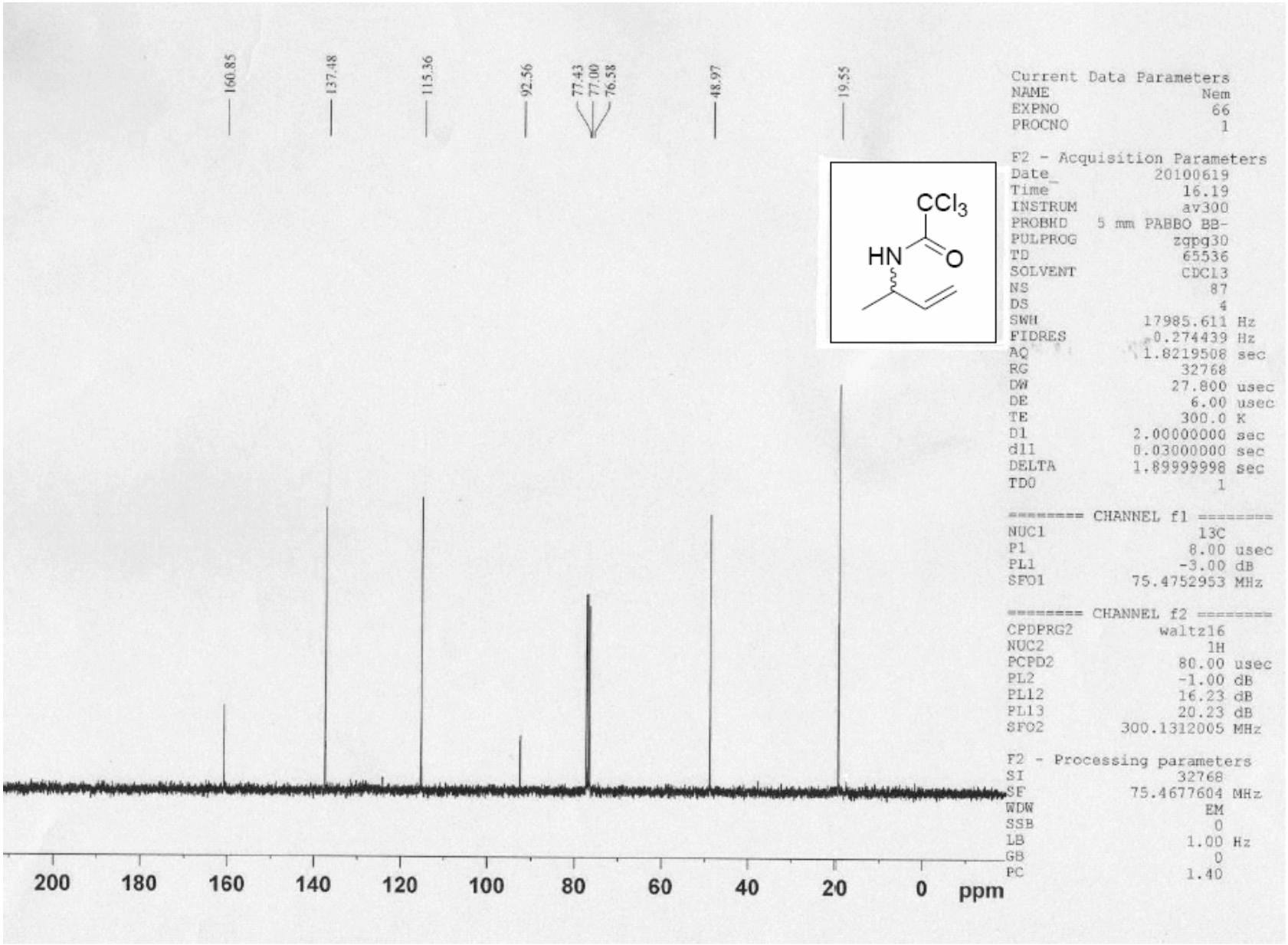
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d11 0.03000000 sec
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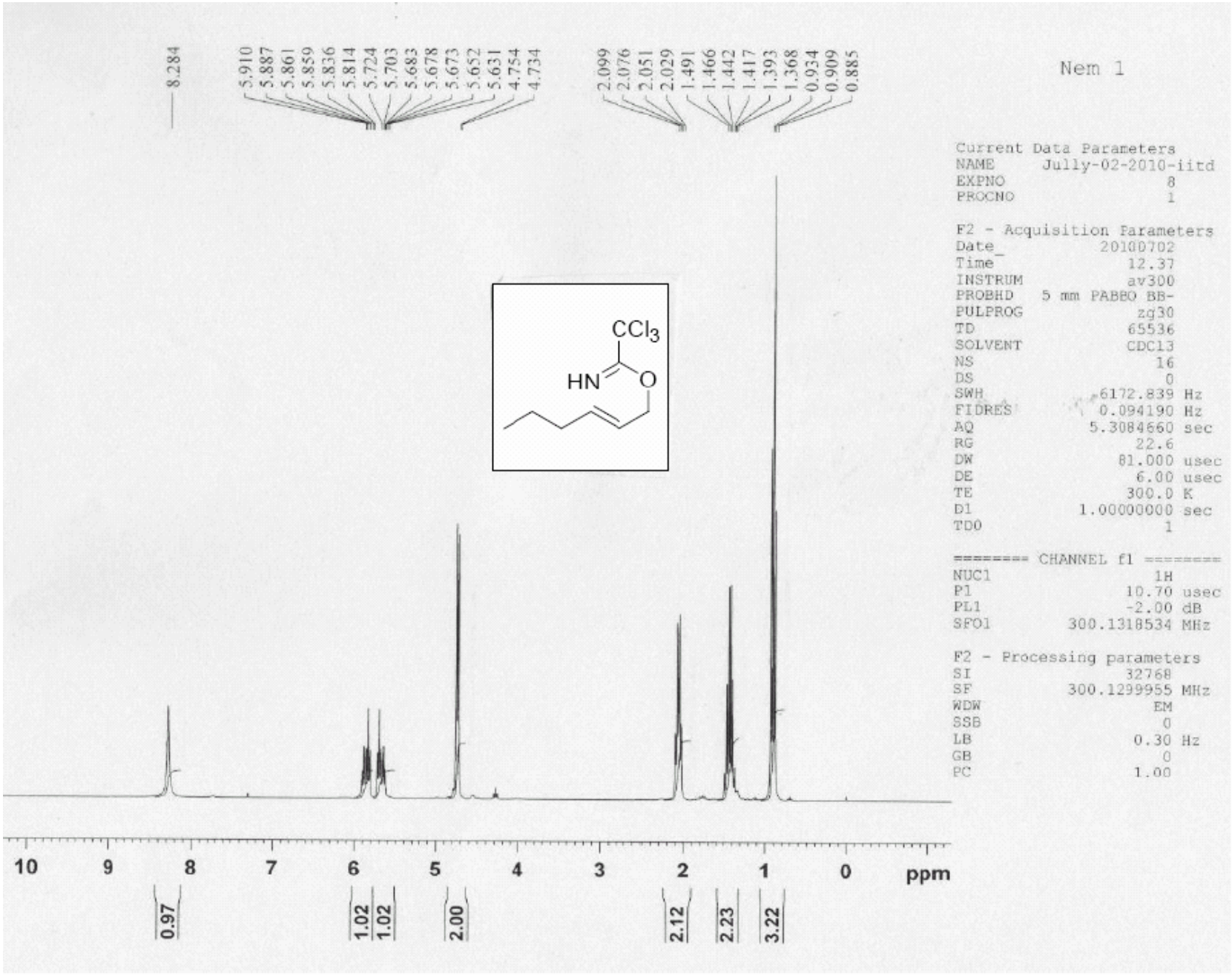
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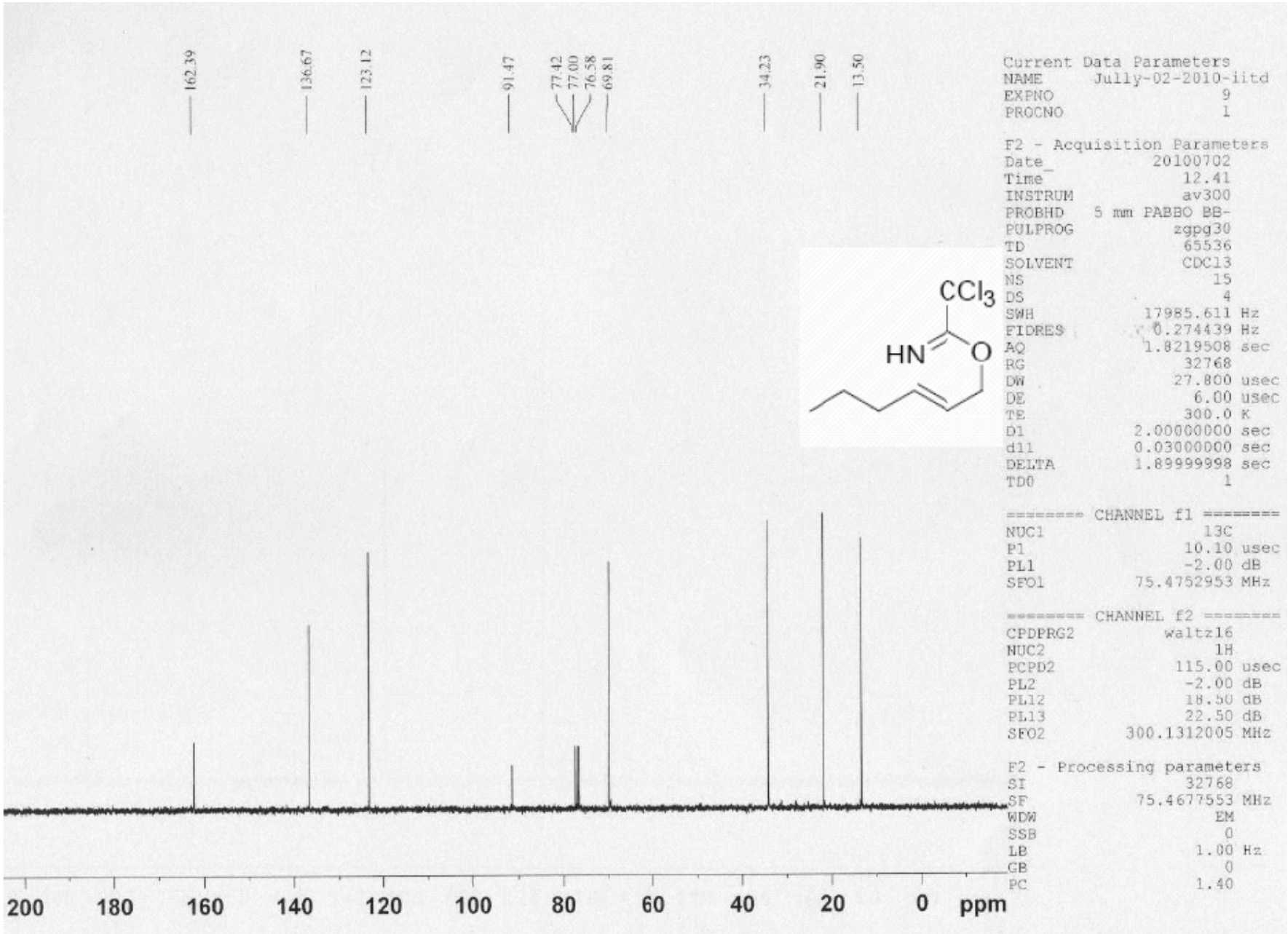
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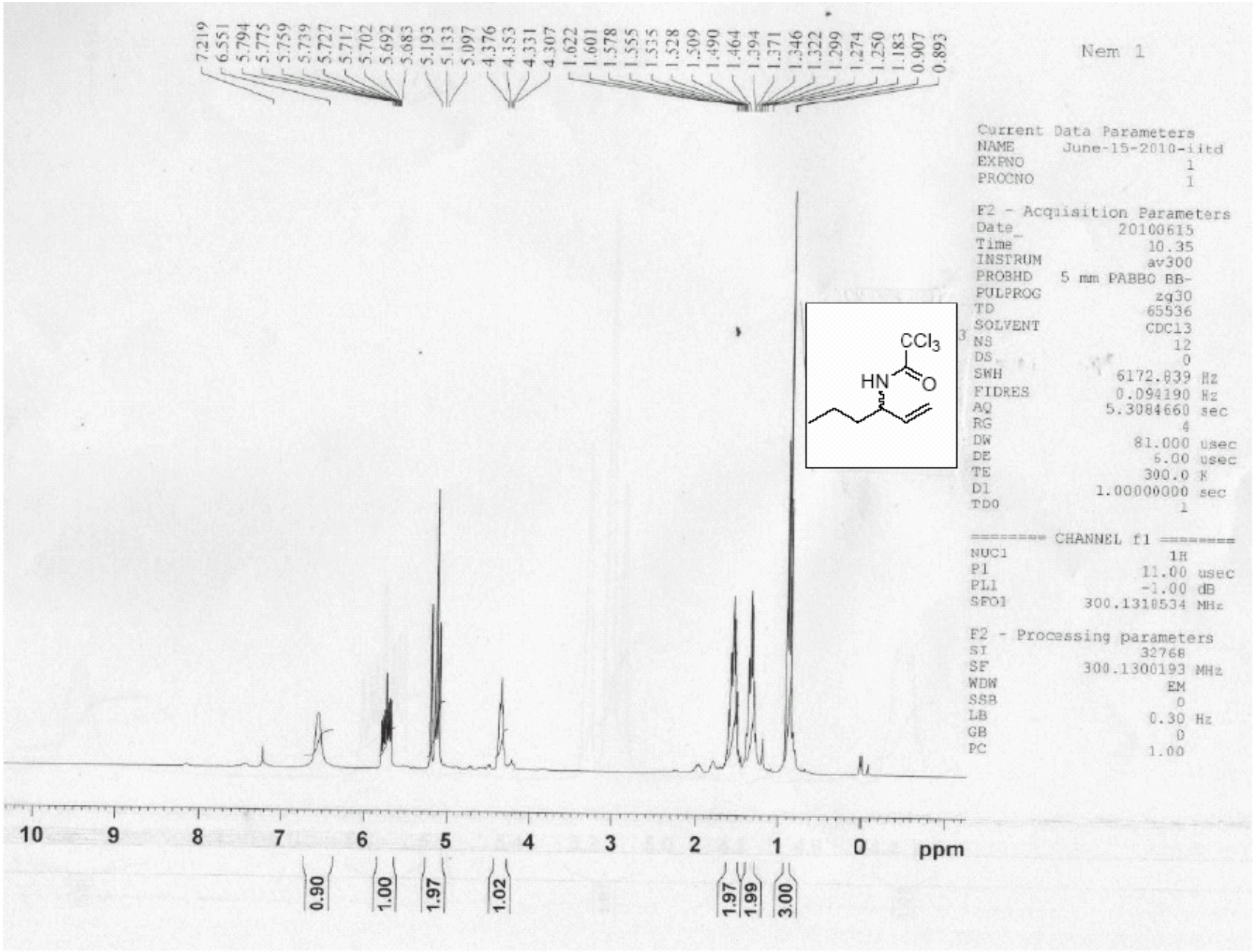
