Supporting Information

Synthesis of propellanes containing bicyclo[2.2.2]octene unit via the Diels–Alder reaction and ring-closing metathesis as key steps

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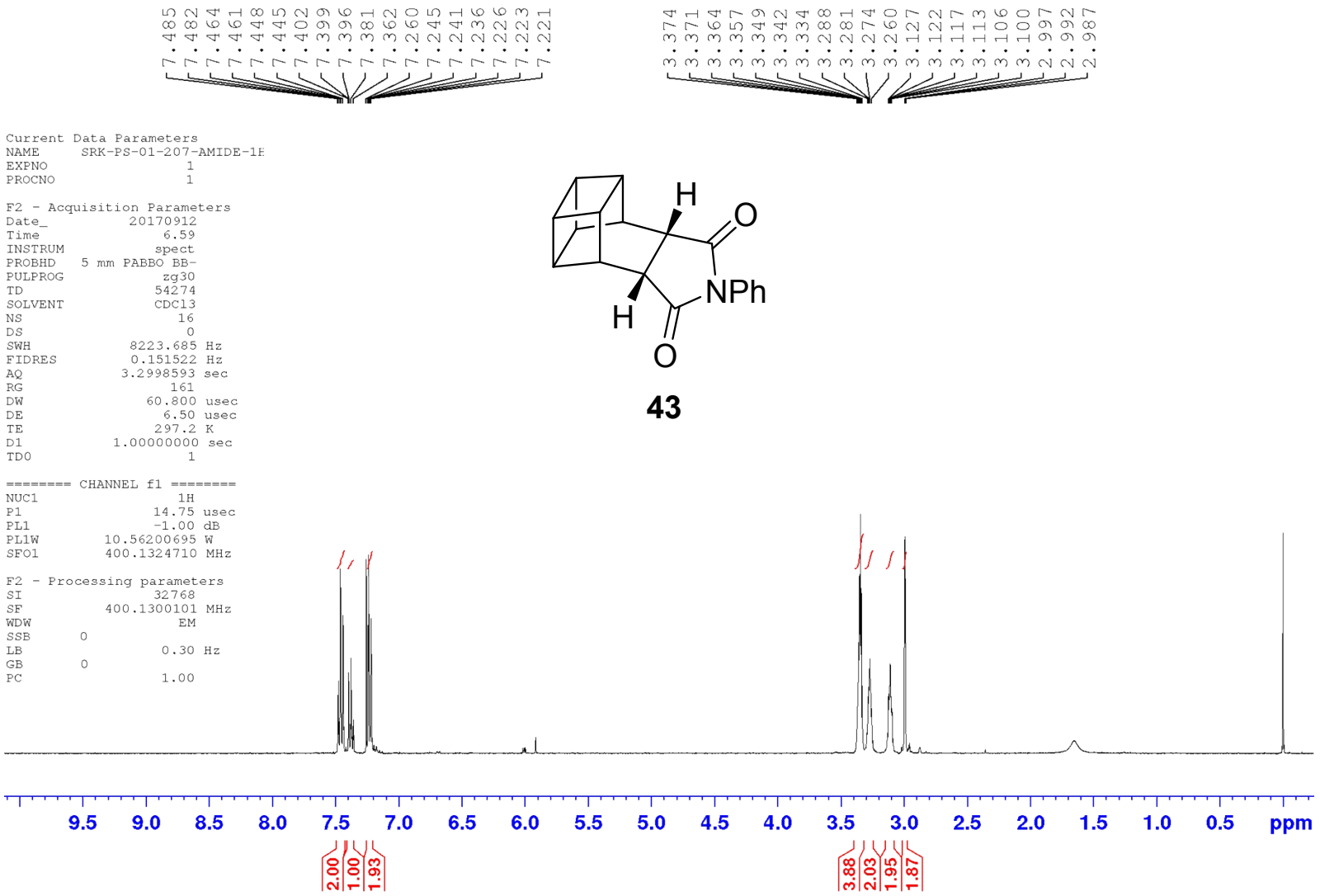
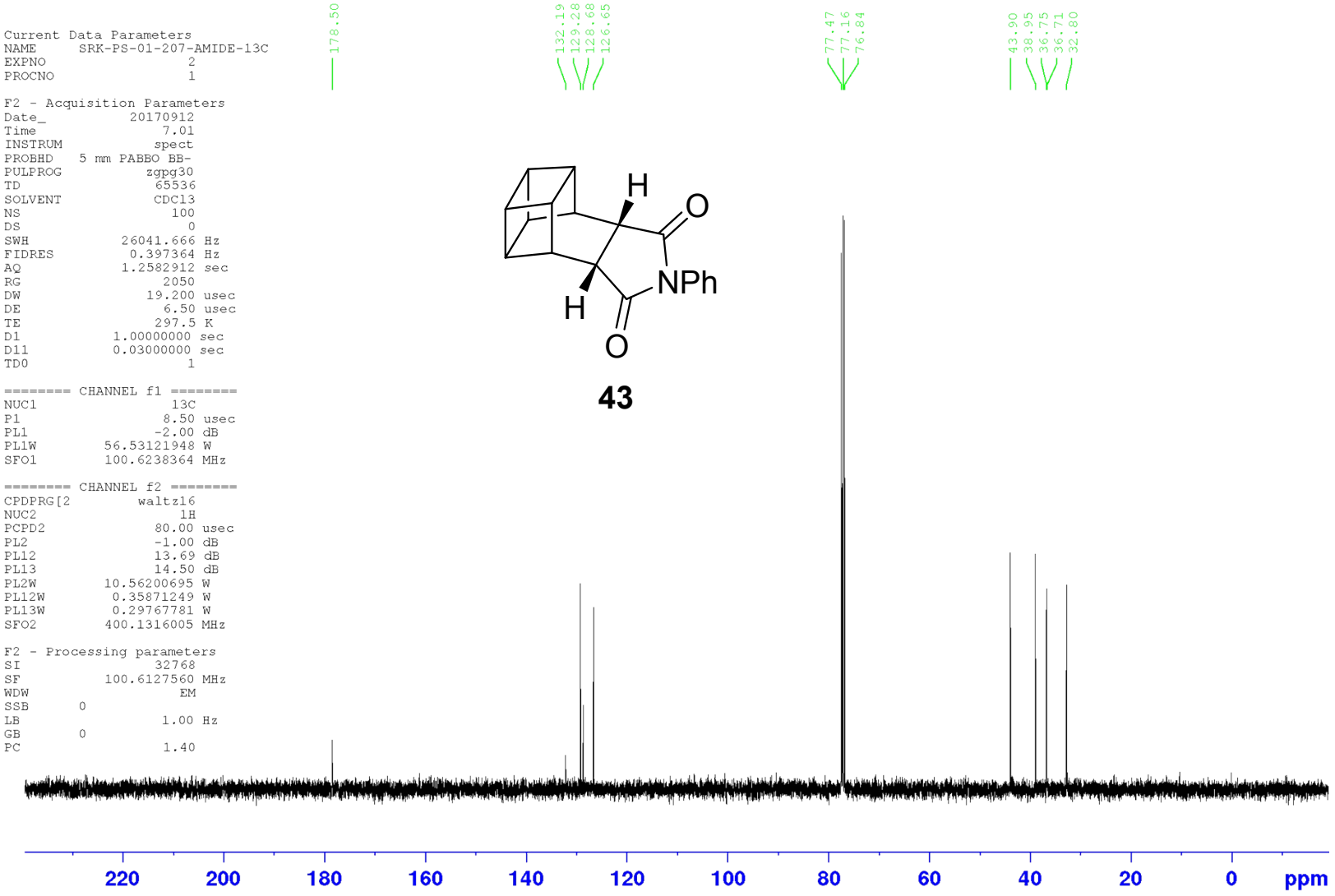
^{1}H NMR of the compound **43**



^{13}C NMR of the compound **43**

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EXPNO                   2
PROCNO                  1

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INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
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                297.5 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

