

# **RING-OPENING METATHESIS OF *N*-ALKENYL $\beta$ -LACTAMS<sup>†</sup>**

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## **Table of Contents**

<sup>1</sup>H and <sup>13</sup>C NMR of the compounds----- 1–21

Energies and Cartesian coordinates of optimized geometries----22–26

# <sup>1</sup>H NMR of the compound 3

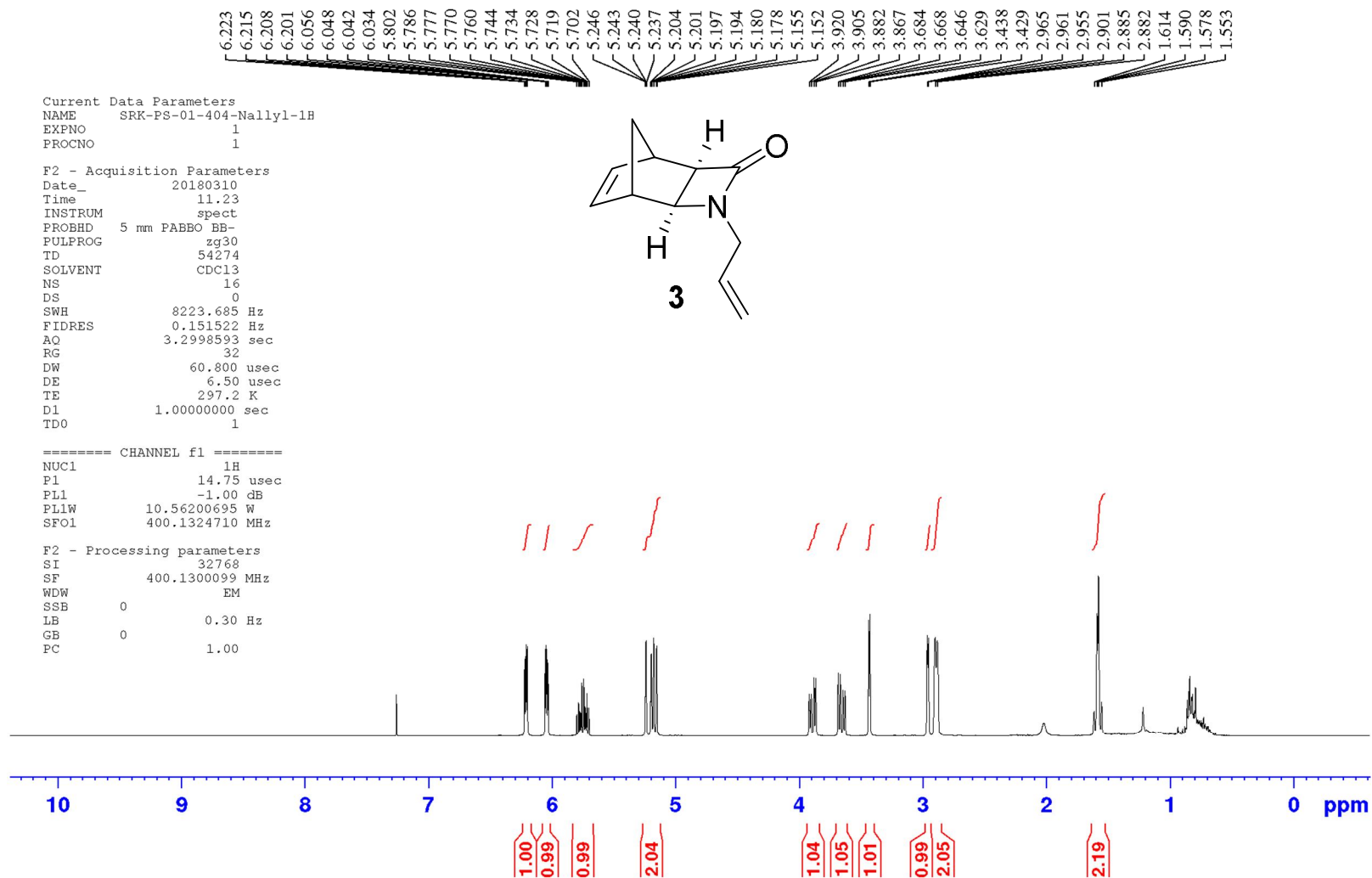
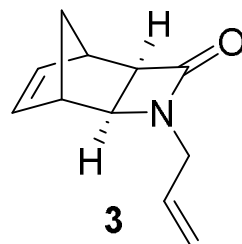
SRK-PS-01-404-Nallyl-1H

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PROCNO 1

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SOLVENT CDC13  
NS 16  
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SWH 8223.685 Hz  
FIDRES 0.151522 Hz  
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RG 32  
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TE 297.2 K  
D1 1.0000000 sec  
TD0 1

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SFO1 400.1324710 MHz

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# <sup>13</sup>C NMR of the compound 3

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EXPNO 2  
PROCNO 1

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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 80  
DS 0  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2582912 sec  
RG 2050  
DW 19.200 usec  
DE 6.50 usec  
TE 297.4 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

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P1 8.50 usec  
PL1 -2.00 dB  
PL1W 56.53121948 W  
SFO1 100.6238364 MHz

===== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 13.69 dB  
PL13 14.50 dB  
PL2W 10.56200695 W  
PL12W 0.35871249 W  
PL13W 0.29767781 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
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SF 100.6127622 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
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PC 1.40

169.54

138.75

135.18

132.21

118.65

77.47

77.16

76.84

56.89

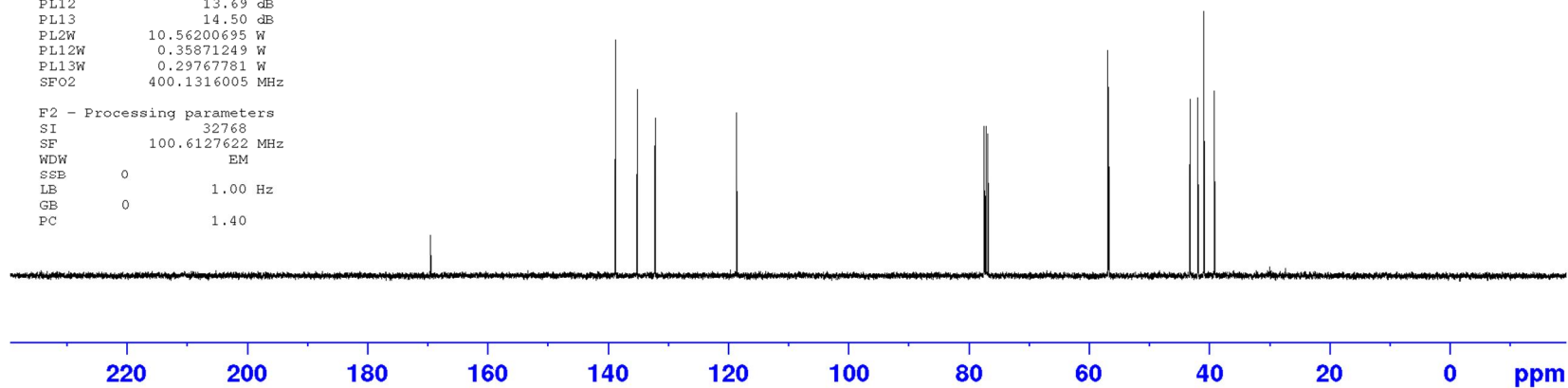
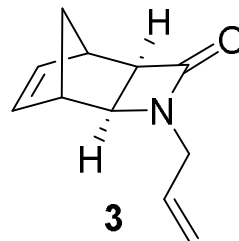
56.76

43.26

41.96

40.96

39.21

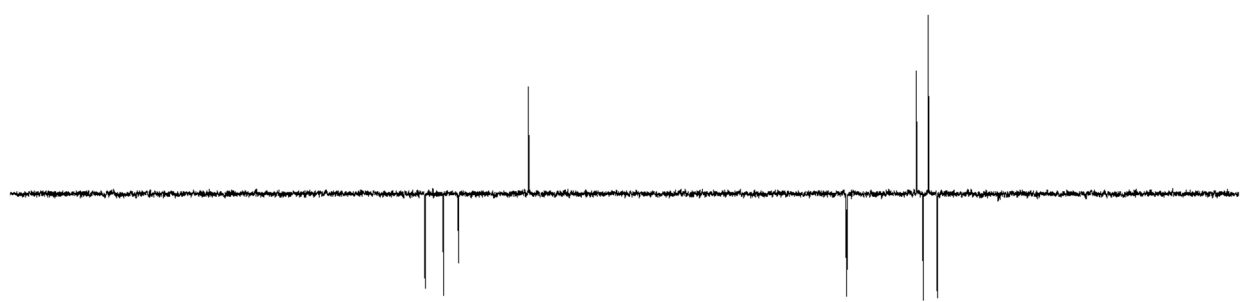
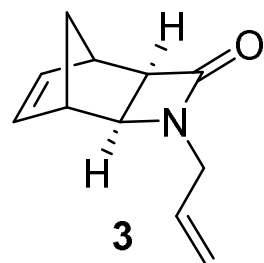


# DEPT NMR of the compound 3

SRK-PS-01-404-Nallyl-DEPT

138.75  
135.18  
132.21  
118.64

56.89  
56.76  
43.26  
41.96  
40.96  
39.21



200 180 160 140 120 100 80 60 40 20 0 ppm

Current Data Parameters  
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EXPNO 3  
PROCNO 1

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SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
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RG 2050  
DW 20.800 usec  
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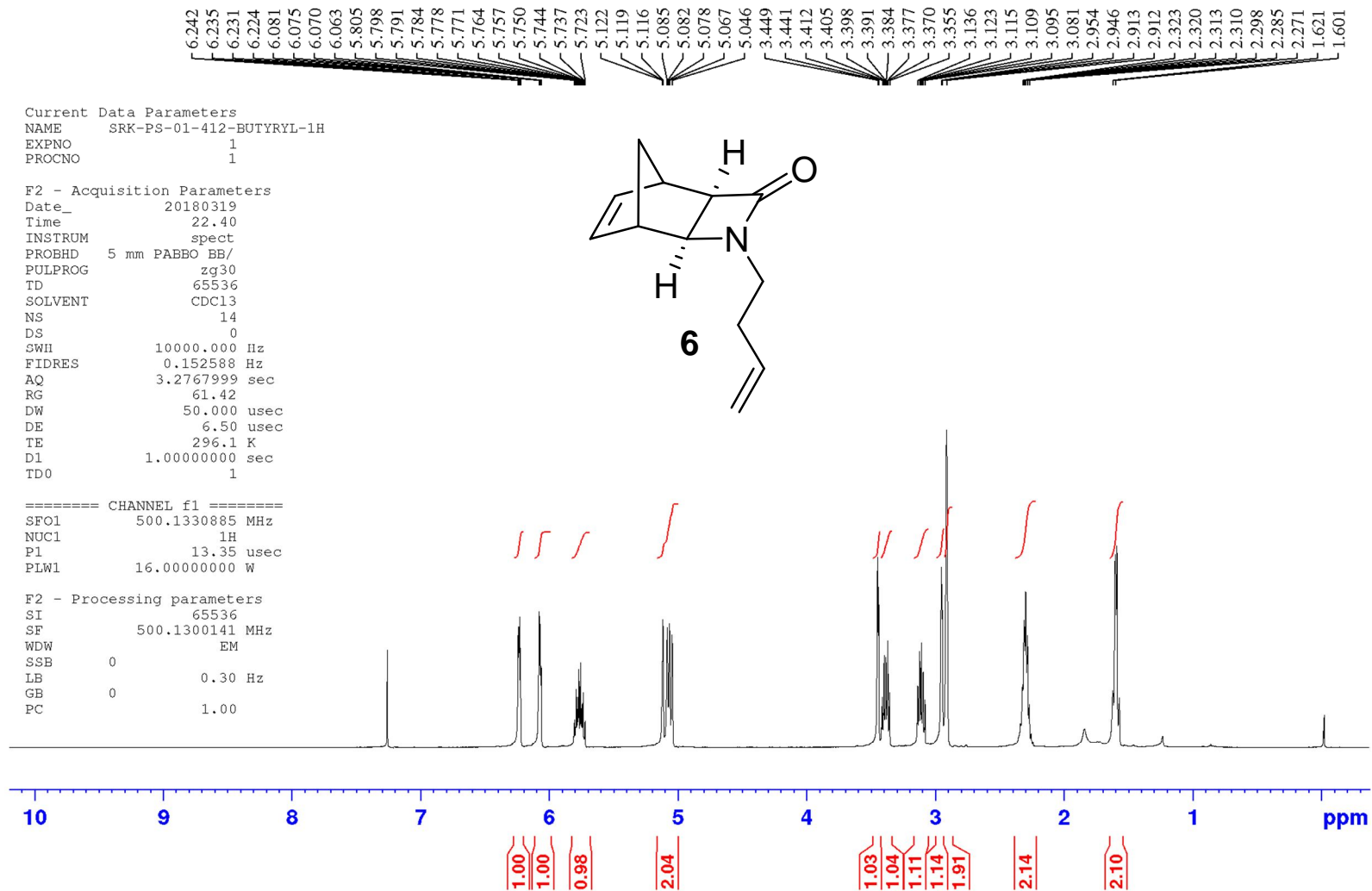
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P2 17.00 usec  
PL1 -2.00 dB  
PL1W 56.53121948 W  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
P3 14.75 usec  
P4 29.50 usec  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 13.69 dB  
PL2W 10.56200695 W  
PL12W 0.35871249 W  
SFO2 400.1316005 MHz