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TE 300.0 K
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TD0 1
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GB 0
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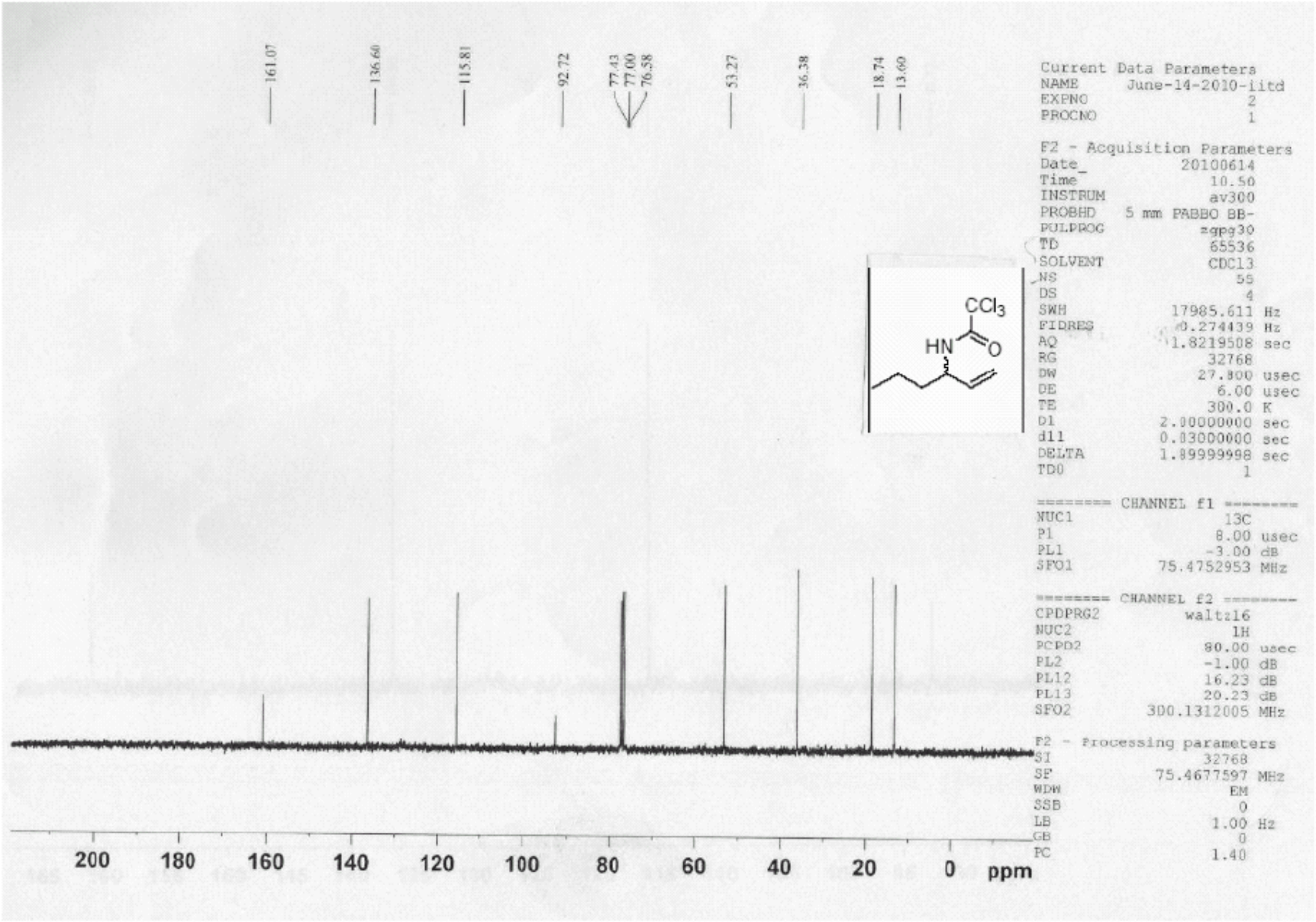
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TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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P1 