F2 - Processing parameters
SI                32768
SF          100.6127560 MHz
WDW                EM
SSB       0
LB                1.00 Hz
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PC                1.40
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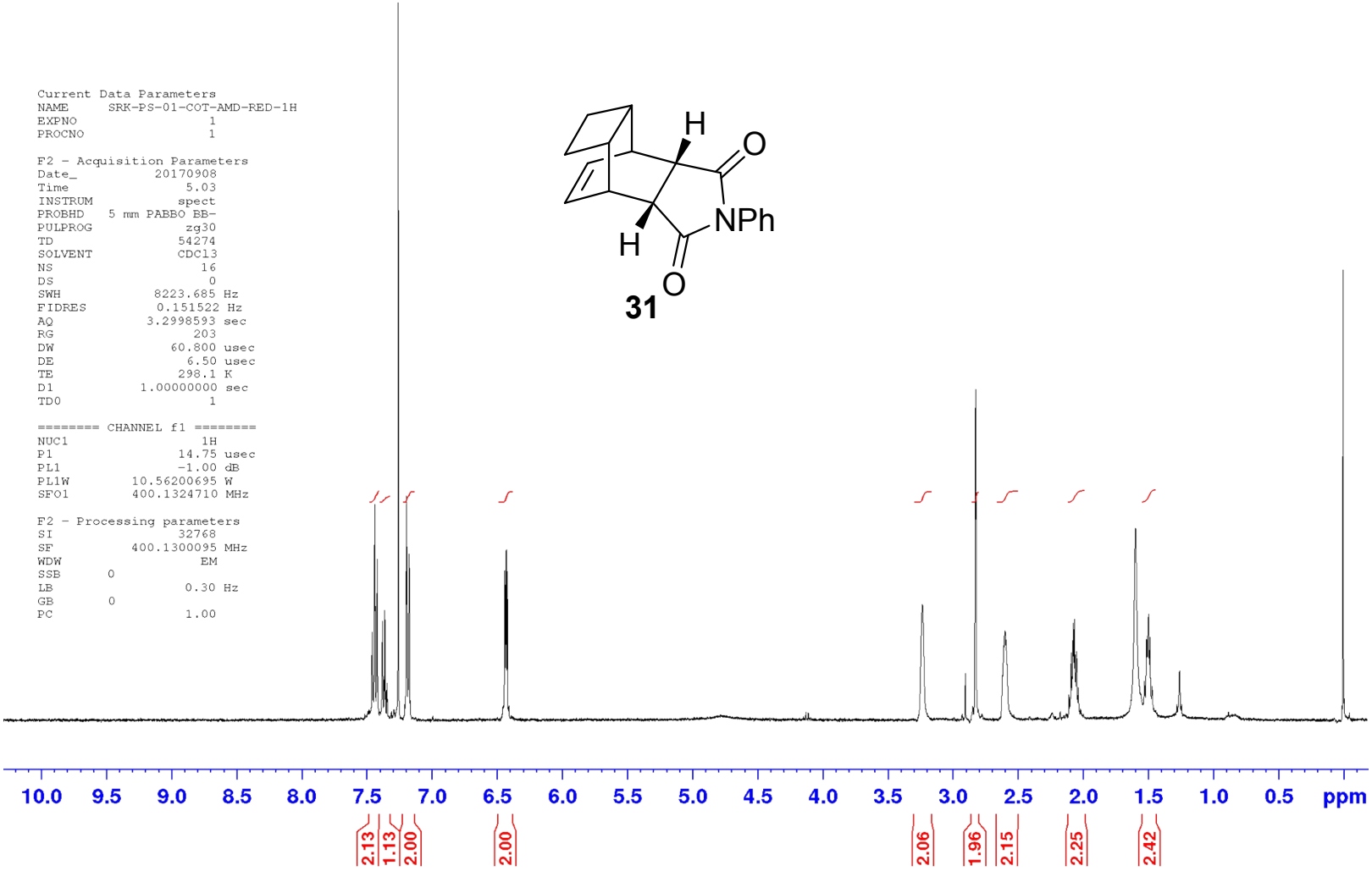
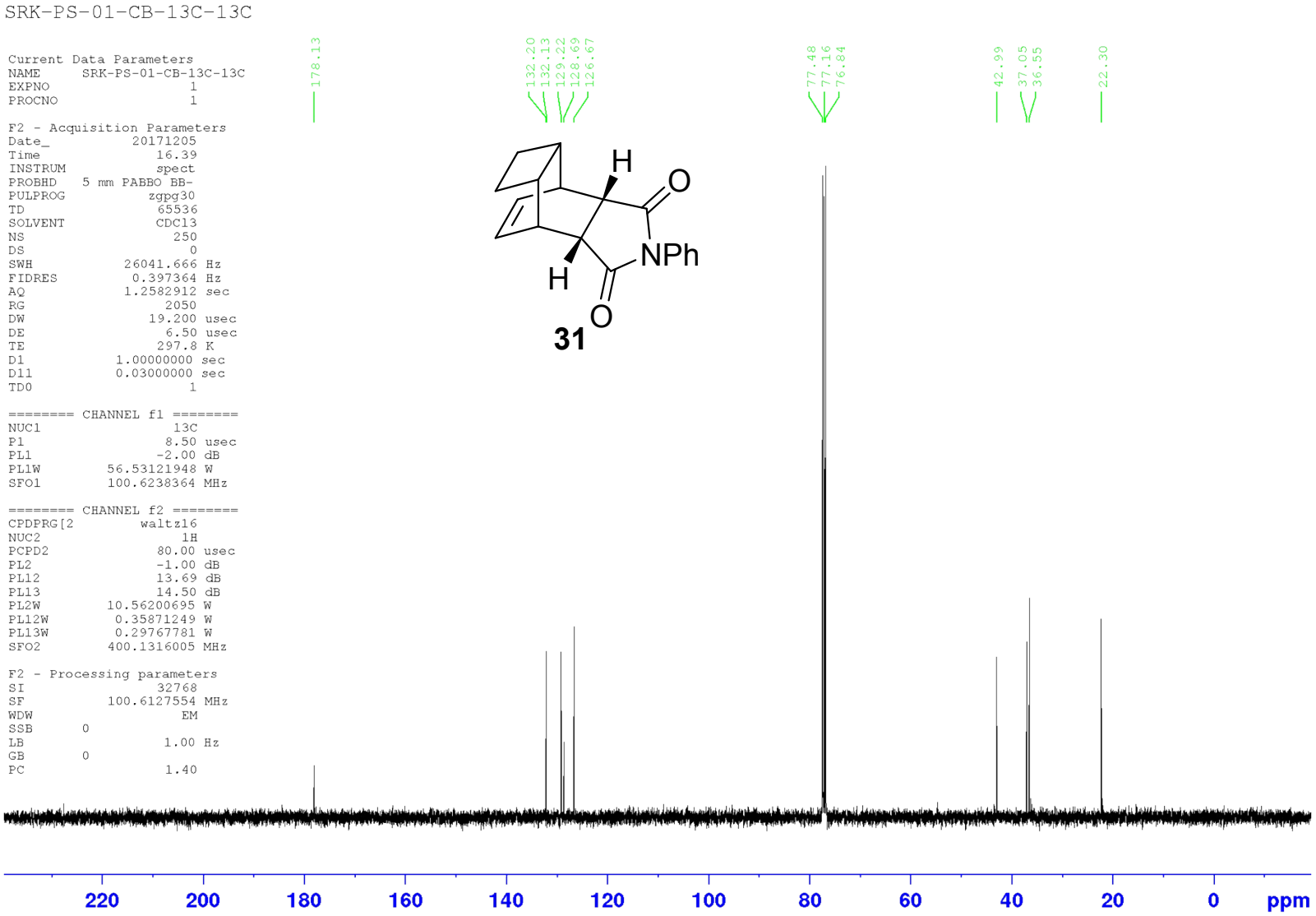
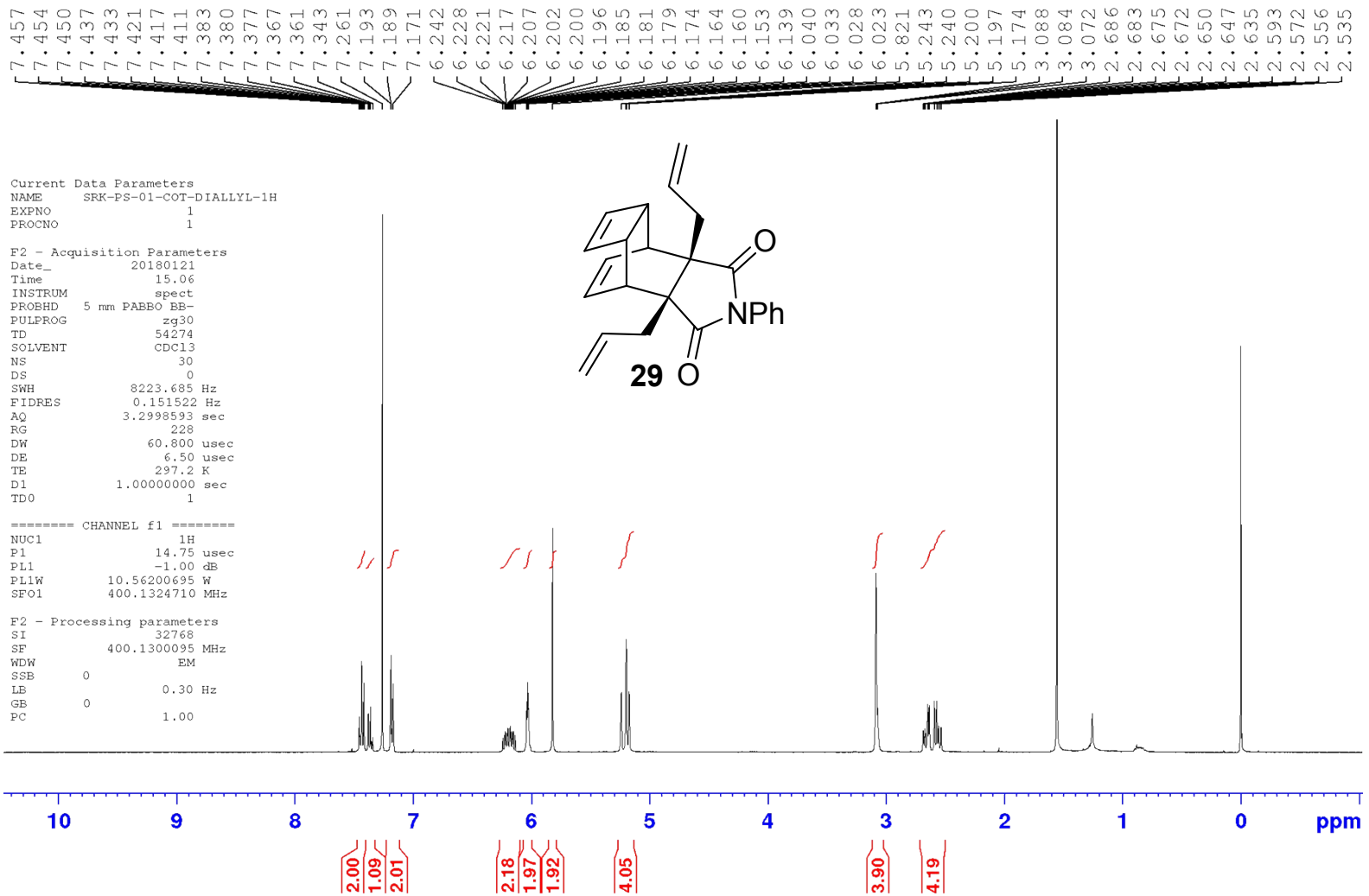
[1]H NMR of the compound **31**