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SF 100.6127622 MHz  
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GB 0  
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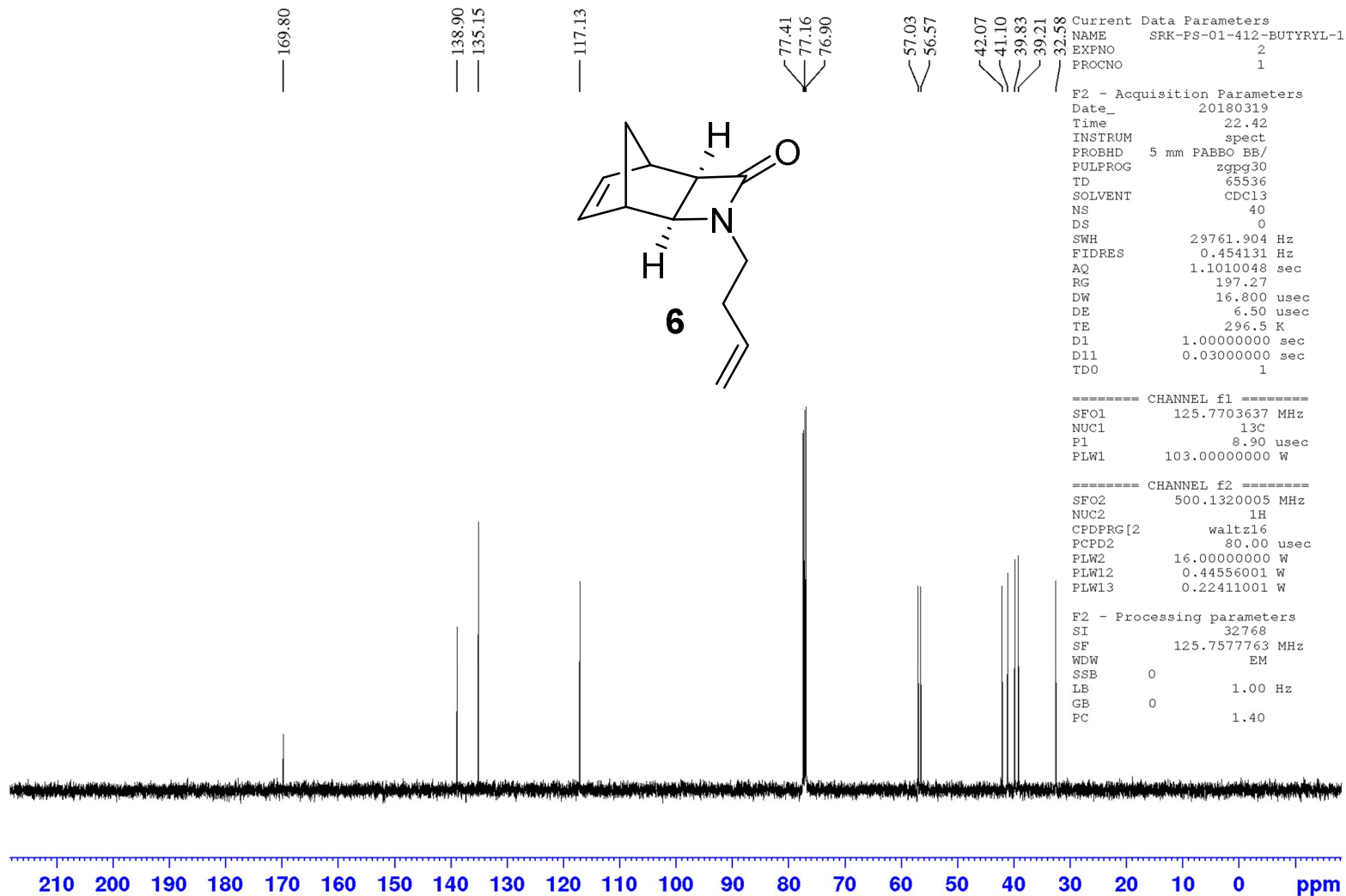
# <sup>1</sup>H NMR of the compound 6

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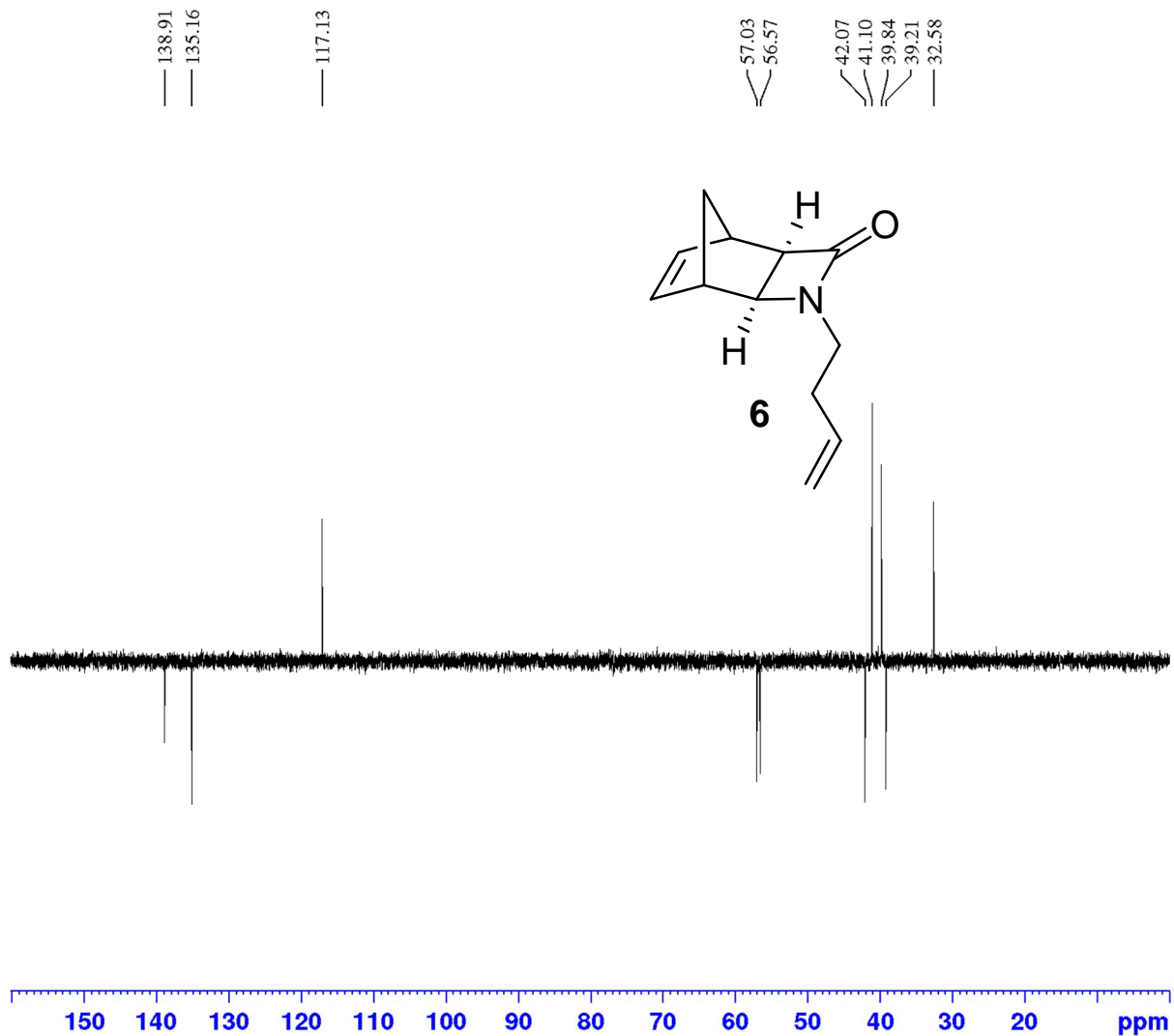
# <sup>13</sup>C NMR of the compound 6