8.00 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.23 dB
PL13 20.23 dB
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F2 - Processing parameters
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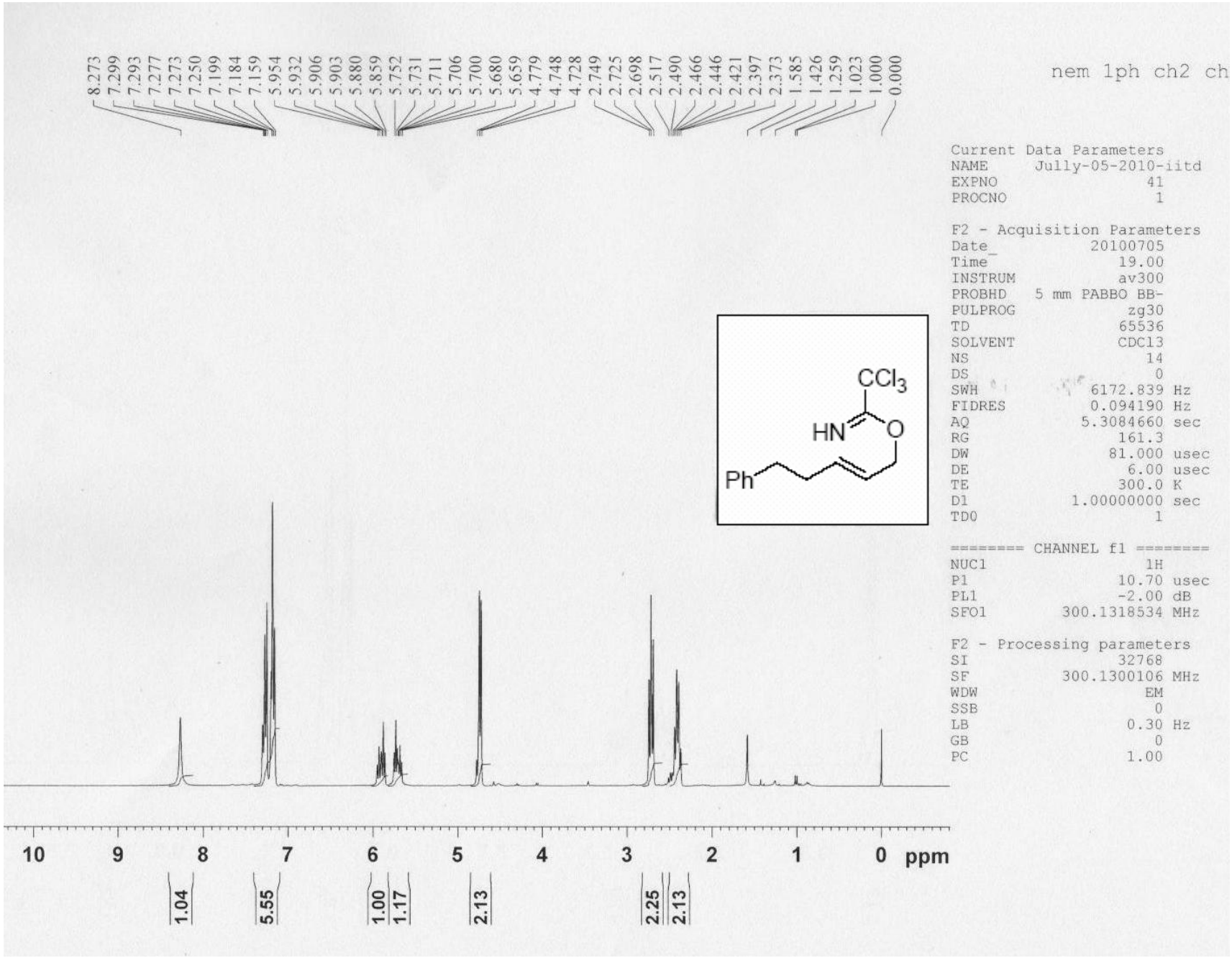
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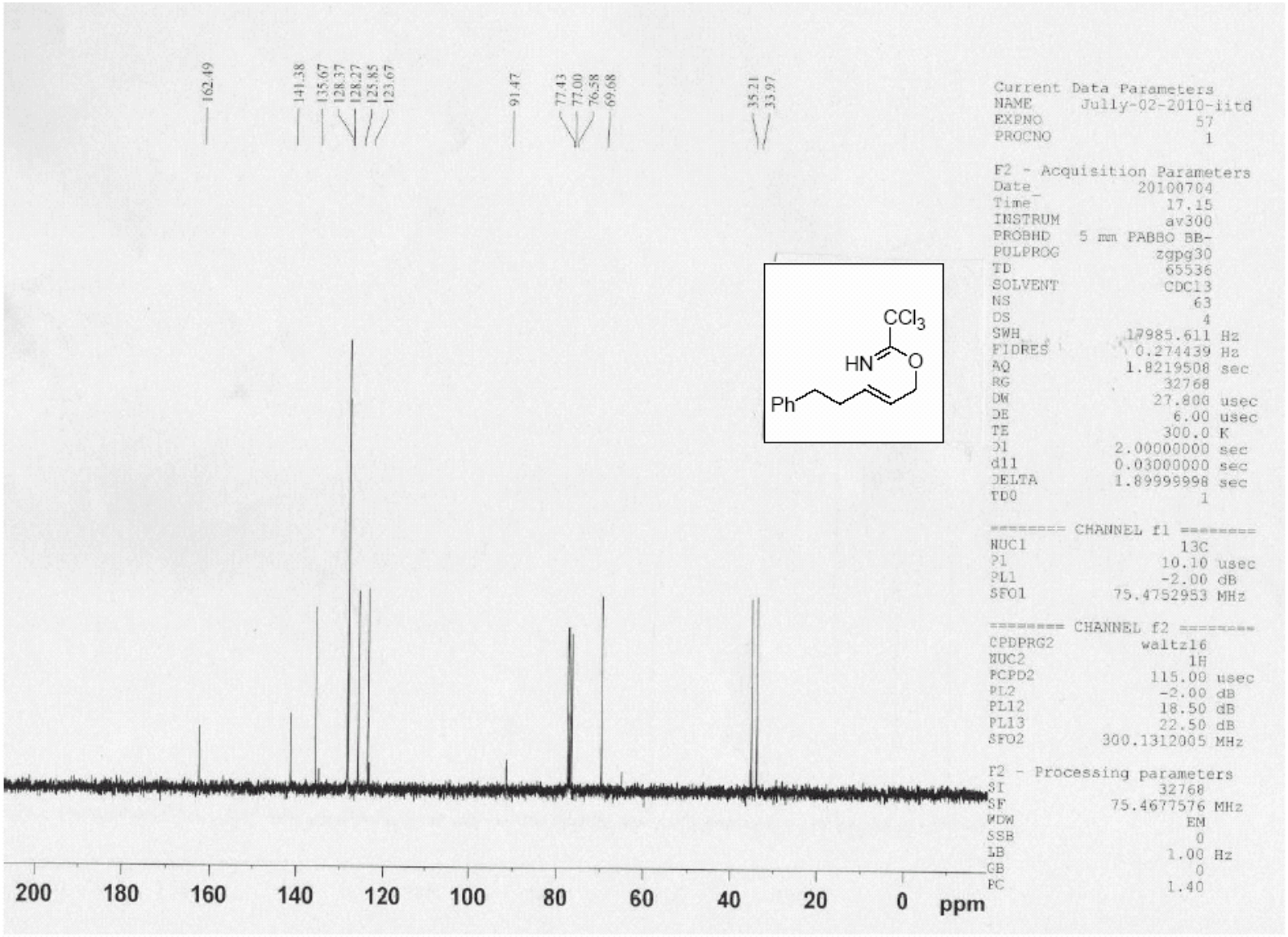
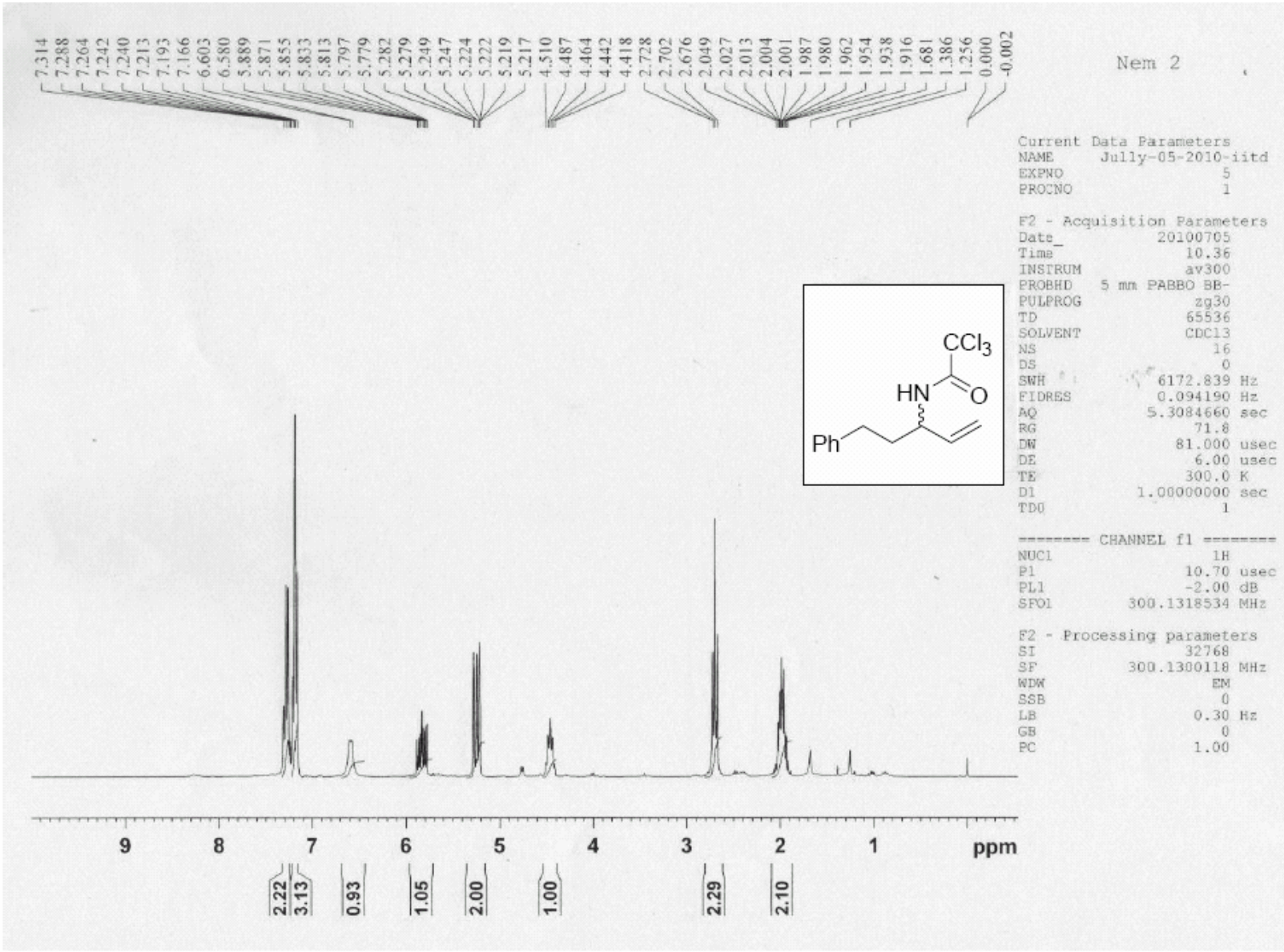