^{13}C NMR of the compound **31**



^{1}H NMR of the compound **29**



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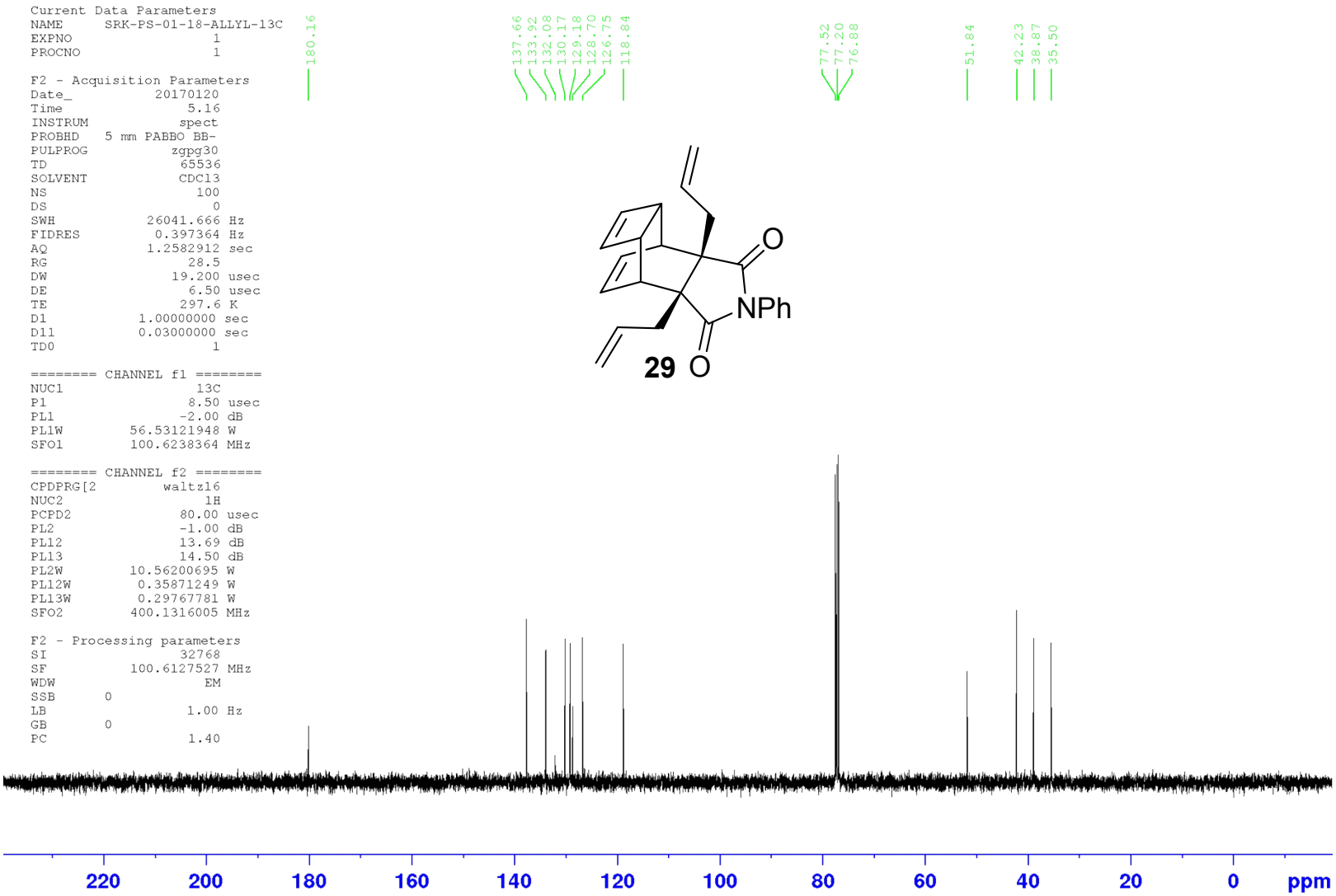