SRK-PS-01-412-BUTYRYL-13C



# DEPT NMR of the compound 6

SRK-PS-01-412-BUTYRYL-DEPT



```

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PROCNO    1

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PULPROG   deptspl35
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SOLVENT   CDCl3
NS         25
DS         0
SWH        20161.291 Hz
FIDRES     0.307637 Hz
AQ         1.6252928 sec
RG         197.27
DW         24.800 usec
DE         6.50 usec
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CNST2     145.0000000
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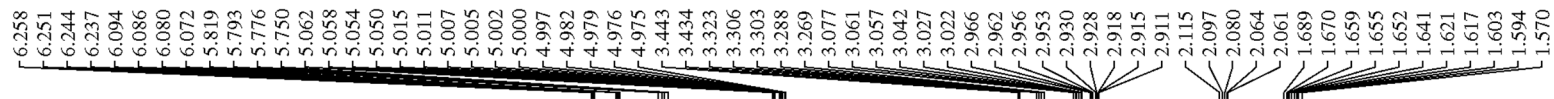
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SPNAM[5]   Crp60comp.4
SPOAL5     0.500
SPOFFS5    0 Hz
SPW5       12.46500015 W

----- CHANNEL f2 -----
SFO2      500.1315995 MHz
NUC2       1H
CPDPRG[2]  waltz16
F3         13.35 usec
F4         26.70 usec
PCPD2      80.00 usec
PLW2       16.00000000 W
PLW12      0.44556001 W

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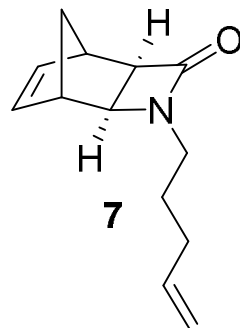
# <sup>1</sup>H NMR of the compound 7

SRK-PS-01-422-PENTENYL-1H



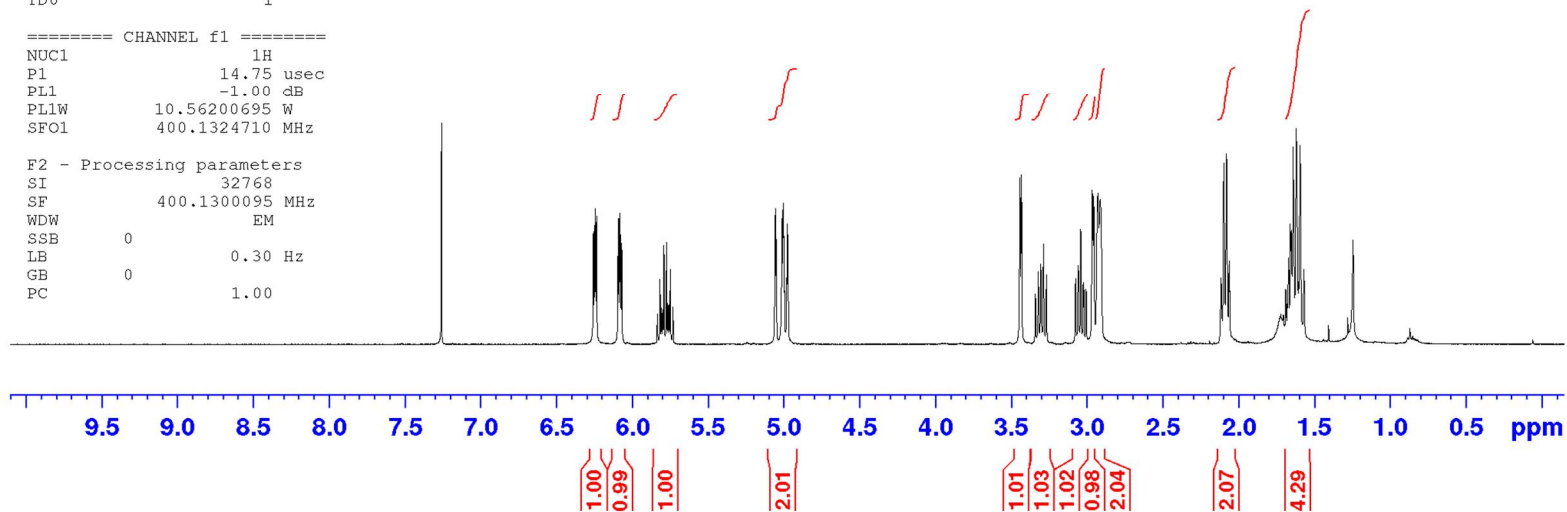
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EXPNO 1  
PROCNO 1

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PULPROG zg30  
TD 54274  
SOLVENT CDCl3  
NS 10  
DS 0  
SWH 8223.685 Hz  
FIDRES 0.151522 Hz  
AQ 3.2998593 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 298.9 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
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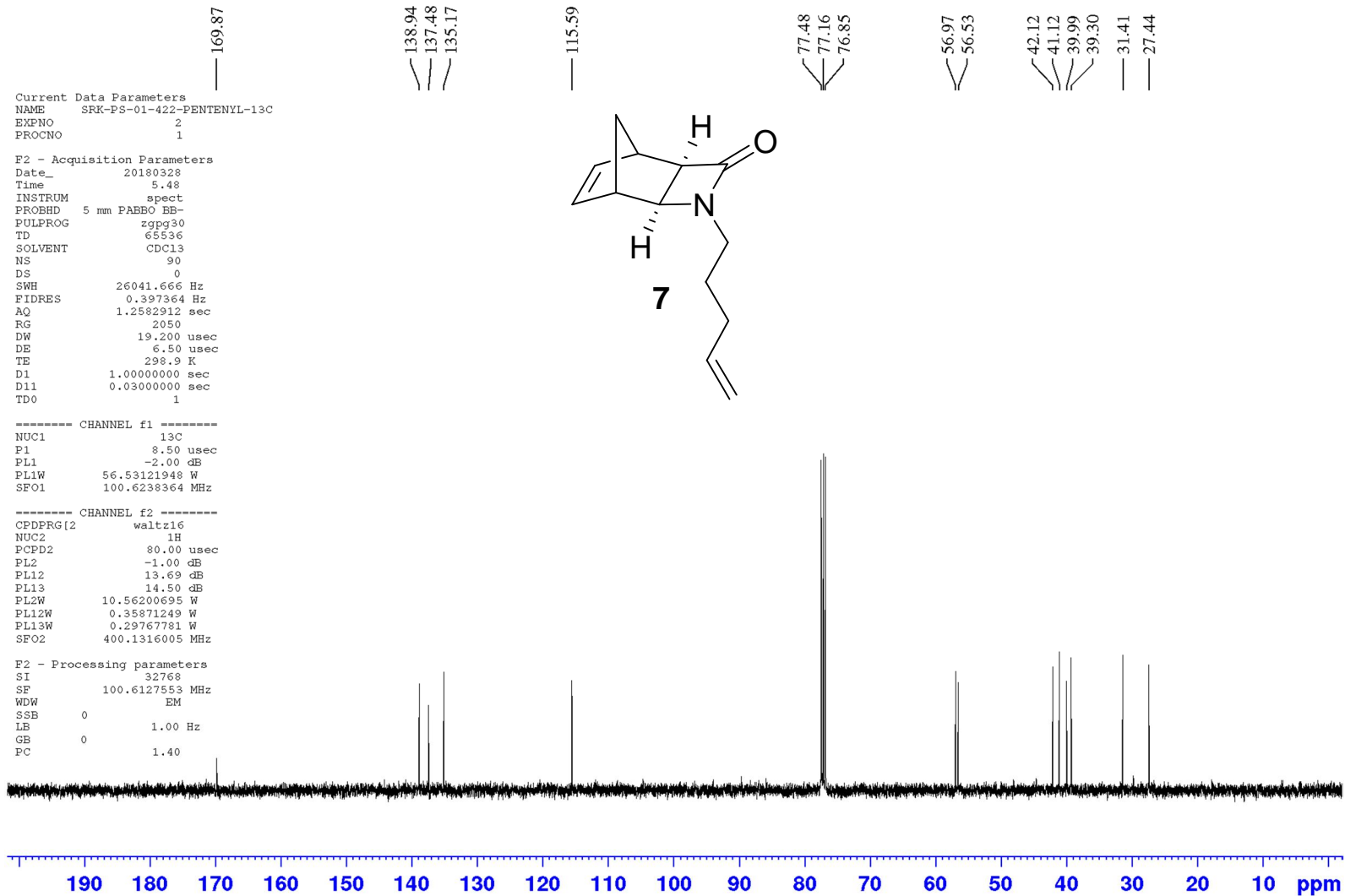
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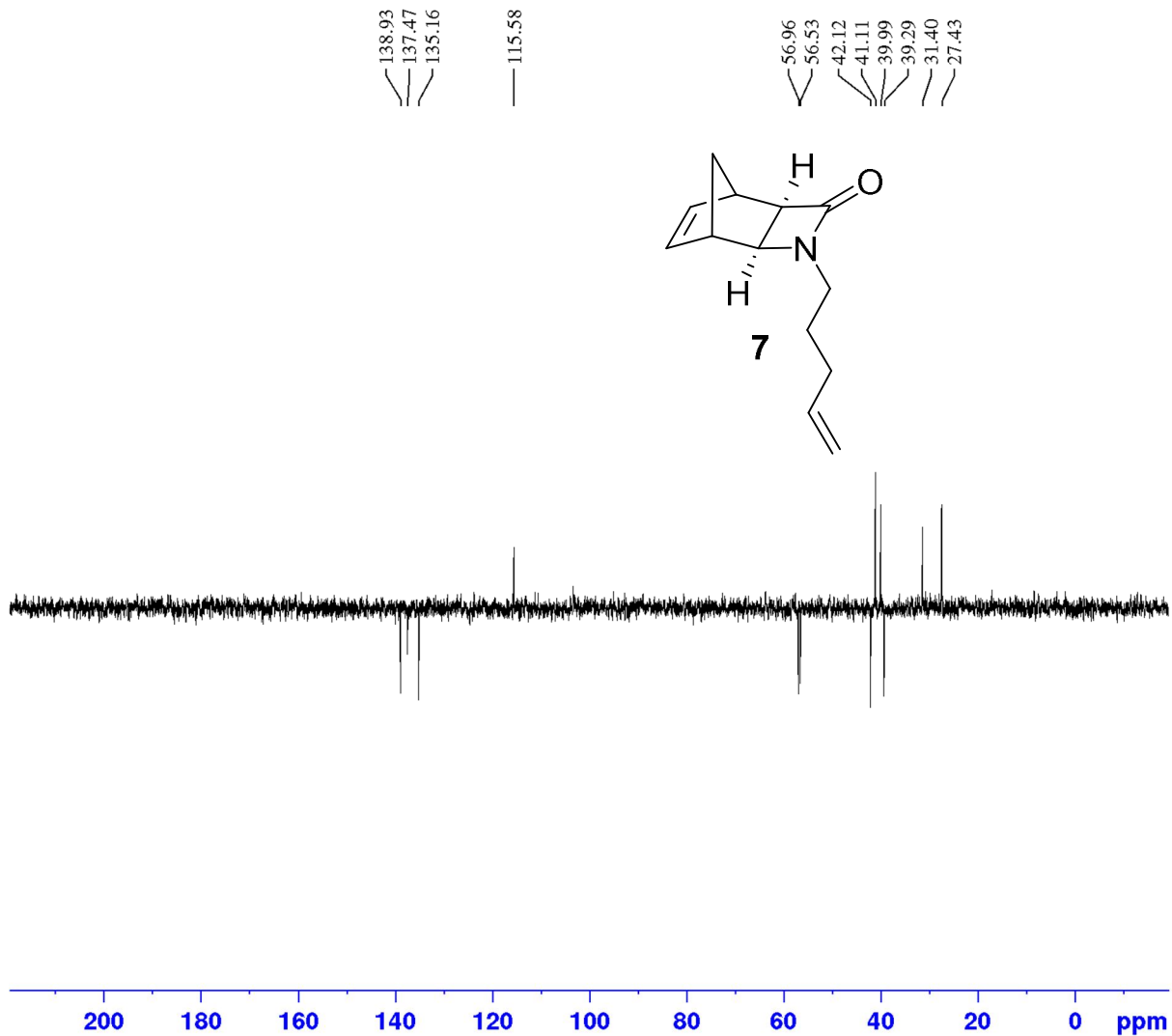
# <sup>13</sup>C NMR of the compound 7

SRK-PS-01-422-PENTENYL-13C



# DEPT NMR of the compound 7

SRK-PS-01-422-PENTENYL-DEPT



Current Data Parameters  
 NAME SRK-PS-01-422-PENTENYL-DEPT  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
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 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG dept135  
 TD 65536  
 SOLVENT CDCl3  
 NS 50  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.2 K  
 CNST2 145.0000000  
 D1 1.00000000 sec  
 D2 0.00344828 sec  
 D12 0.00002000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.50 usec  
 F2 17.00 usec  
 FL1 -2.00 dB  
 PLLW 56.53121948 W  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 P3 14.75 usec  
 P4 29.50 usec  
 PCPD2 80.00 usec  
 FL2 -1.00 dB  
 FL12 13.69 dB  
 FL2W 10.56200695 W  
 PLL2W 0.35871249 W  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
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# <sup>1</sup>H NMR of the compound 8

SRK-PS-01-510-HEX-1H

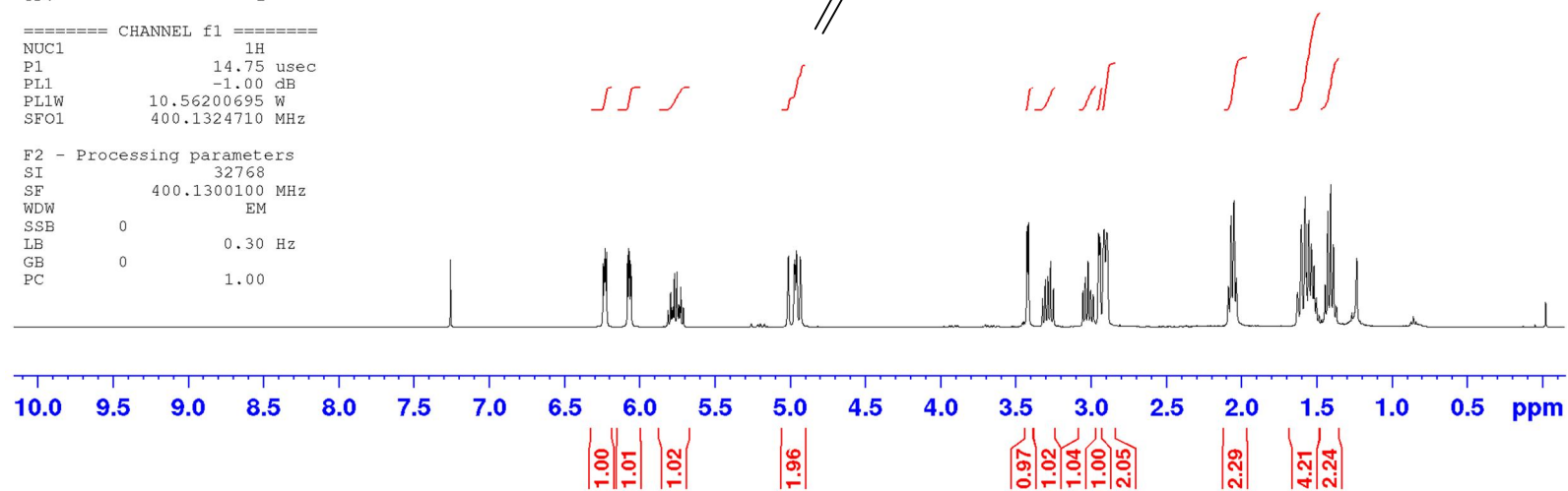
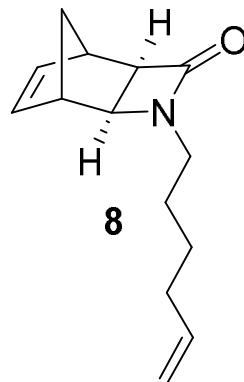


Current Data Parameters  
NAME SRK-PS-01-510-HEX-1H  
EXPNO 1  
PROCNO 1

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Date\_ 20180601  