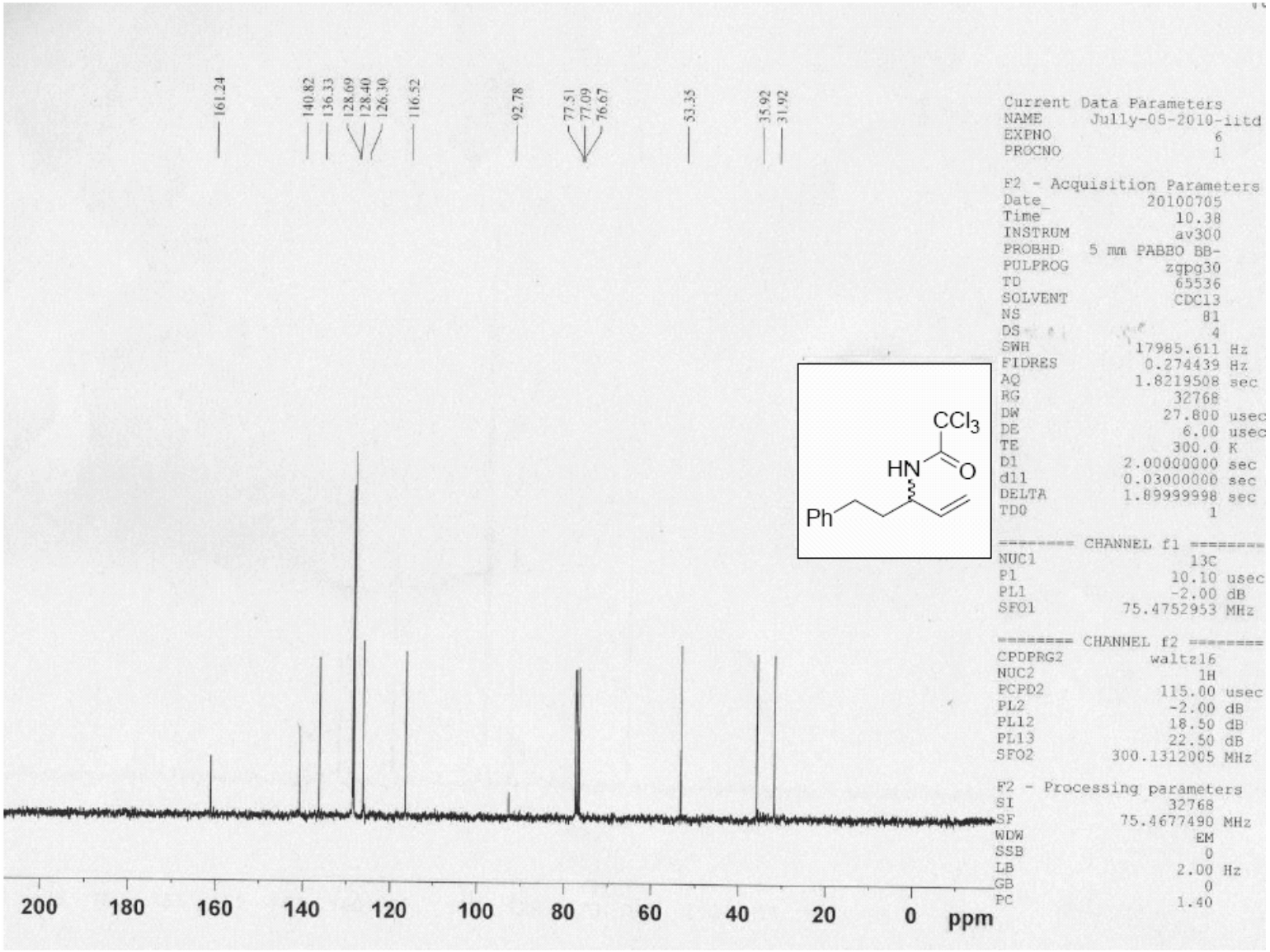
1.259
1.023
1.000
0.000
nem 1ph ch2 ch
Current Data Parameters
NAME Jully-05-2010-iitd
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100705
Time 19.00
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 14
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CCl3
HN
O
Ph
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
5.55
1.00
1.17
2.13
2.25
2.13