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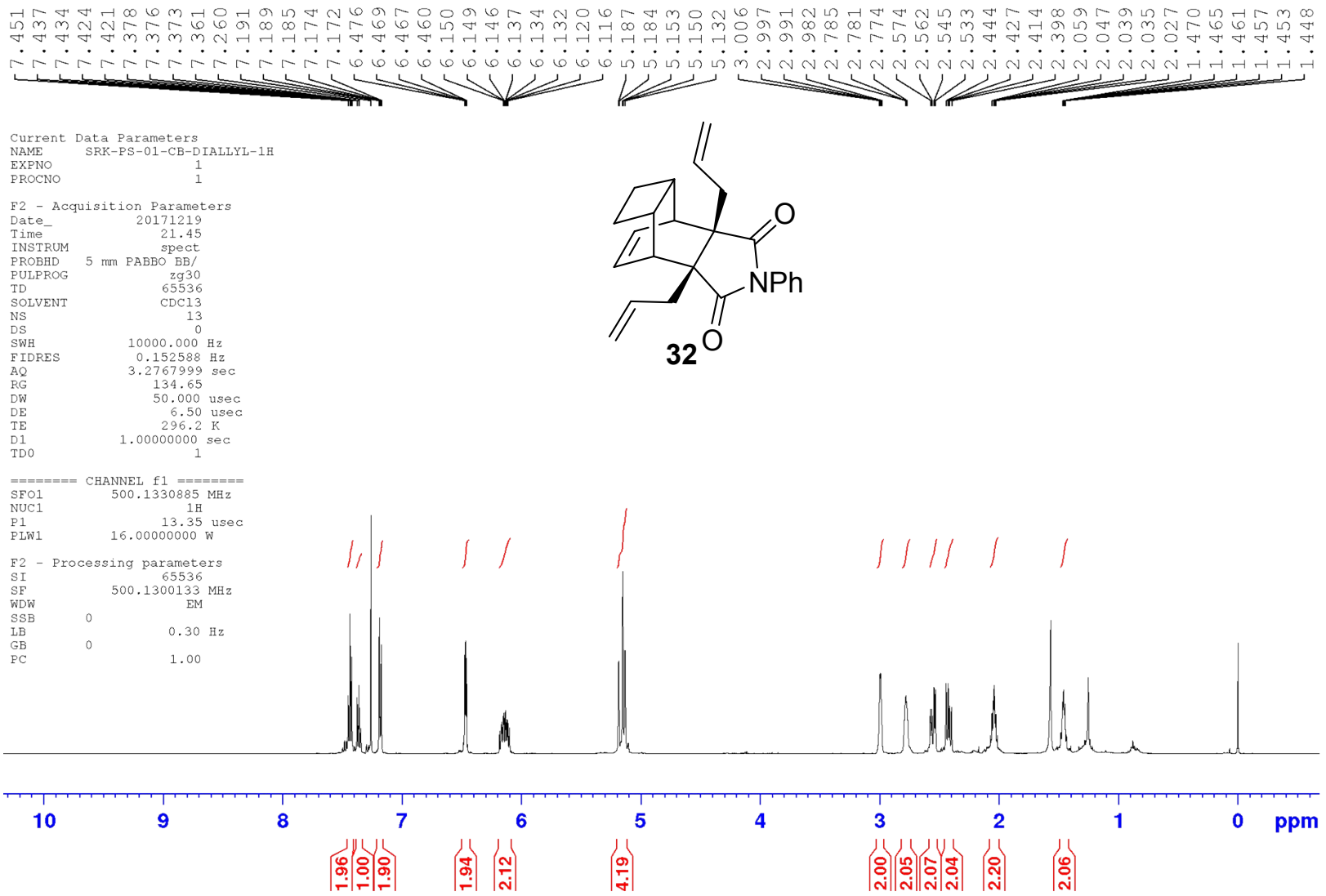

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