Time 11.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 54274  
SOLVENT CDCl3  
NS 12  
DS 0  
SWH 8223.685 Hz  
FIDRES 0.151522 Hz  
AQ 3.2998593 sec  
RG 71.8  
DW 60.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PL1 -1.00 dB  
PL1W 10.56200695 W  
SFO1 400.1324710 MHz

F2 - Processing parameters  
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SF 400.1300100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



# <sup>13</sup>C NMR of the compound 8

SRK-PS-01-510-HEX-13C

Current Data Parameters  
 NAME SRK-PS-01-510-HEX-13C  
 EXPNO 3  
 PROCNO 1

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 Time\_ 11.04  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 50  
 DS 0  
 SWH 26041.666 Hz  
 FIDRES 0.397364 Hz  
 AQ 1.2582912 sec  
 RG 2050  
 DW 19.200 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.50 usec  
 PL1 -2.00 dB  
 PL1W 56.53121948 W  
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 13.69 dB  
 PL13 14.50 dB  
 PL2W 10.56200695 W  
 PL12W 0.35871249 W  
 PL13W 0.29767781 W  
 SFO2 400.1316005 MHz

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 PC 1.40

169.87

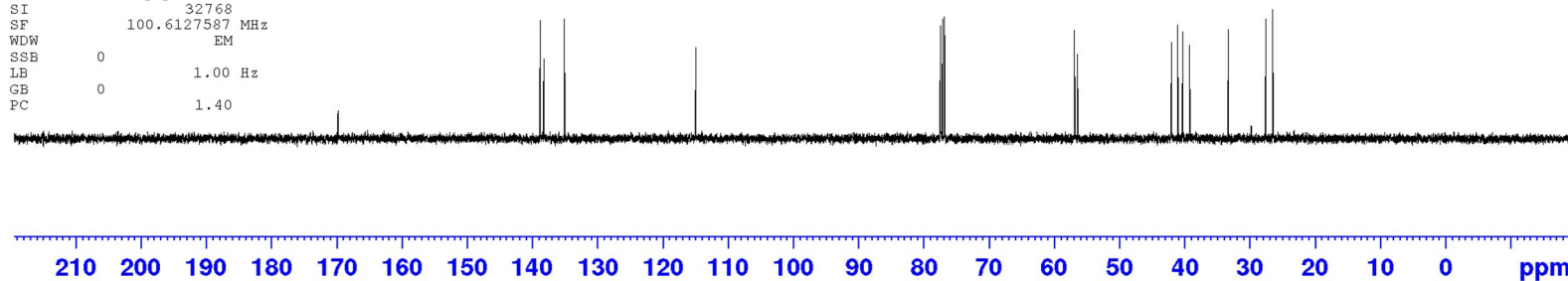
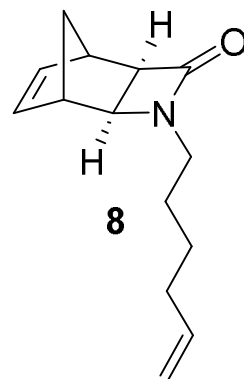
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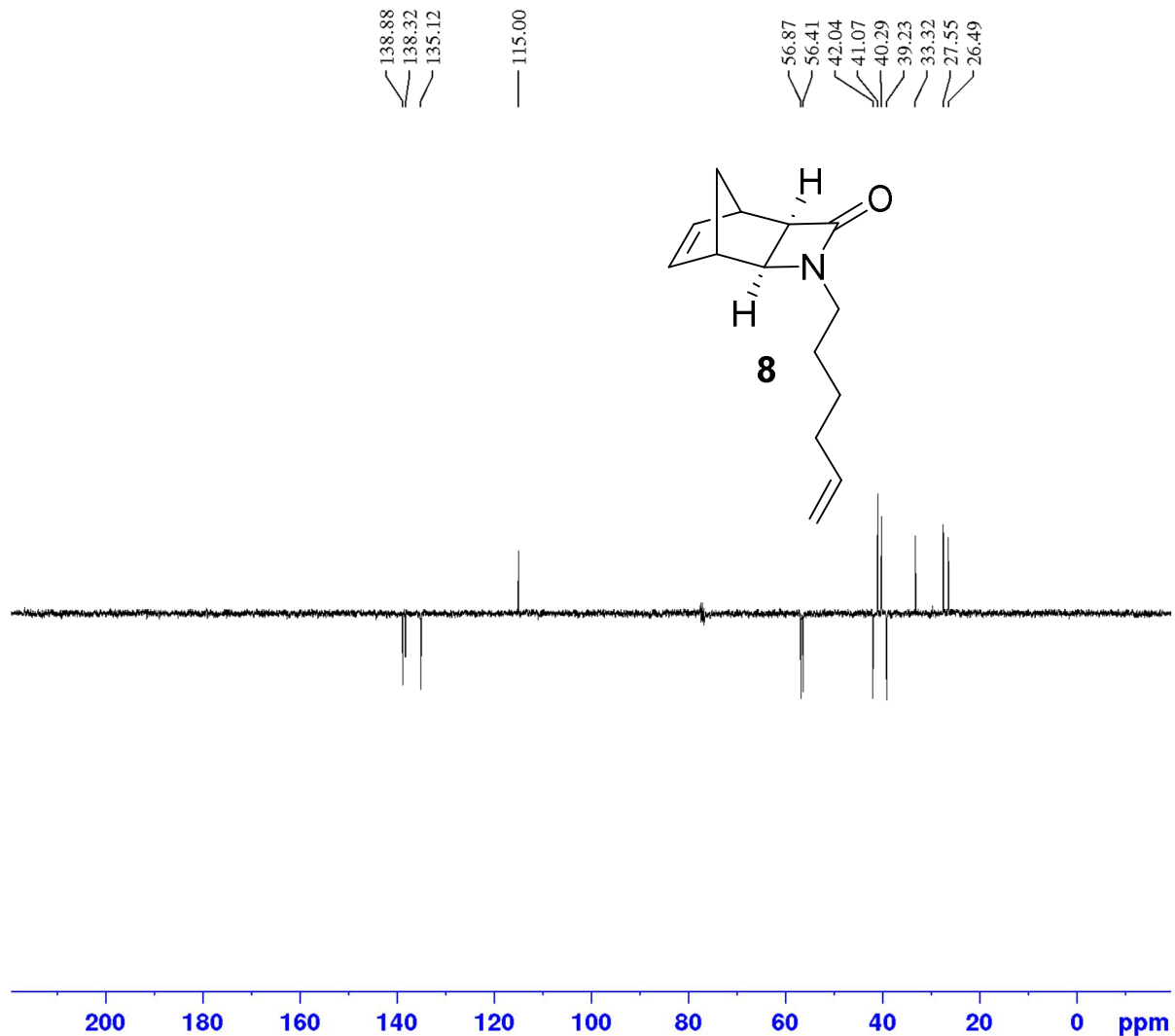
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 56.42

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 33.33  
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# DEPT NMR of the compound 8

SRK-PS-01-510-HEX-DEPT



Current Data Parameters  
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 EXPNO 2  
 PROCNO 1

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 TD 65536  
 SOLVENT CDC13  
 NS 50  
 DS 0  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 CNST2 145.0000000  
 D1 1.0000000 sec  
 D2 0.00344828 sec  
 D12 0.00002000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.50 usec  
 P2 17.00 usec  
 PL1 -2.00 dB  
 PL1W 56.53121948 W  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 P3 14.75 usec  
 P4 29.50 usec  
 FCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 13.69 dB  
 PL2W 10.56200695 W  
 PL12W 0.35871249 W  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
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 SF 100.6127596 MHz  
 WDW EM  
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 CB 0  
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# <sup>1</sup>H NMR of the compound 4

SRK-PS-01-414-GH-I-1H

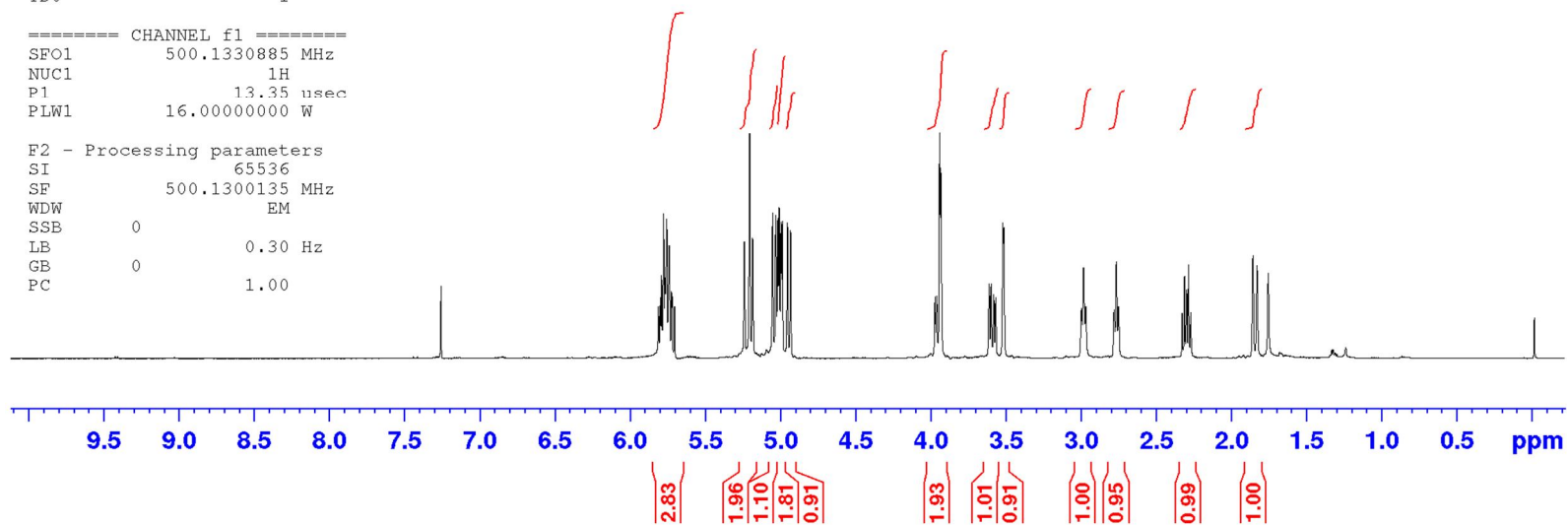
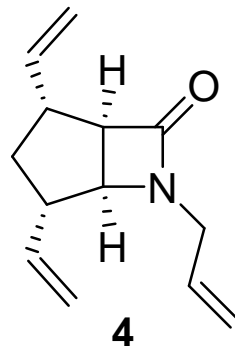
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PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 15  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 53.37  
DW 50.000 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
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P1 13.35 usec  
PLW1 16.00000000 W

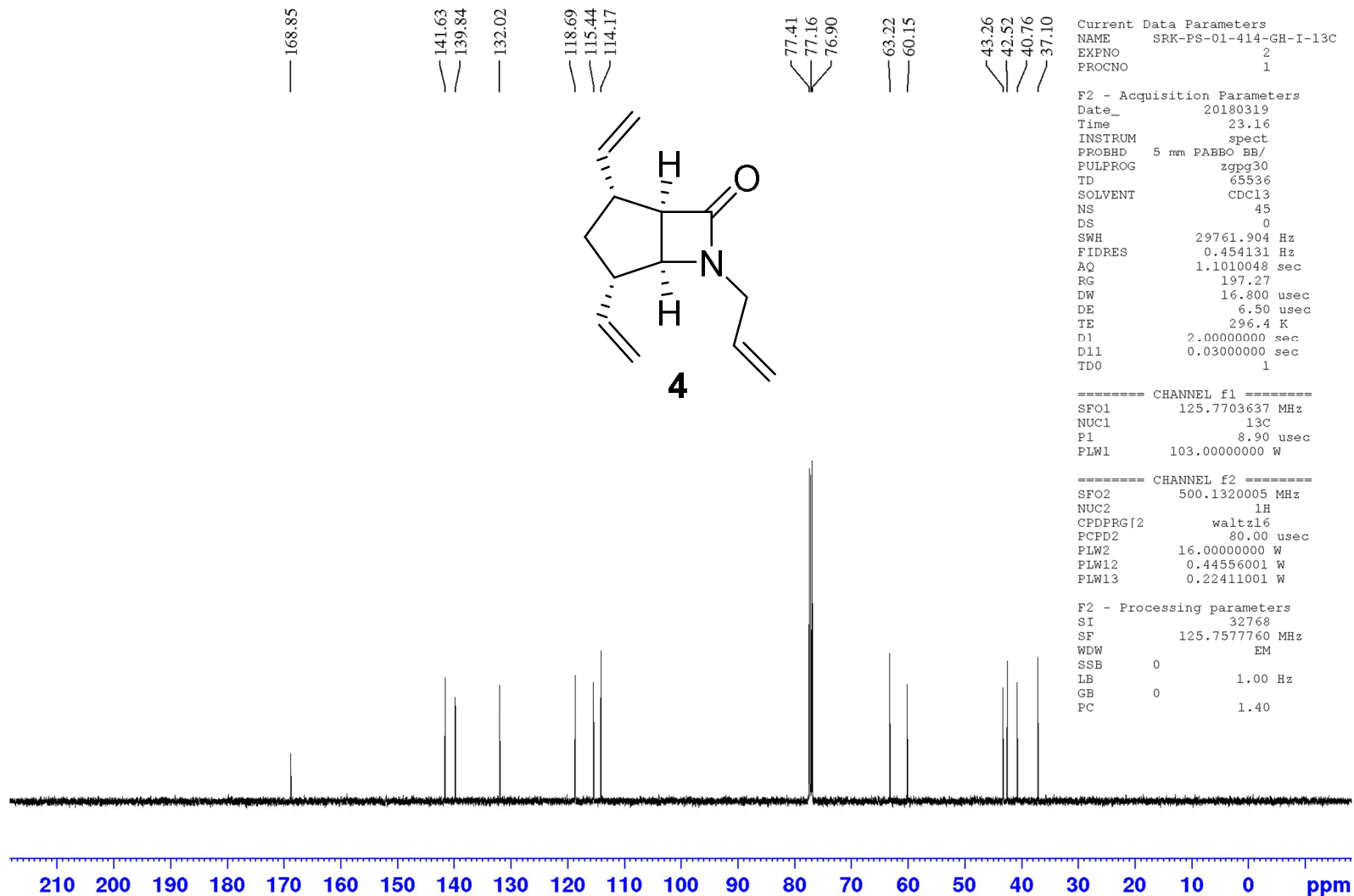
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GB 0  