162.49
141.38
135.67
128.57
128.27
125.85
123.67
91.47
77.43
77.00
76.58
69.68
35.21
33.97
CCl3
HN
O
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Jully-02-2010-iitd
EXPNO 57
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100704
Time_ 17.15
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 63
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


7.314
7.288
7.264
7.242
7.240
7.213
7.193
7.166
6.603
6.580
5.889
5.871
5.855
5.833
5.813
5.797
5.779
5.282
5.279
5.249
5.247
5.224
5.222
5.219
5.217
4.510
4.487
4.464
4.442
4.418
2.728
2.702
2.676
2.049
2.027
2.013
2.004
2.001
1.987
1.980
1.962
1.954
1.938
1.916
1.681
1.386
1.256
0.000
-0.002
Nem 2
Current Data Parameters
NAME Jully-05-2010-iitd
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100705
Time 10.36
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 71.8
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CCl3
HN
O
Ph
9
8
7
6
5
4
3
2
1
ppm
2.22
3.13
0.93
1.05
2.00
1.00
2.29
2.10

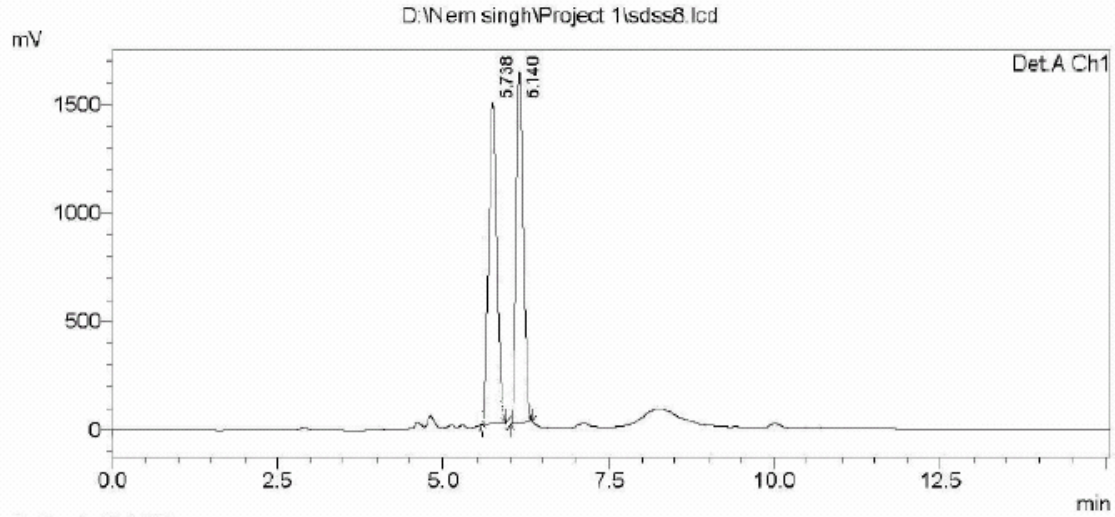

161.24
140.82
136.33
128.69
128.40
126.30
116.52
92.78
77.51
77.09
76.67
53.35
35.92
31.92
CCl3
HN
O
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Jully-05-2010-iitd
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100705
Time 10.38
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 81
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss8.lcd