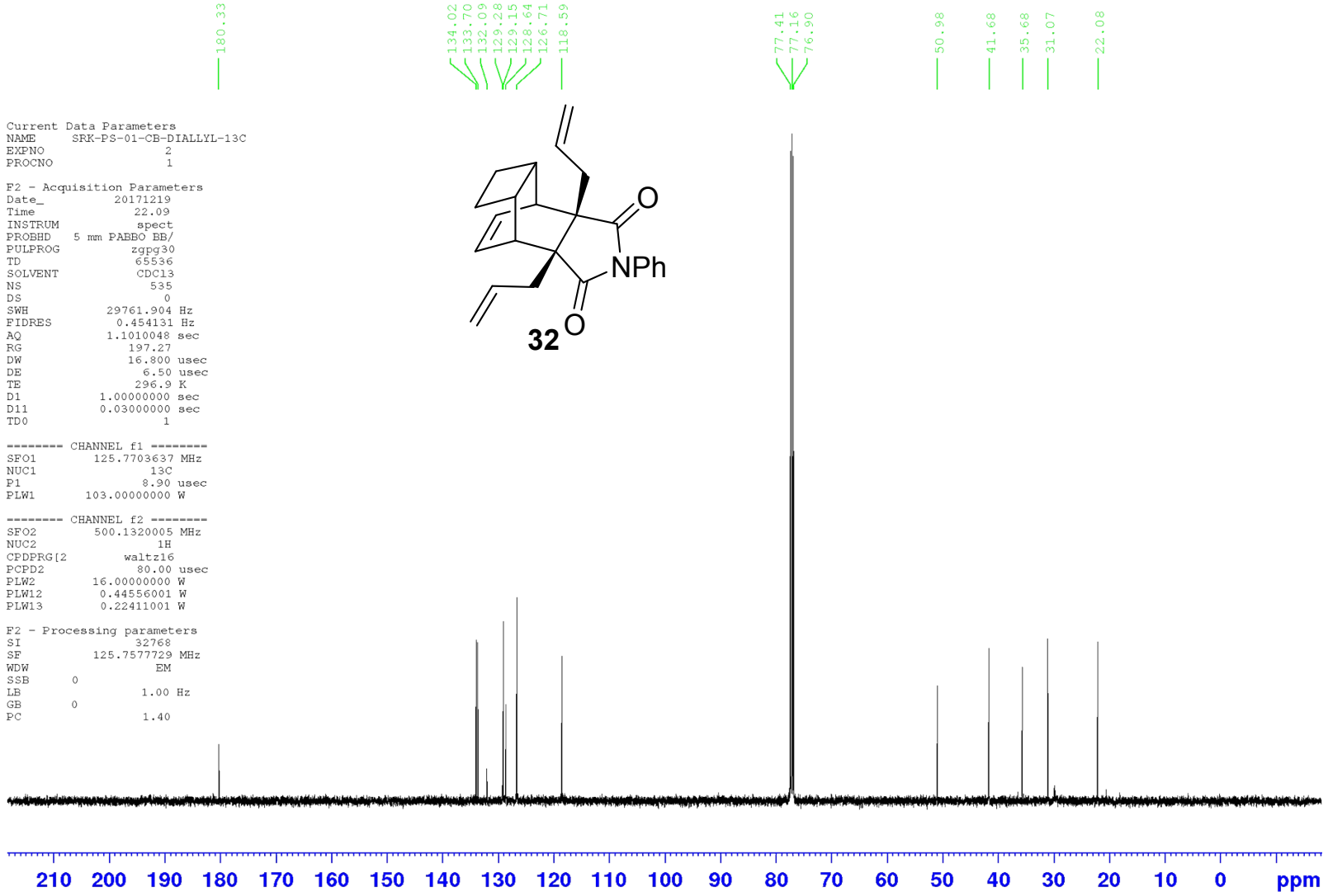
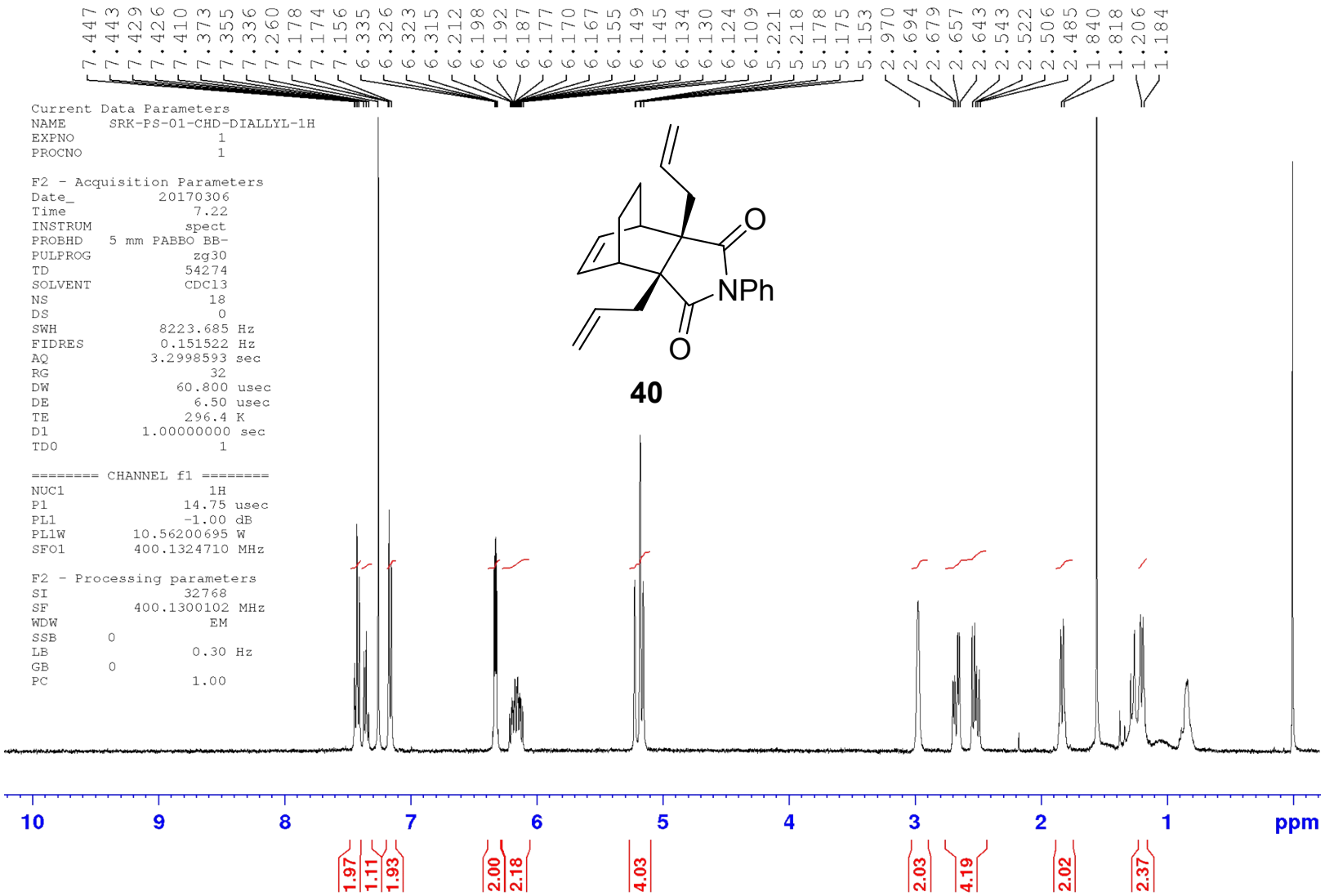
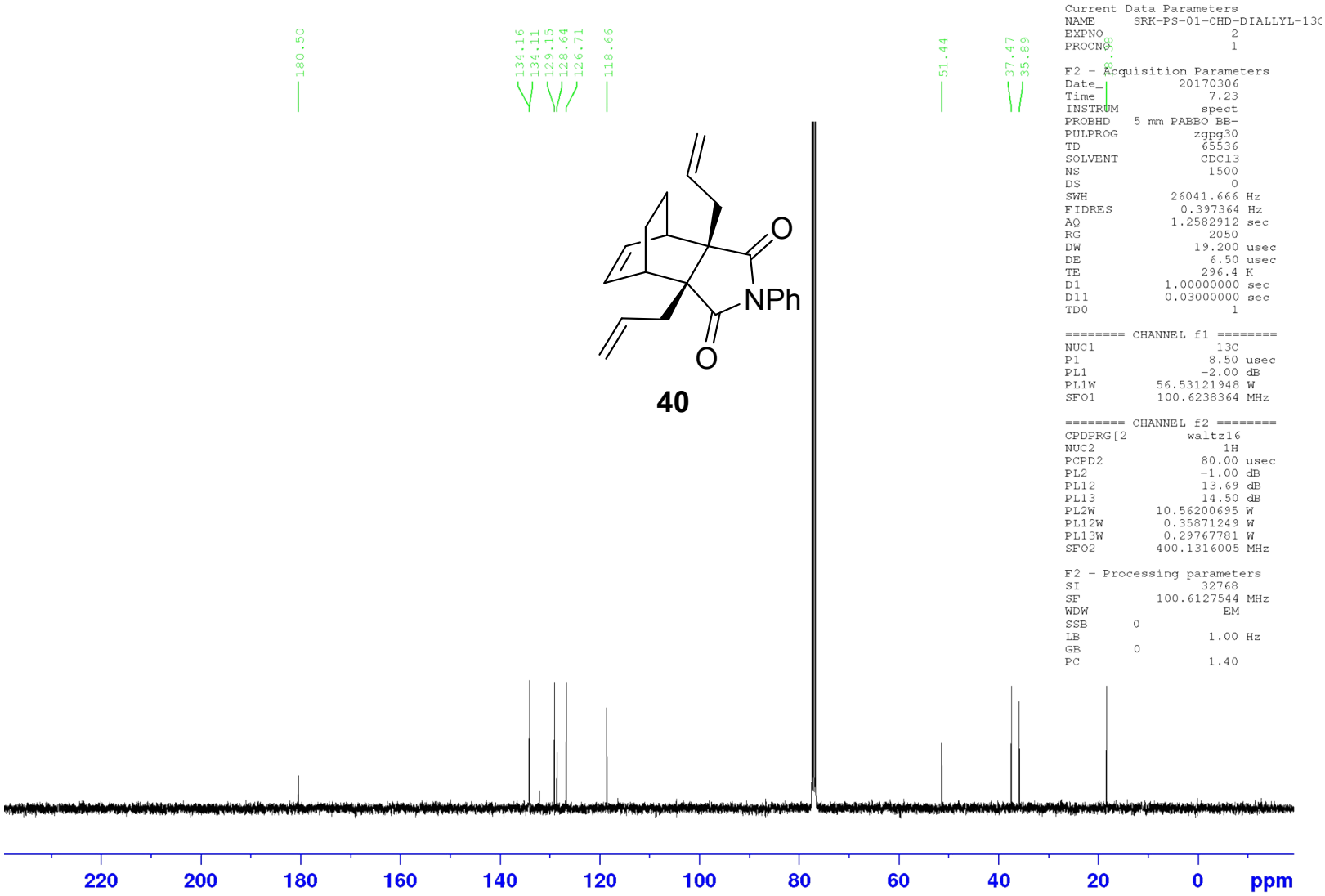