PC 1.00

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5.792  
5.779  
5.769  
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5.758  
5.744  
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5.726  
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4.988  
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3.972  
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1.829



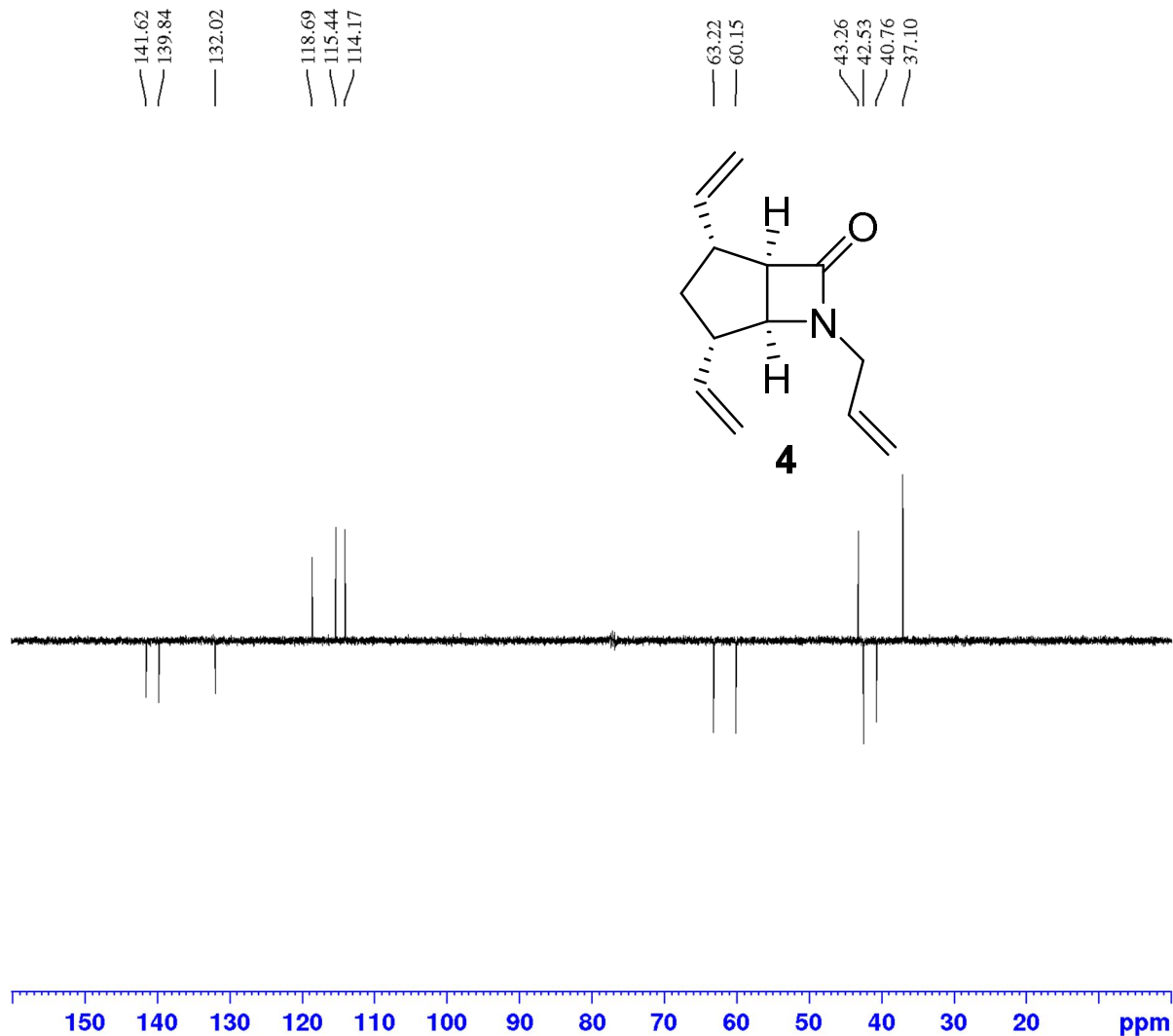
# <sup>13</sup>C NMR of the compound 4

SRK-PS-01-414-GH-I-13C



# DEPT NMR of the compound 4

SRK-PS-01-414-GH-I-DEPT



Current Data Parameters  
 NAME SRK-PS-01-414-GH-I-DEPT  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time\_ 23.19  
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 PULPROG deptsp135  
 TD 65536  
 SOLVENT CDC13  
 NS 30  
 DS 0  
 SWH 20161.291 Hz  
 FIDRES 0.307637 Hz  
 AQ 1.6252928 sec  
 RG 197.27  
 DW 24.800 usec  
 DE 6.50 usec  
 TE 296.6 K  
 CNST2 145.000000  
 D1 1.0000000 sec  
 D2 0.00344828 sec  
 D12 0.00002000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 125.7678486 MHz  
 NUC1 13C  
 P1 8.90 usec  
 P13 2000.00 usec  
 PLW0 0 W  
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 SPNAM[5] Crp60comp.4  
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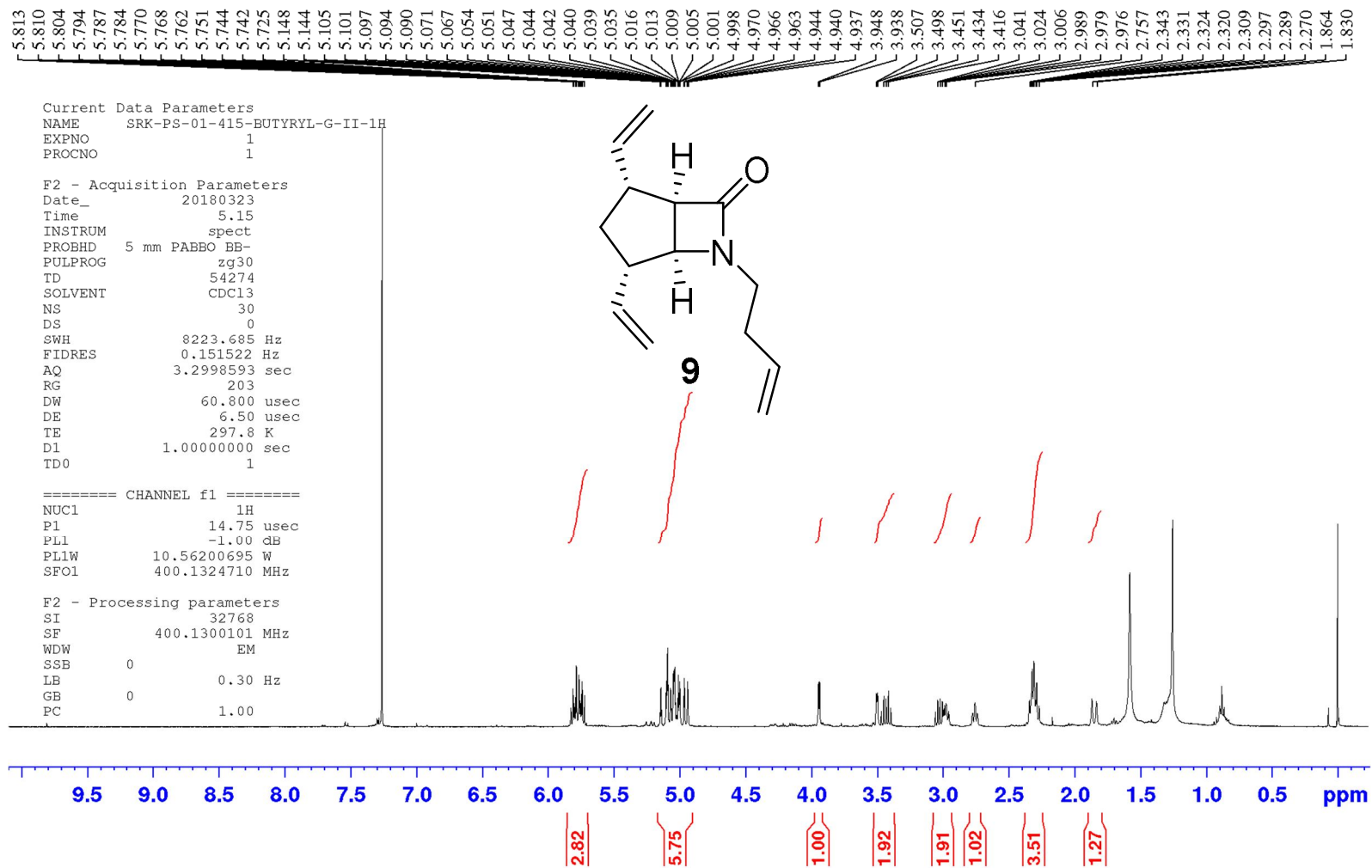
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 PCPD2 80.00 usec  
 PLW2 16.0000000 W  
 PLW12 0.44556001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577762 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



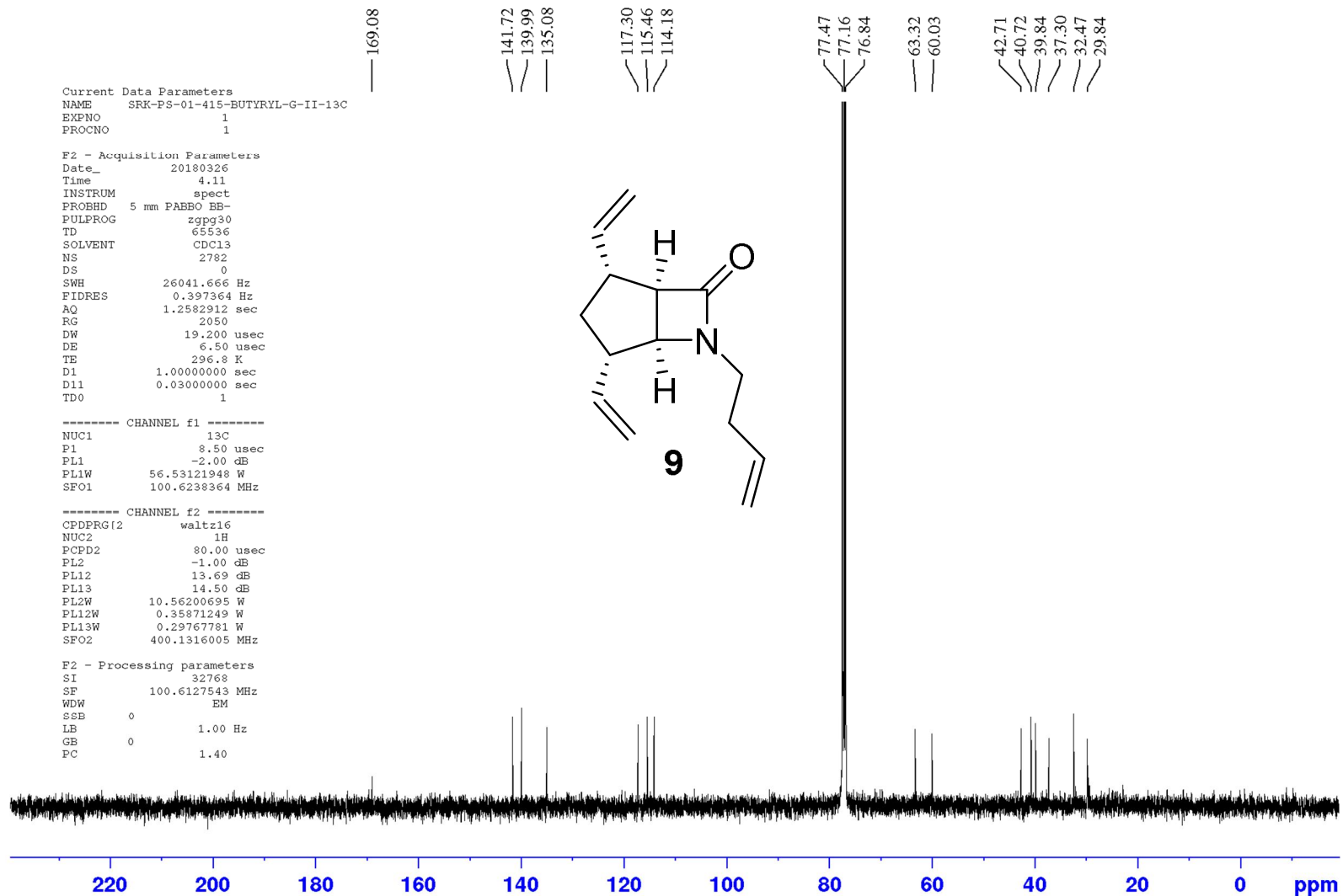
# <sup>1</sup>H NMR of the compound 9

SRK-PS-01-415-BUTYRYL-G-II-1H



# <sup>13</sup>C NMR of the compound 9

SRK-PS-01-415-BUTYRYL-G-II-13C



# <sup>1</sup>H NMR of the compound 10

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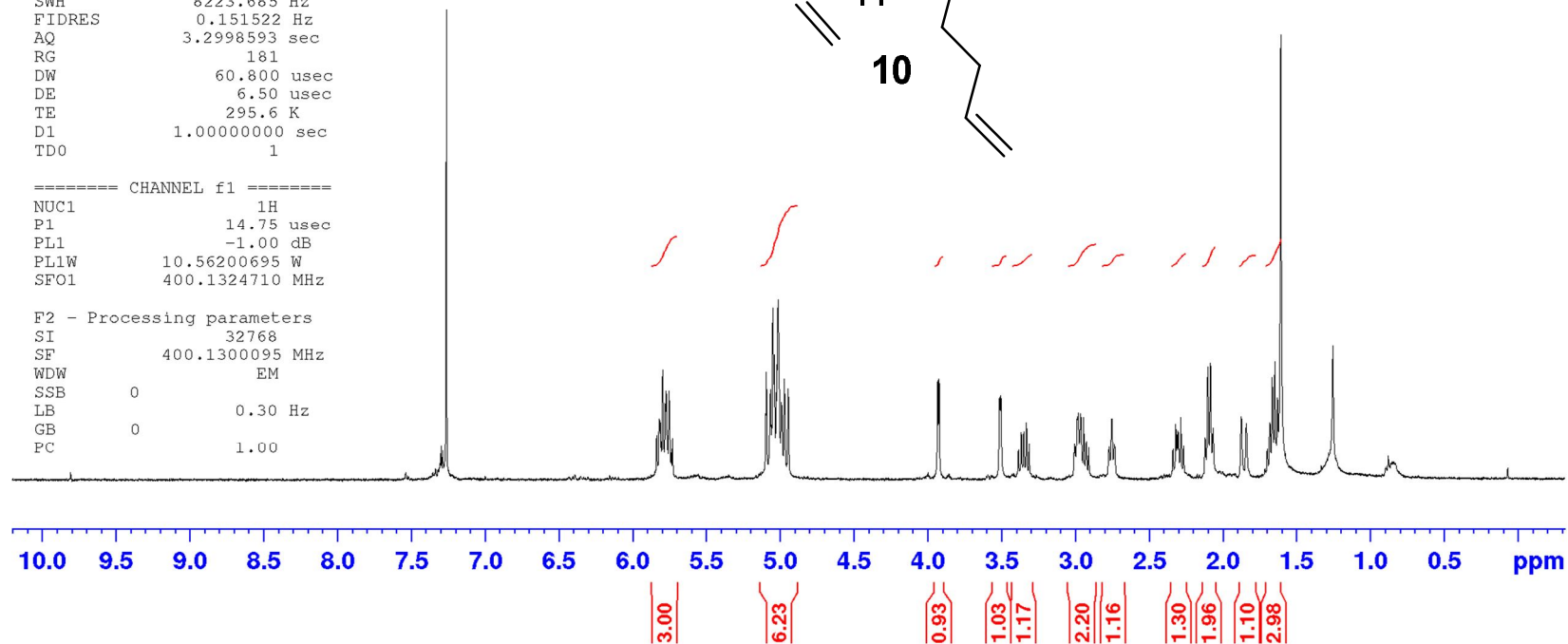
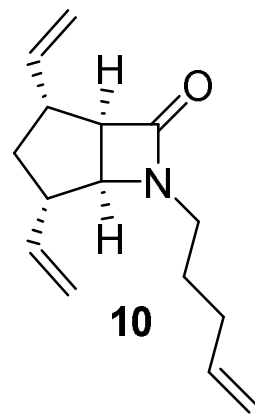
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5.090  
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5.063  
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5.039  
5.036  
5.024  
5.020  
5.016  
5.013  
5.010  
5.006  
5.002  
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4.973  
4.970  
4.967  
4.947  
4.944  
4.941  
3.931  
3.922  
3.511  
3.503  
3.365  
3.347  
3.330  
2.983  
2.978  
2.961  
2.958  
2.942  
2.751  
2.317  
2.309  
2.301  
2.283  
2.099  
2.082  
2.064  
1.873  
1.839  
1.678  
1.664  
1.645  
1.626

Current Data Parameters  
NAME SRK-PS-01-PENTENYL-RCM-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180403  
Time 6.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 54274  
SOLVENT CDC13  
NS 11  
DS 0  
SWH 8223.685 Hz  
FIDRES 0.151522 Hz  
AQ 3.2998593 sec  
RG 181  
DW 60.800 usec  
DE 6.50 usec  
TE 295.6 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.75 usec  
PL1 -1.00 dB  
PL1W 10.56200695 W  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300095 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