Sample ID	**: Me RAC**
Acquired by	: Admin
Sample Name	: nem
Injection Volume	: 20 uL
Data File Name	: sdss8.lcd
Method File Name	: method 5 percent 1 ml.lcm
Report File Name	: Default.lcr
Data Acquired	: 6/28/2010 10:01:33 PM
Data Processed	: 6/29/2010 11:58:06 AM

<Chromatogram>

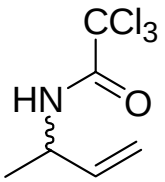


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.738	12041643	1412058	50.895	46.612
2	6.140	11618078	1617317	49.105	53.388
Total		23659722	3029376	100.000	100.000



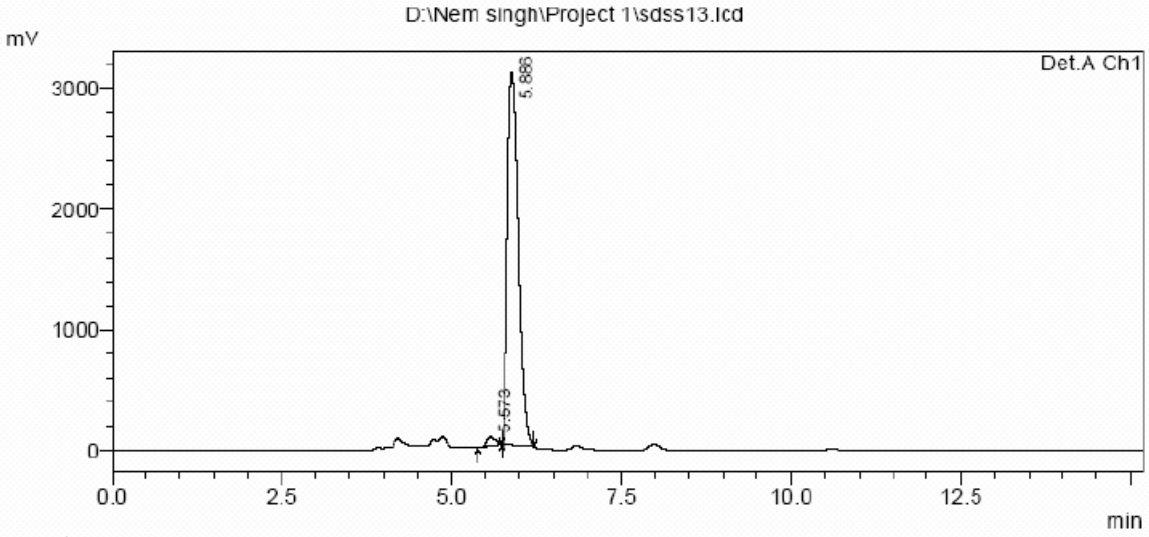
Racemic

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss13.lcd

Sample ID	: Me OAc
Acquired by	: Admin
Sample Name	: nem
Injection Volume	: 20 uL
Data File Name	: sdss13.lcd
Method File Name	: method 5 percent 1 ml.lcm
Report File Name	: Default.lcr
Data Acquired	: 6/28/2010 11:23:14 PM
Data Processed	: 6/29/2010 5:12:42 PM

<Chromatogram>

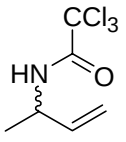


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.573	626881	73931	1.822	2.339
2	5.886	33772332	3086941	98.178	97.661
Total		34399214	3160872	100.000	100.000



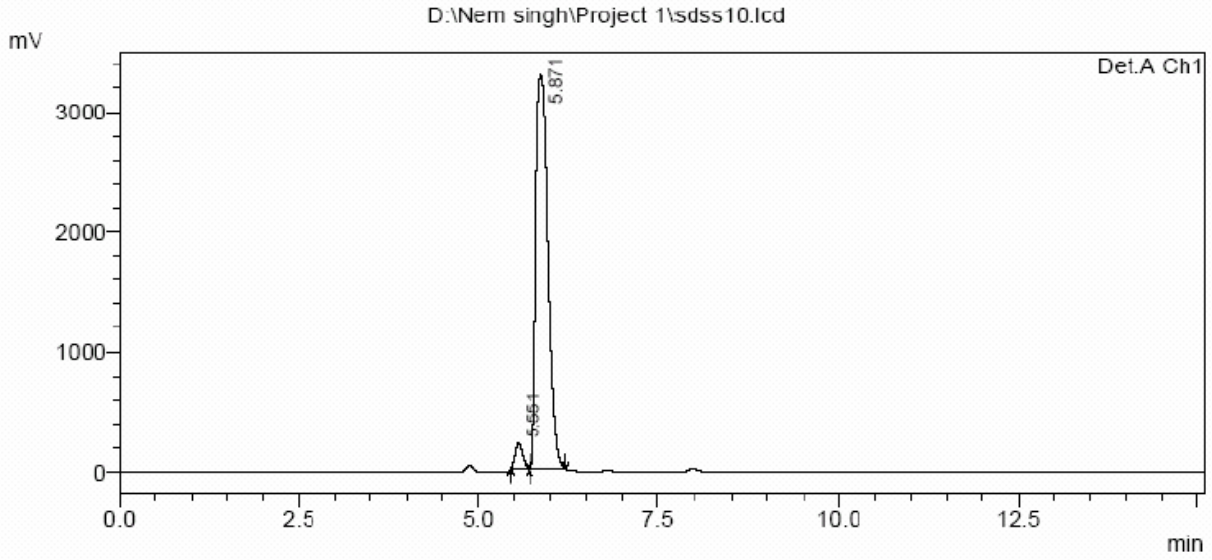
Catalyst used
Palladacycle **4**

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss10.lcd

Sample ID	**: Me Cl**
Acquired by	: Admin
Sample Name	: nem
Injection Volume	: 20 uL
Report File Name	: Default.lcr
Data Acquired	: 6/28/2010 10:36:18 PM
Data Processed	: 6/29/2010 12:19:43 PM

<Chromatogram>

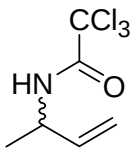


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.551	1550022	217255	3.935	6.205
2	5.871	37837562	3284228	96.065	93.795
Total		39387584	3501483	100.000	100.000