^{1}H NMR of the compound **40**



^{13}C NMR of the compound **40**

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PROCNO                1

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INSTRUM           spect
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TD              65536
SOLVENT         CDCl3
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SWH         26041.666 Hz
FIDRES       0.397364 Hz
AQ           1.2582912 sec
RG              2050
DW             19.200 usec
DE              6.50 usec
TE             296.4 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

F2 - Processing parameters
SI               32768
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WDW                EM
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LB                1.00 Hz
GB        0
PC                1.40
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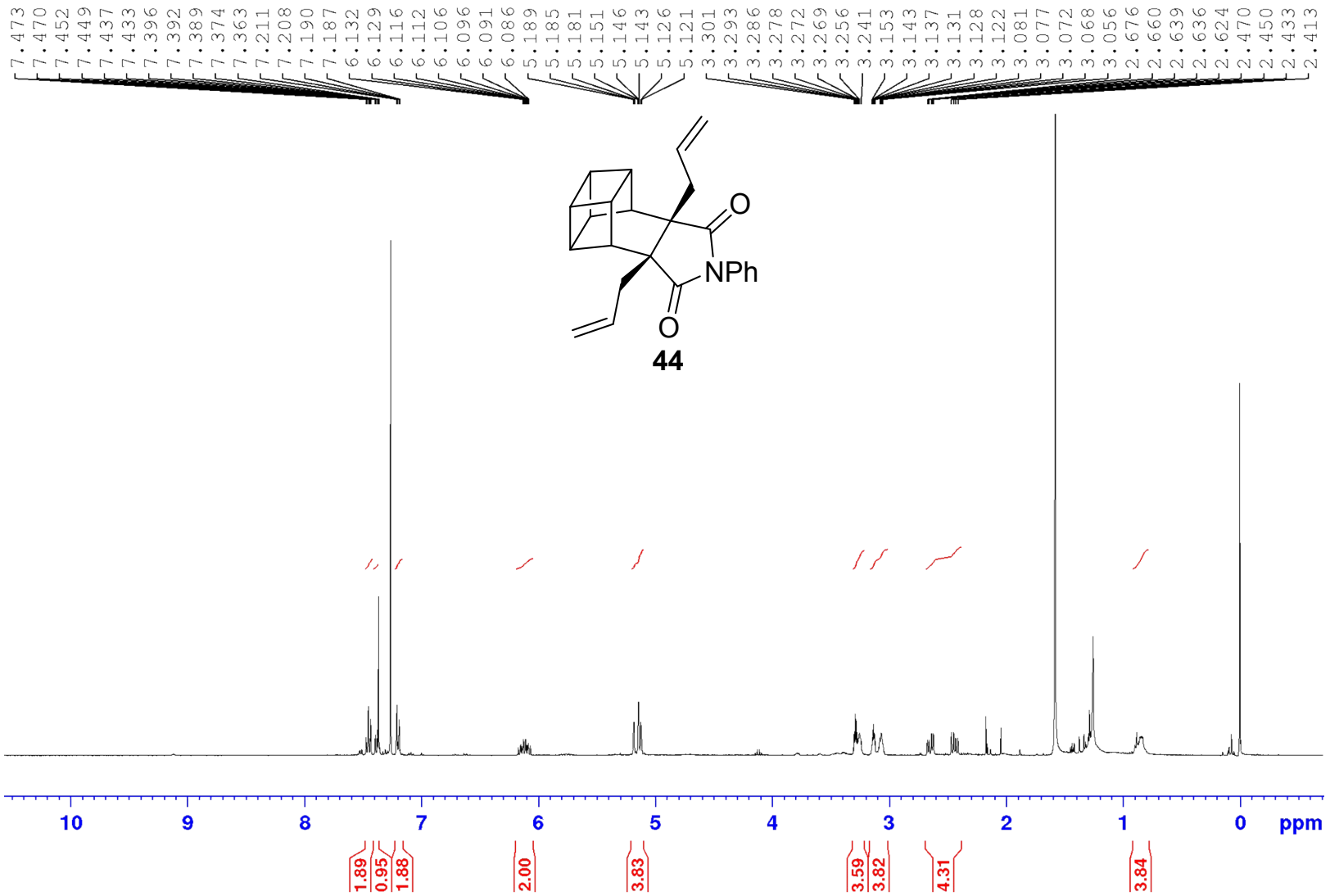
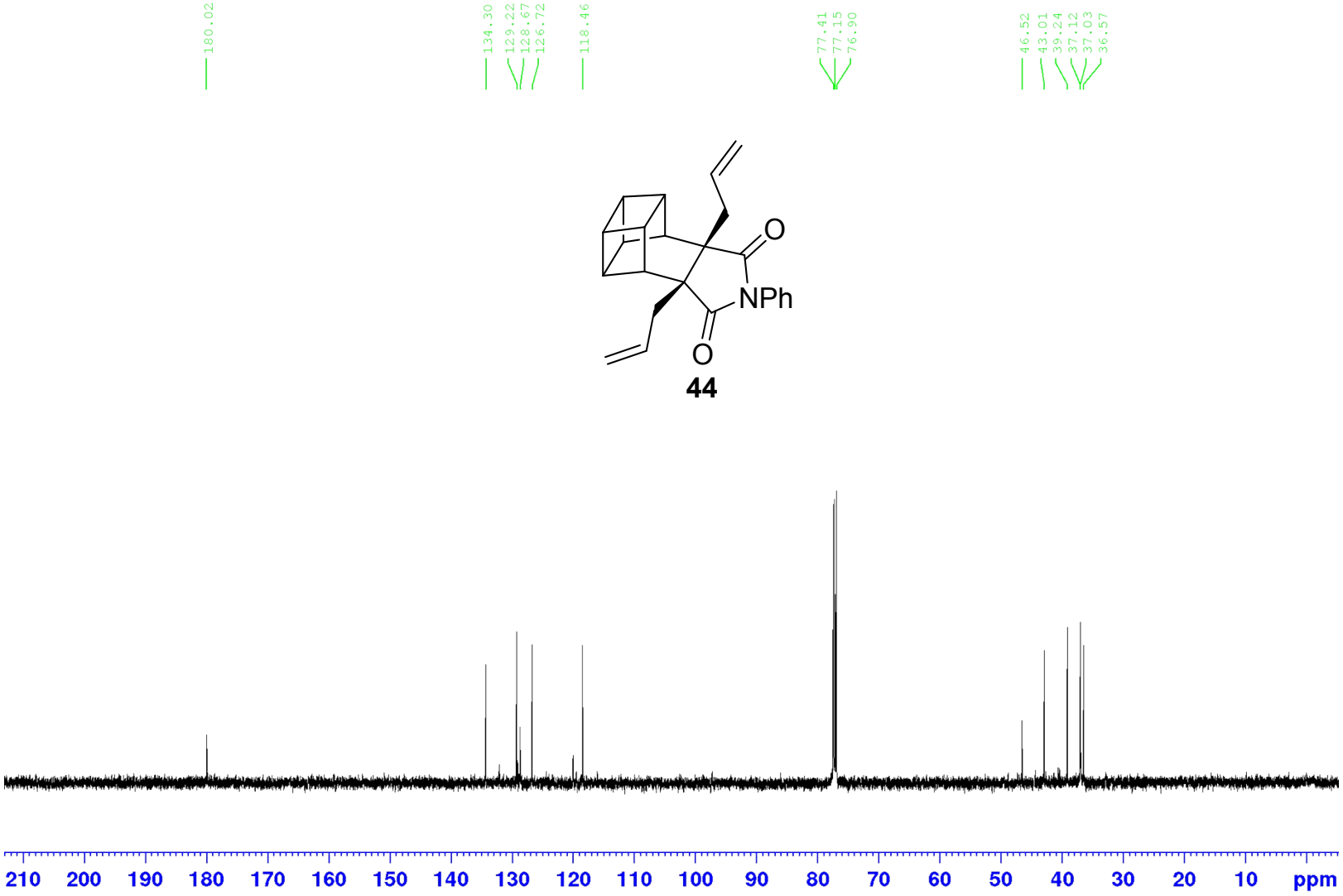
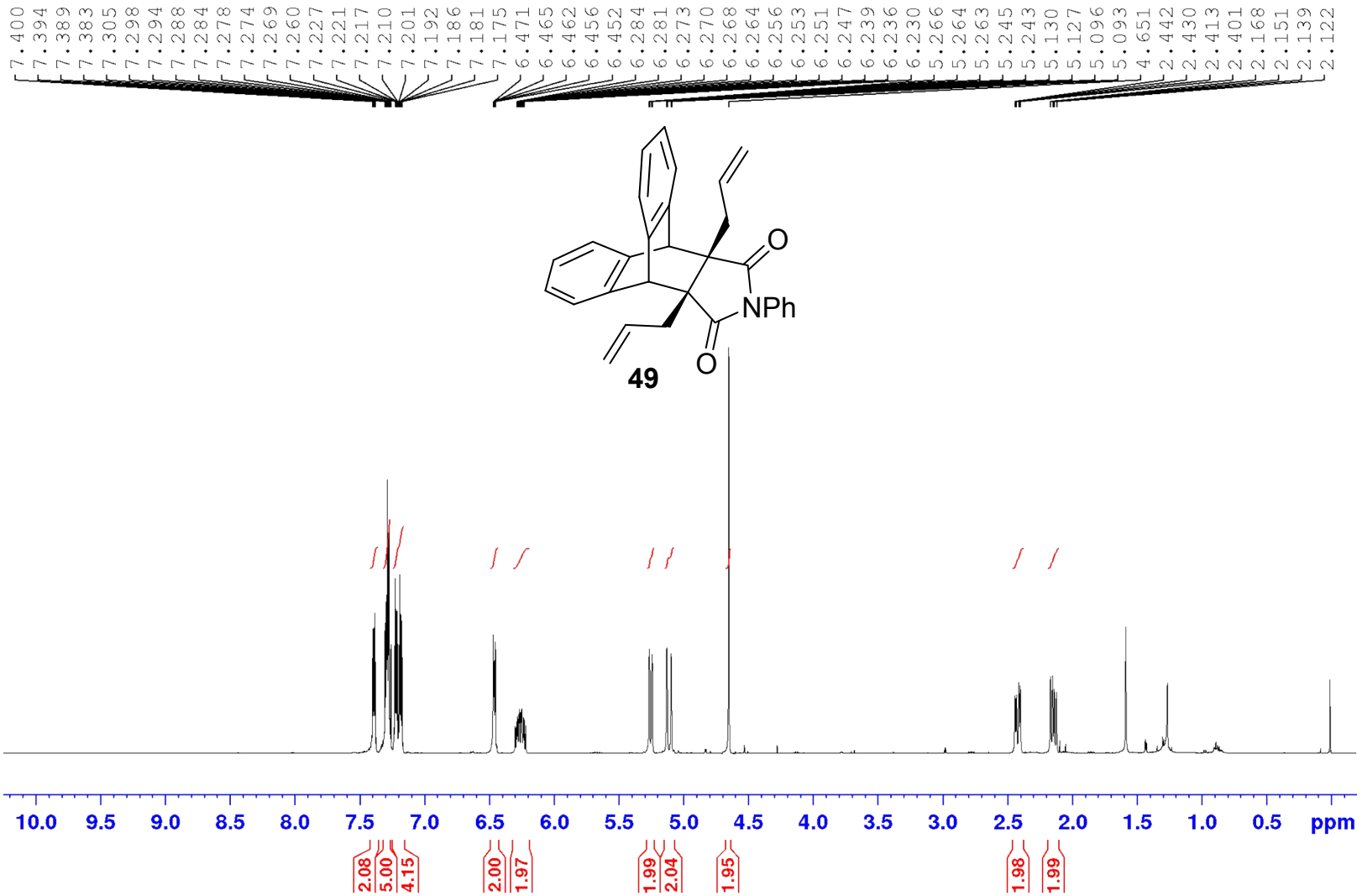
[1]H NMR of the compound **44**