# <sup>1</sup>H NMR of the compound 11

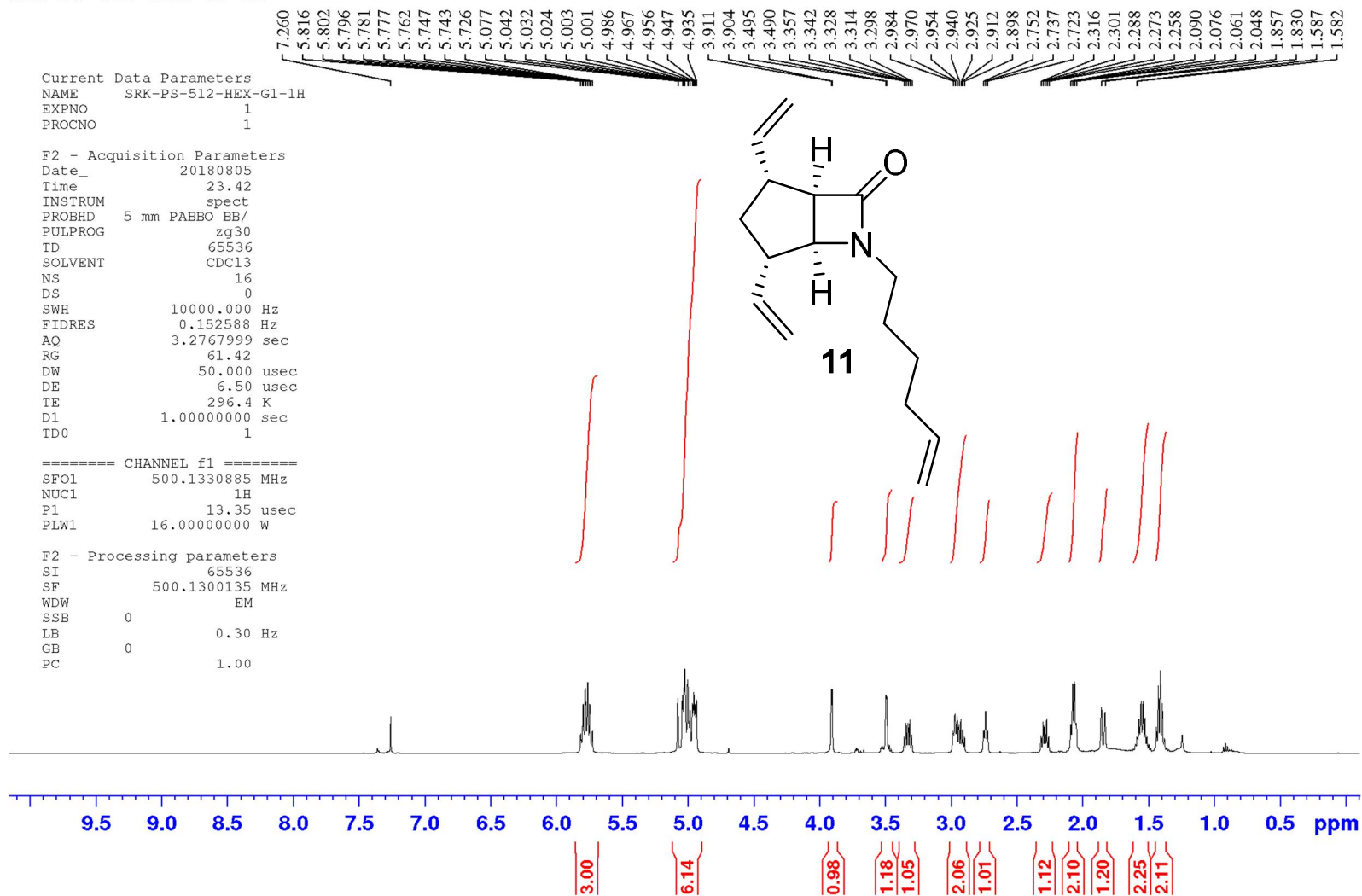
SRK-PS-512-HEX-G1-1H

Current Data Parameters  
NAME SRK-PS-512-HEX-G1-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180805  
Time\_ 23.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 61.42  
DW 50.000 usec  
DE 6.50 usec  
TE 296.4 K  
D1 1.00000000 sec  
TD0 1

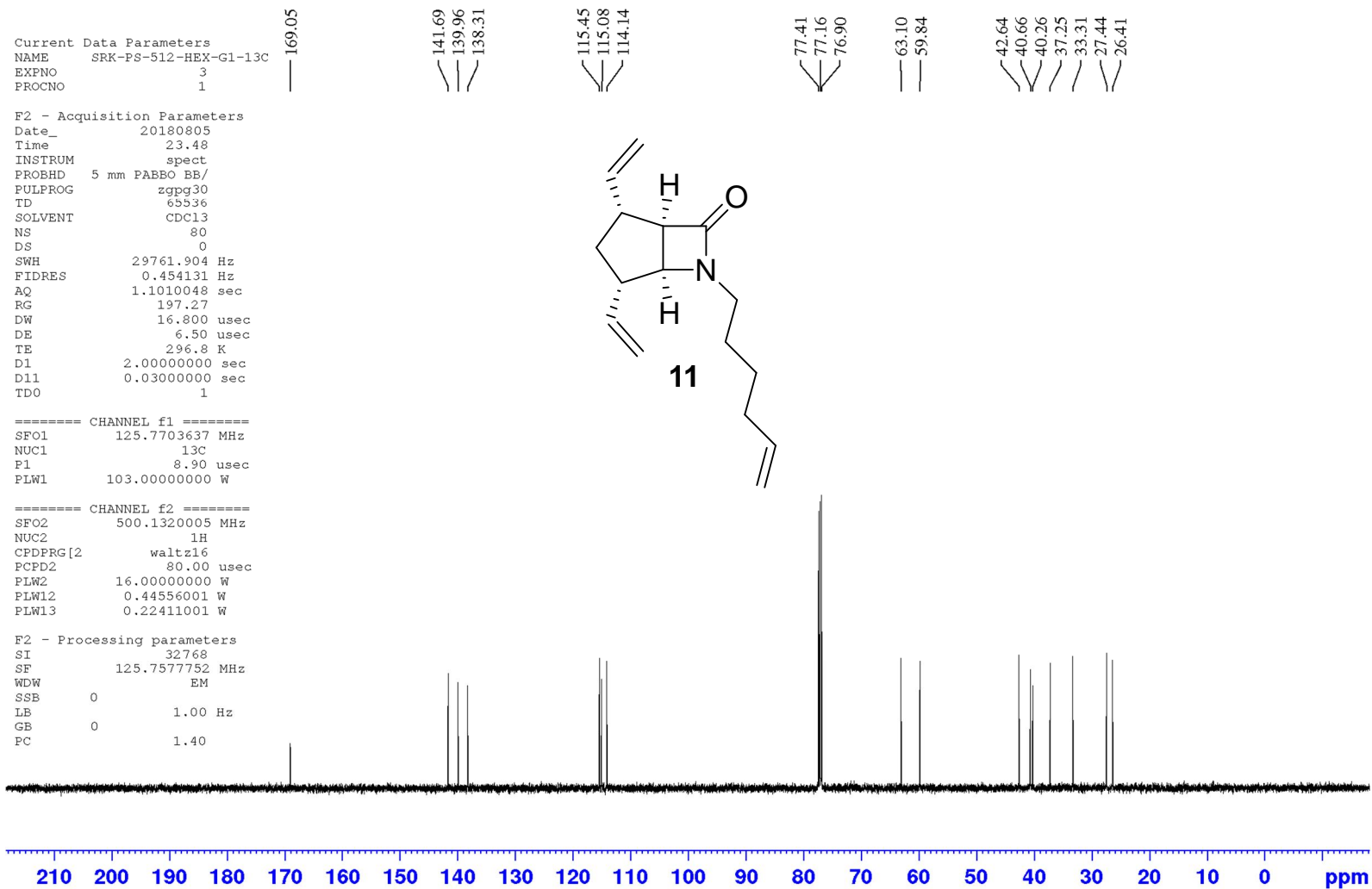
===== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 13.35 usec  
PLW1 16.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300135 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



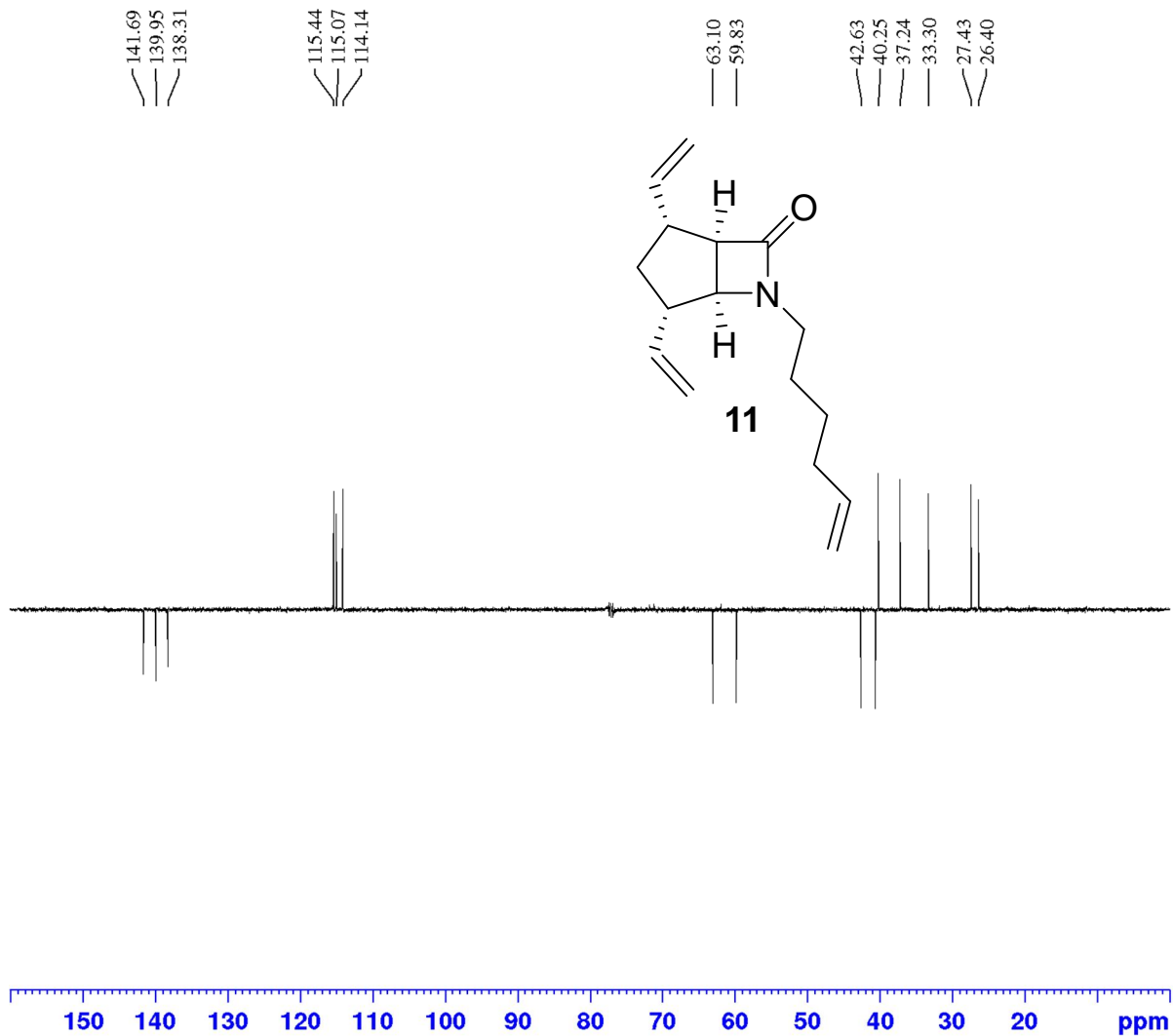
# <sup>13</sup>C NMR of the compound 11

SRK-PS-512-HEX-G1-13C



# DEPT NMR of the compound 11

SRK-PS-512-HEX-G1-DEPT



Current Data Parameters  
 NAME SRK-PS-512-HEX-G1-DEPT  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180805  
 Time 23.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG deptsp135  
 TD 65536  
 SOLVENT CDCl3  
 NS 80  
 DS 0  
 SWH 20161.291 Hz  
 FIDRES 0.307637 Hz  
 AQ 1.6252928 sec  
 RG 197.27  
 DW 24.800 usec  
 DE 6.50 usec  
 TE 296.4 K  
 CNST2 145.0000000  
 D1 2.00000000 sec  
 D2 0.00344828 sec  
 D12 0.00002000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 125.7678486 MHz  
 NUC1 13C  
 P1 8.90 usec  
 P13 2000.00 usec  
 PLW0 0 W  
 PLW1 103.00000000 W  
 SPNAM[5] Crp60comp.4  
 SPOALS 0.500  
 SPOFFS5 0 Hz  
 SPW5 12.46500015 W

===== CHANNEL f2 =====  
 SFO2 500.1315995 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 P3 13.35 usec  
 P4 26.70 usec  
 PCPD2 80.00 usec  
 PLW2 16.00000000 W  
 PLW12 0.44556001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577765 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

## Energies and cartesian coordinates of optimized geometries of 4, 9, 10, and 11.

Compound 4			
Zero-point correction=	0.275534 (Hartree/Particle)		
Thermal correction to Energy=	0.290404		
Thermal correction to Enthalpy=	0.291348		
Thermal correction to Gibbs Free Energy=	0.231841		
Sum of electronic and zero-point Energies=	-634.972971		
Sum of electronic and thermal Energies=	-634.958101		
Sum of electronic and thermal Enthalpies=	-634.957157		
Sum of electronic and thermal Free Energies=	-635.016664		
0 1			
C	-0.40479700	0.19193600	-0.65983200
C	0.57836300	-1.01809200	-0.76550400
C	1.70903900	-0.78539200	0.25143600
C	1.07931100	0.22385300	1.24759400
C	0.14862100	1.13343000	0.42565700
H	-0.69925200	0.70344300	-1.58154800
H	0.91292500	-1.32117800	-1.75865600
H	1.94074600	-1.72358700	0.76835600
H	0.47330600	-0.33625000	1.96845800
H	1.83110200	0.77154200	1.82022100
H	-0.69210500	1.48364800	1.04301800
C	-0.57913000	-1.84546300	-0.17961800
O	-0.72935200	-2.97646100	0.21039200
N	-1.41122900	-0.75707900	-0.17373000
C	-2.67831700	-0.53589400	0.48438600
H	-3.09559700	-1.53086600	0.67556300
H	-2.53545900	-0.04141700	1.45655400
C	-3.59152300	0.28947300	-0.37724400