Catalyst used
Palladacycle **5**

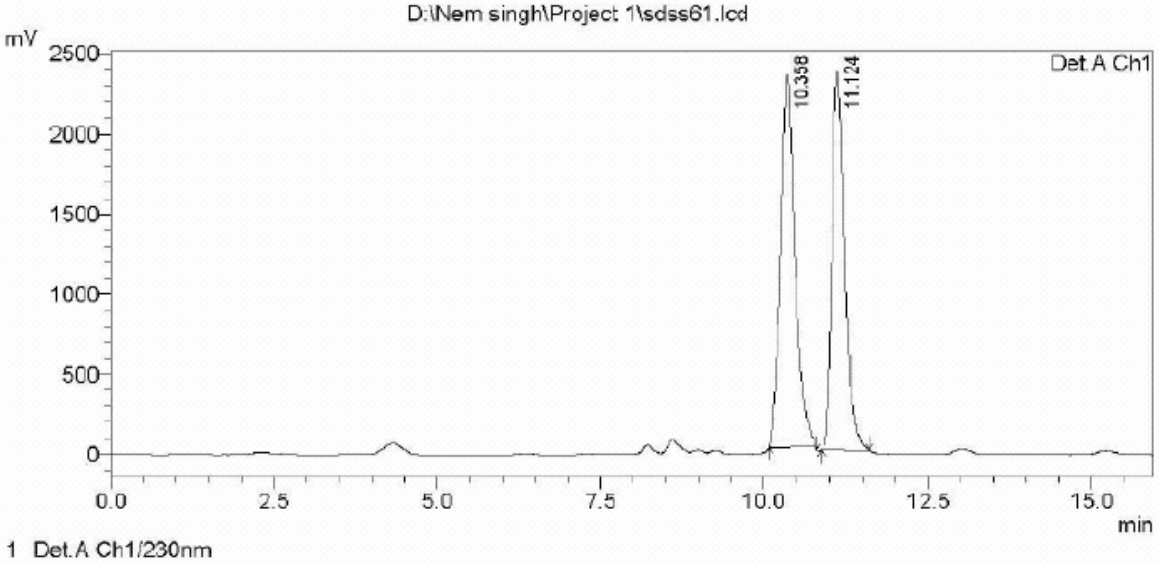
7/8/2010 11:21:20

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss61.lcd

Sample ID : nPr rac f 1 ipa10%
Injection Volume : 20 uL

<Chromatogram>

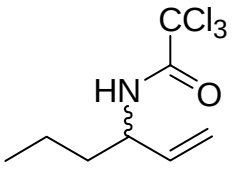


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.358	34310339	2296135	52.152	49.356
2	11.124	31478715	2356016	47.848	50.644
Total		65789054	4652151	100.000	100.000



Racemic

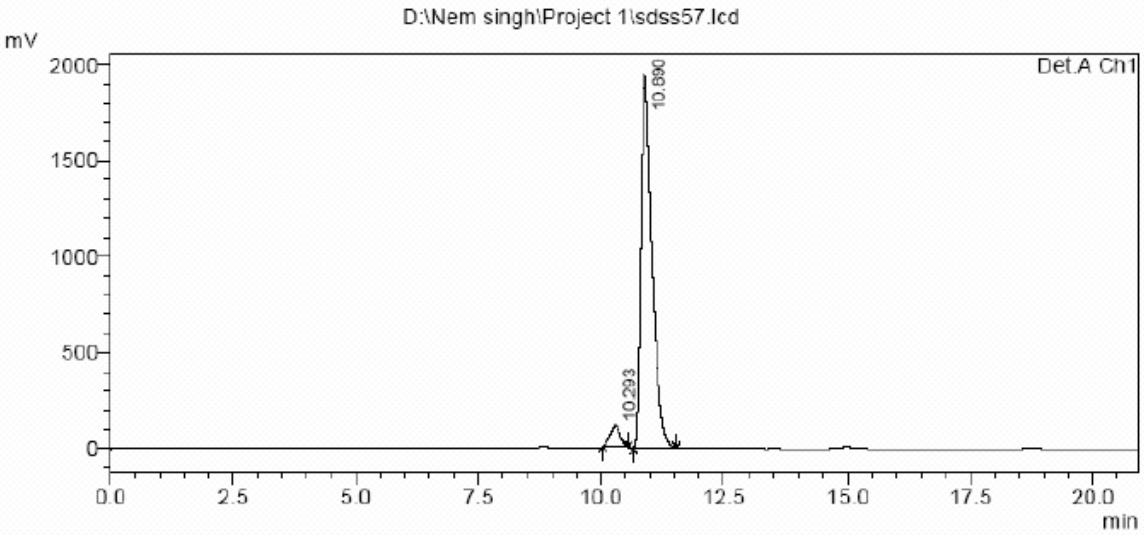
==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss57.lcd

Sample ID : nPr OAc f 1 ipa10%

Injection Volume : 20 uL

<Chromatogram>

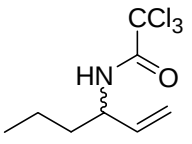


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.293	1559121	109478	4.883	5.328
2	10.890	30367539	1945350	95.117	94.672
Total		31926660	2054827	100.000	100.000



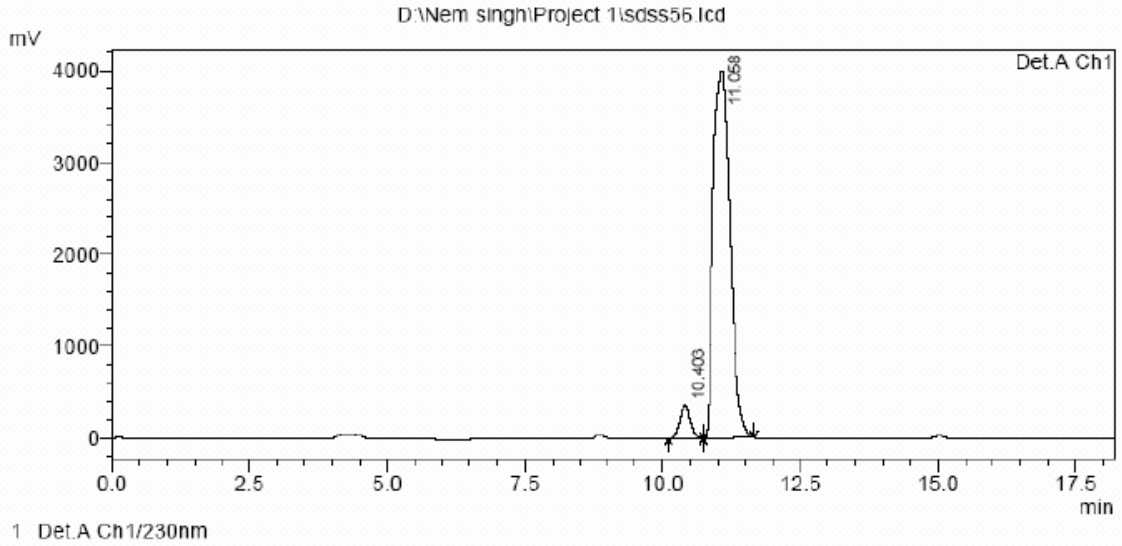
Catalyst used
Palladacycle **4**

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss56.lcd

Sample ID : nPr Cl f 1 ipa10%
Injection Volume : 20 uL

<Chromatogram>

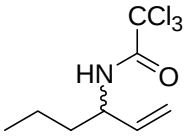


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.403	4840598	374837	5.311	8.570
2	11.058	86297235	3998743	94.689	91.430
Total		91137832	4373580	100.000	100.000



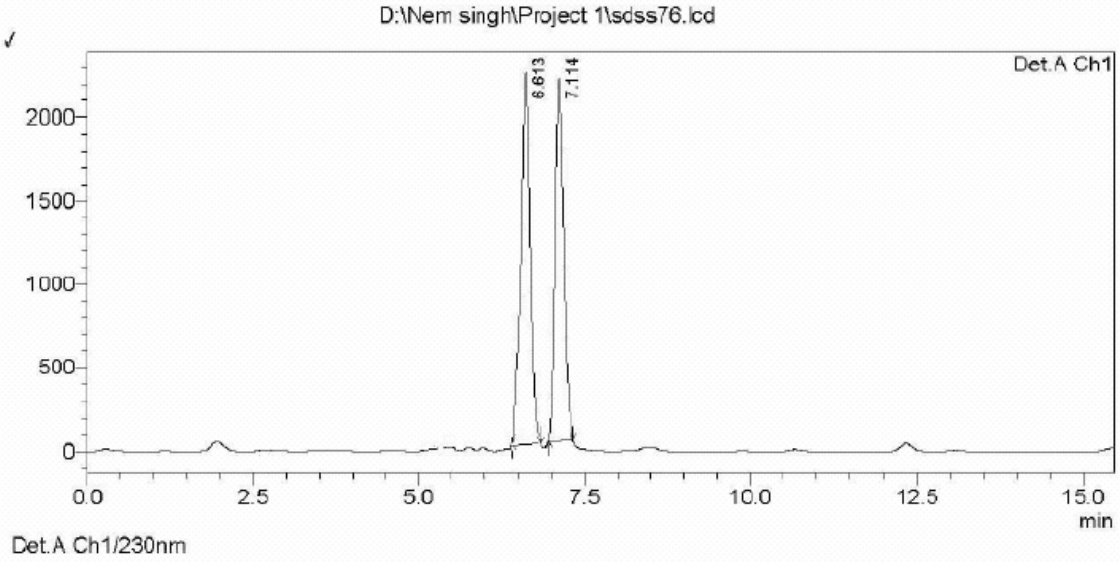
Catalyst used
Palladacycle **5**

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss76.lcd

Sample ID	**: PhCH2CH2 rac**
Acquired by	: Admin
Sample Name	: nem
Injection Volume	: 20 uL
Data File Name	: sdss76.lcd
Data Acquired	: 7/8/2010 12:18:06 AM
Data Processed	: 7/8/2010 1:14:52 AM