^{13}C NMR of the compound **44**



^{1}H NMR of the compound **49**



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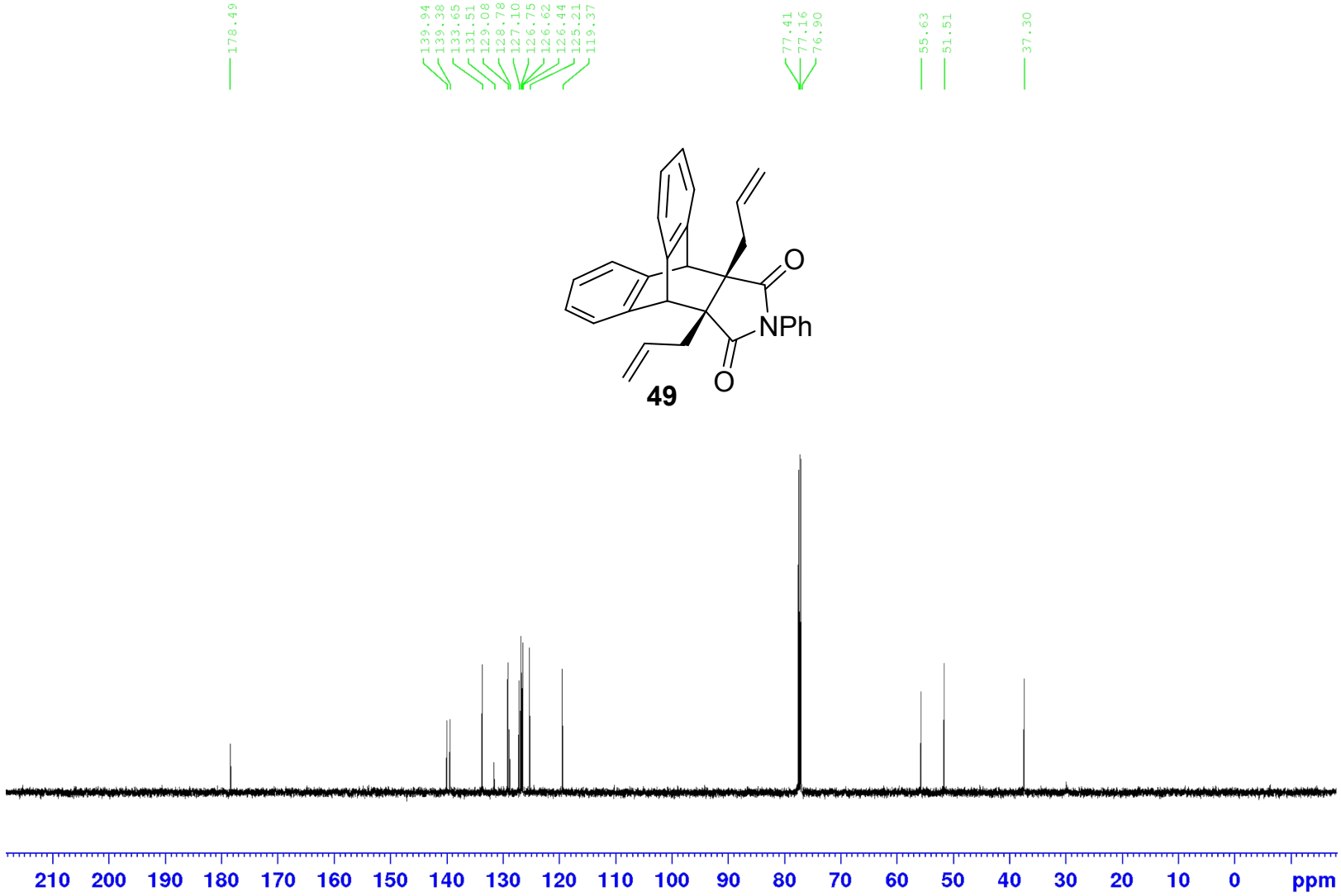