H	-3.83644500	-0.13238100	-1.35058100
C	-4.06329700	1.47819500	-0.01729300
H	-3.81648800	1.91145200	0.94906700
H	-4.71578900	2.05514400	-0.66367400
C	4.17658300	-0.77402400	-0.15863200
H	5.06103700	-0.38900700	-0.65510800
H	4.32332400	-1.57789500	0.55831000
C	2.96512600	-0.28845200	-0.41249600
H	2.84748200	0.51490400	-1.13832600
C	1.98856200	2.84897500	0.02731100
H	2.70678300	2.35607400	0.67550600
H	2.31442000	3.76561100	-0.45303800
C	0.76978800	2.36343000	-0.18668600
H	0.10346600	2.91015700	-0.85562200

**Compound 9**

Zero-point correction= 0.304496 (Hartree/Particle)

Thermal correction to Energy= 0.320725

Thermal correction to Enthalpy= 0.321669

Thermal correction to Gibbs Free Energy= 0.258756

Sum of electronic and zero-point Energies= -674.238695

Sum of electronic and thermal Energies= -674.222466

Sum of electronic and thermal Enthalpies= -674.221522

Sum of electronic and thermal Free Energies= -674.284434

O 1

C	0.10282300	0.33213400	-0.59317100
C	0.95072700	-0.97316700	-0.71826300
C	2.13336000	-0.85584800	0.25636500
C	1.64955800	0.22155400	1.26311200
C	0.78846800	1.21871800	0.46443400
H	-0.15613200	0.86238200	-1.51590000
H	1.21914400	-1.30894700	-1.72114900
H	2.28437300	-1.80978000	0.77406400
H	1.01395400	-0.26441100	2.01098500
H	2.47366600	0.69384100	1.80254900
H	0.01485200	1.65763300	1.11177100
C	-0.27471400	-1.67540300	-0.10858500
O	-0.54159000	-2.79189500	0.26078300
N	-0.98100800	-0.50316800	-0.06708600
C	-2.25985800	-0.18403000	0.51562800
H	-2.64670900	-1.11414000	0.94252900
H	-2.12968500	0.52985900	1.34194800
C	4.57547000	-1.09293900	-0.23968300
H	5.47282500	-0.80276800	-0.77587700
H	4.67168800	-1.89771800	0.48474800
C	3.40797600	-0.49574600	-0.45797900
H	3.34035400	0.30546800	-1.19264100
C	2.78979800	2.71550800	-0.03359900
H	3.48032100	2.14071600	0.57601300
H	3.19300500	3.58998400	-0.53342100
C	1.51377900	2.37322700	-0.18146500
H	0.88232400	2.99467000	-0.81826300
C	-3.24544800	0.38375400	-0.51288200
H	-3.41627800	-0.36327400	-1.29454100
H	-2.78443200	1.25841200	-0.99177600
C	-4.54334100	0.78037700	0.12812400
H	-4.48600600	1.56839200	0.87970500
C	-5.71962600	0.22534600	-0.14382200
H	-5.81307400	-0.56402300	-0.88498200
H	-6.62825500	0.54013200	0.35828900



### Compound 10

Zero-point correction=	0.352954 (Hartree/Particle)
Thermal correction to Energy=	0.369851
Thermal correction to Enthalpy=	0.370795
Thermal correction to Gibbs Free Energy=	0.305462
Sum of electronic and zero-point Energies=	-709.188587
Sum of electronic and thermal Energies=	-709.171690
Sum of electronic and thermal Enthalpies=	-709.170746
Sum of electronic and thermal Free Energies=	-709.236079

0 1

C	0.54981800	0.41160500	-0.27797600
C	1.44188600	-0.79066600	-0.70182100
C	2.70666800	-0.77665100	0.17905800
C	2.30091200	0.12601800	1.37293100
C	1.28990700	1.16942100	0.82971900
H	0.15159700	1.03750200	-1.06438100
H	1.63379600	-0.92896500	-1.75768900
H	2.92029700	-1.78155300	0.52756000
H	1.81260500	-0.48517100	2.12497400