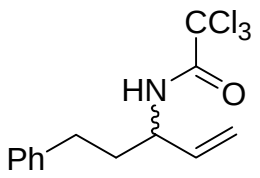
<Chromatogram>



PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.613	19842889	2174051	50.968	50.051
2	7.114	19089422	2169662	49.032	49.949
Total		38932311	4343713	100.000	100.000



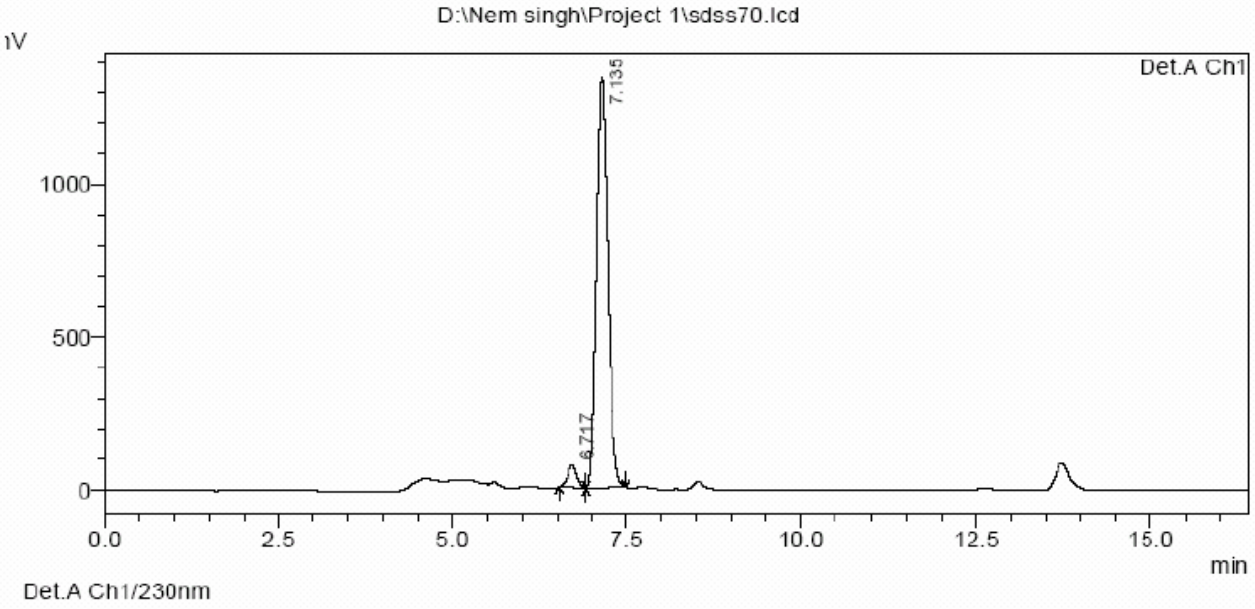
Racemic

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss70.lcd

Sample ID	**: PhCH2CH2 OAc**
Acquired by	: Admin
Sample Name	: nem
Injection Volume	: 20 uL
Report File Name	: Default.lcr
Data Acquired	: 7/7/2010 10:54:31 PM
Data Processed	: 7/7/2010 11:57:09 PM

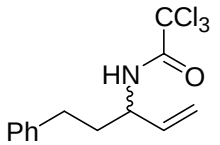
<Chromatogram>



PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.717	656788	71203	4.102	5.028
2	7.135	15355526	1345009	95.898	94.972
Total		16012314	1416212	100.000	100.000



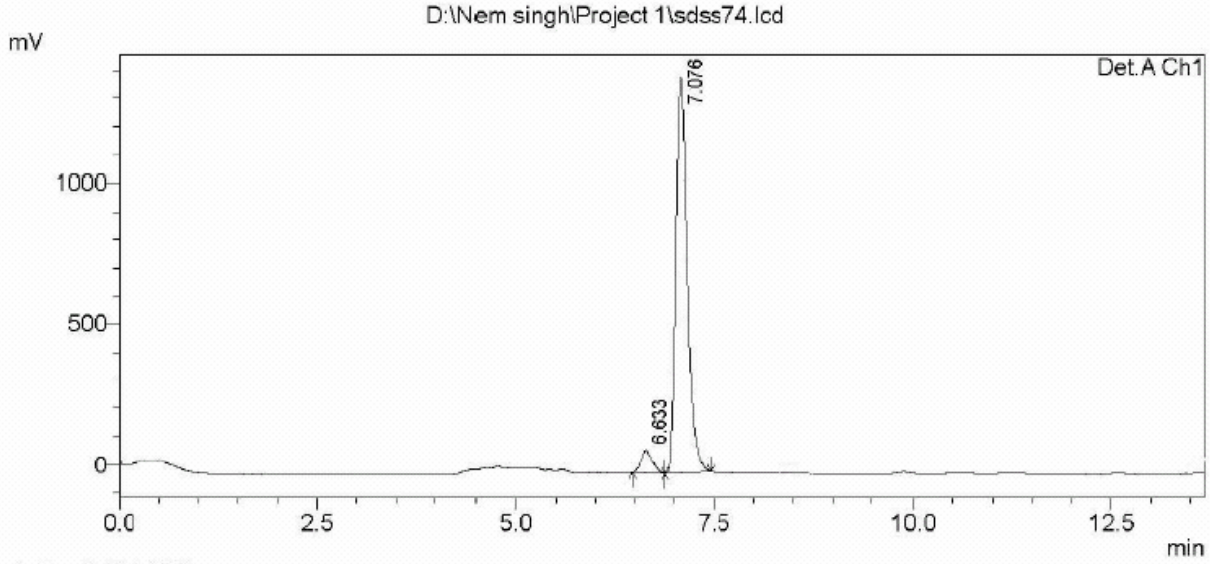
Catalyst used
Palladacycle **4**

==== Shimadzu LCsolution Analysis Report ====

D:\Nem singh\Project 1\sdss74.lcd

Sample ID	**: PhCH2CH2 Cl**
Acquired by	: Admin
Sample Name	: nem
Injection Volume	: 20 uL
Report File Name	: Default.lcr
Data Acquired	: 7/7/2010 11:51:47 PM
Data Processed	: 7/8/2010 12:15:59 AM

<Chromatogram>

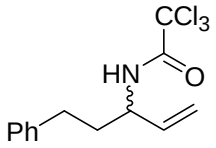


1 Det.A Ch1/230nm

PeakTable

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.633	884755	84099	6.064	5.637
2	7.076	13704628	1407688	93.936	94.363
Total		14589383	1491786	100.000	100.000



Catalyst used
Palladacycle **5**