H	3.15970100	0.58732400	1.84792300
H	0.59519300	1.43924100	1.62277700
C	0.30501700	-1.65831500	-0.16110600
O	0.10080500	-2.83028400	-0.06195700
N	-0.41704100	-0.57590600	0.20495000
C	-1.71383100	-0.46431900	0.82563300
H	-1.96175600	-1.45070800	1.20056500
H	-1.64479300	0.20082400	1.68368500
C	5.03175900	-0.96941500	-0.72893600
H	5.86878100	-0.56596400	-1.27126400
H	5.14572600	-1.96264900	-0.32731700
C	3.91757600	-0.27583100	-0.56771300
H	3.85315200	0.71424500	-0.99005100
C	1.89286500	3.08756600	-0.75813600
H	1.32889300	2.72521200	-1.59868500
H	2.41953900	4.01400700	-0.90532500
C	1.96221400	2.45615700	0.40221300
H	2.56143200	2.90694600	1.17958500
C	-2.79911600	0.02698600	-0.13183800
H	-2.85662200	-0.64866900	-0.98051400
H	-2.52261600	1.00440400	-0.52310300
C	-4.16975500	0.11899900	0.54872400
H	-4.46611700	-0.86078700	0.91413200
H	-4.09212600	0.77016300	1.41918500
C	-5.23430300	0.65822500	-0.36729200
H	-5.06241300	1.65051900	-0.75878700
C	-6.33512700	0.01683600	-0.72020500
H	-7.05621100	0.46229600	-1.38273000
H	-6.55415500	-0.97430400	-0.35906500

### Compound 11

Zero-point correction=	0.383191 (Hartree/Particle)
Thermal correction to Energy=	0.401406
Thermal correction to Enthalpy=	0.402350
Thermal correction to Gibbs Free Energy=	0.333514
Sum of electronic and zero-point Energies=	-748.196674
Sum of electronic and thermal Energies=	-748.178460
Sum of electronic and thermal Enthalpies=	-748.177515
Sum of electronic and thermal Free Energies=	-748.246351

0 1

C	0.98869700	0.37476900	-0.30179800
C	1.98542600	-0.75338700	-0.69503900
C	3.21477700	-0.64313700	0.22822900
C	2.70061800	0.22386200	1.40672500
C	1.63037300	1.18641500	0.82880800
H	0.56869200	0.96887600	-1.10150900
H	2.22336400	-0.87362400	-1.74375600
H	3.49356100	-1.62904200	0.58489900
H	2.23640000	-0.42422400	2.14291000
H	3.50481600	0.74975300	1.90938300
H	0.89070000	1.40042600	1.59781900
C	0.90124300	-1.70792100	-0.19380500
O	0.78375100	-2.89277700	-0.10529300
N	0.08693700	-0.68597900	0.15058200
C	-1.23815000	-0.67673200	0.72062400
H	-1.40686300	-1.66693100	1.12810700
H	-1.26292600	0.02431900	1.55160400
C	5.57714900	-0.65437600	-0.60068600
H	6.39828700	-0.18660400	-1.11490900
H	5.75393800	-1.63645500	-0.19439100
C	4.40790100	-0.04921000	-0.47780100
H	4.28139700	0.93359600	-0.90309200
C	2.13560000	3.14736200	-0.74073600
H	1.62984600	2.74326200	-1.59911300
H	2.59330500	4.11211400	-0.87156400
C	2.21479300	2.52190200	0.42220300
H	2.75073700	3.01699600	1.21858600
C	-2.32888200	-0.32901400	-0.29219600
H	-2.28671900	-1.04557800	-1.10907900
H	-2.12527200	0.65061000	-0.72137000
C	-3.72405700	-0.33178500	0.33274000
H	-3.92448800	-1.31192400	0.76289300
H	-3.76121100	0.37970200	1.15554800
C	-4.82724200	0.01300200	-0.67500600
H	-4.78129900	-0.69375400	-1.50254400
H	-4.64876900	1.00015700	-1.09390500
C	-6.20303800	-0.03521400	-0.06845400
H	-6.50197400	-0.98589400	0.34902900
C	-7.04893200	0.97932600	-0.00859300
H	-6.80143200	1.94798700	-0.41054600
H	-8.02031600	0.87511900	0.44197400