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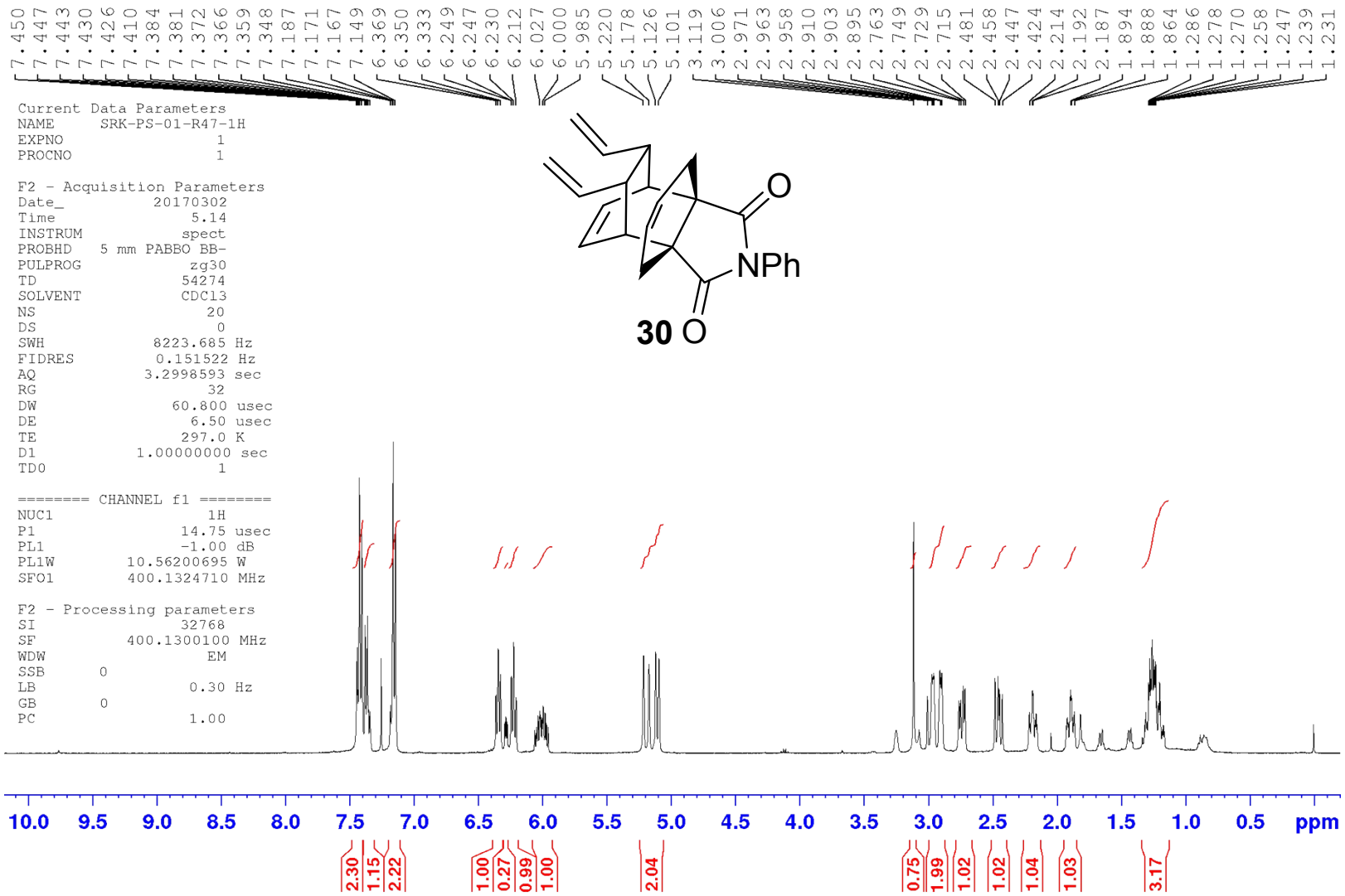
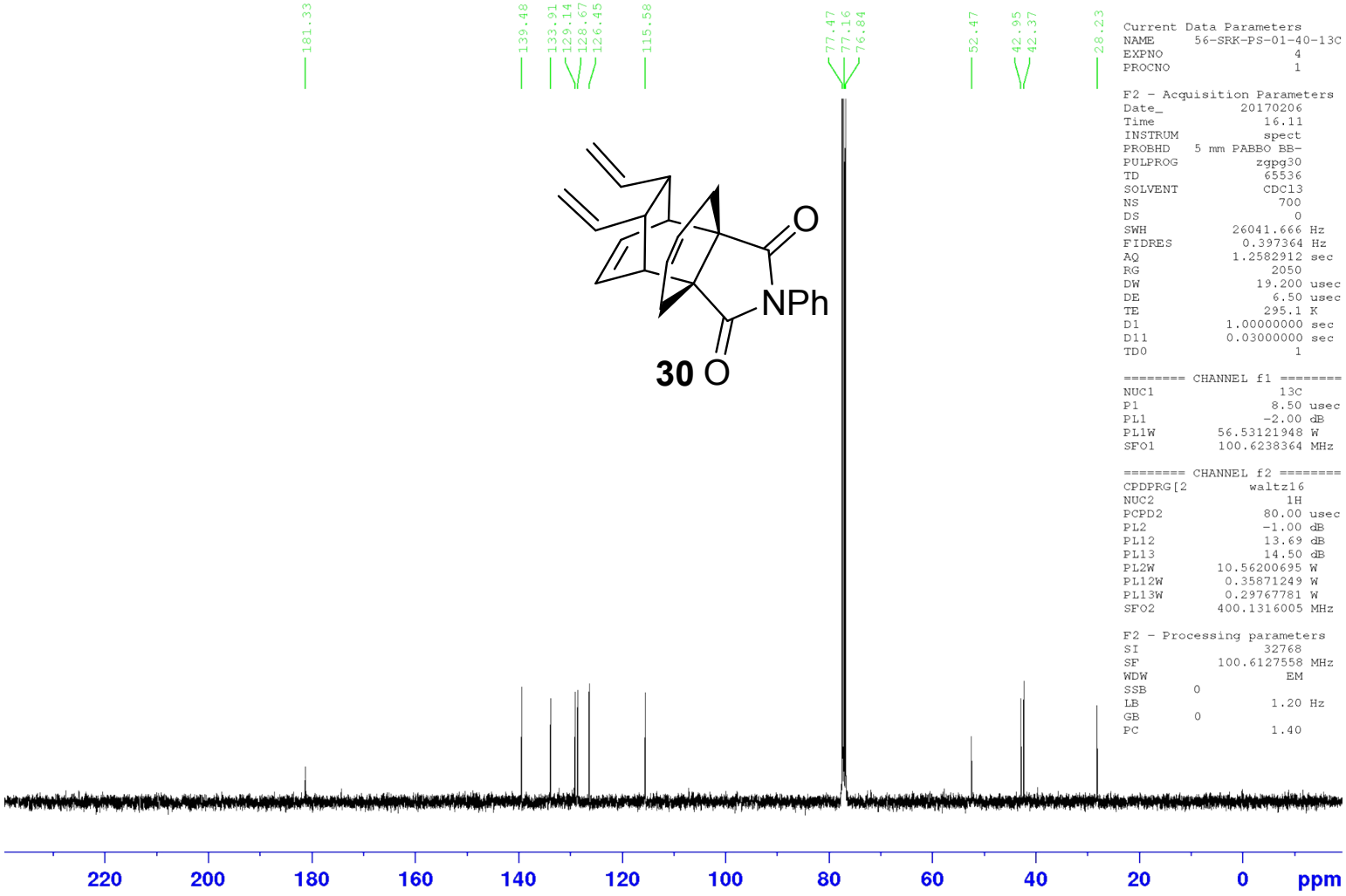


^{13}C NMR of the compound **30**

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PROCNO                      1

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Time                  16.11
INSTRUM               spect
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TD                   65536
SOLVENT              CDCl3
NS                     700
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                  295.1 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

F2 - Processing parameters
SI                     32768
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WDW                       EM
SSB       0
LB                    1.20 Hz
GB        0
PC                    1.40
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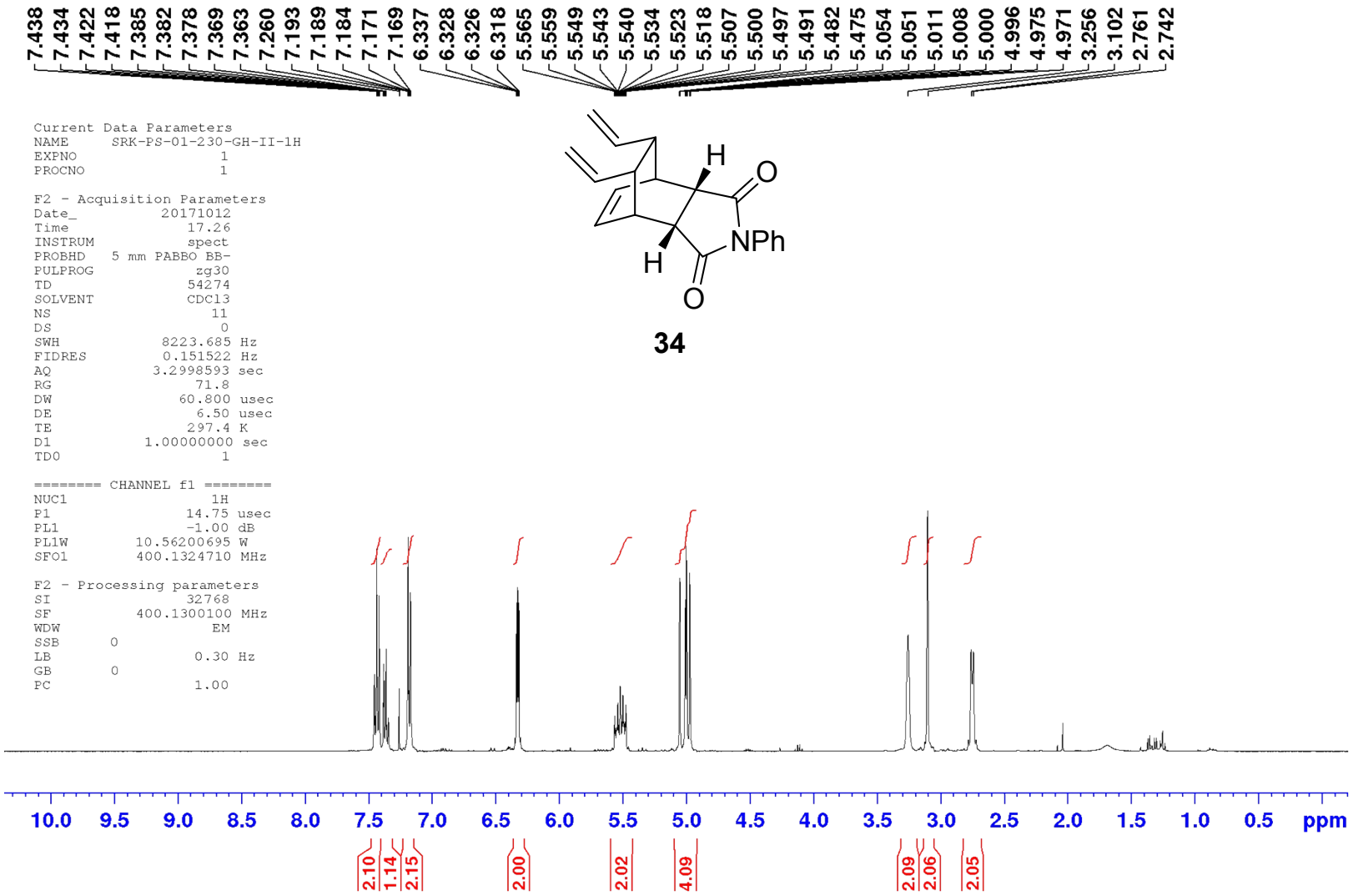
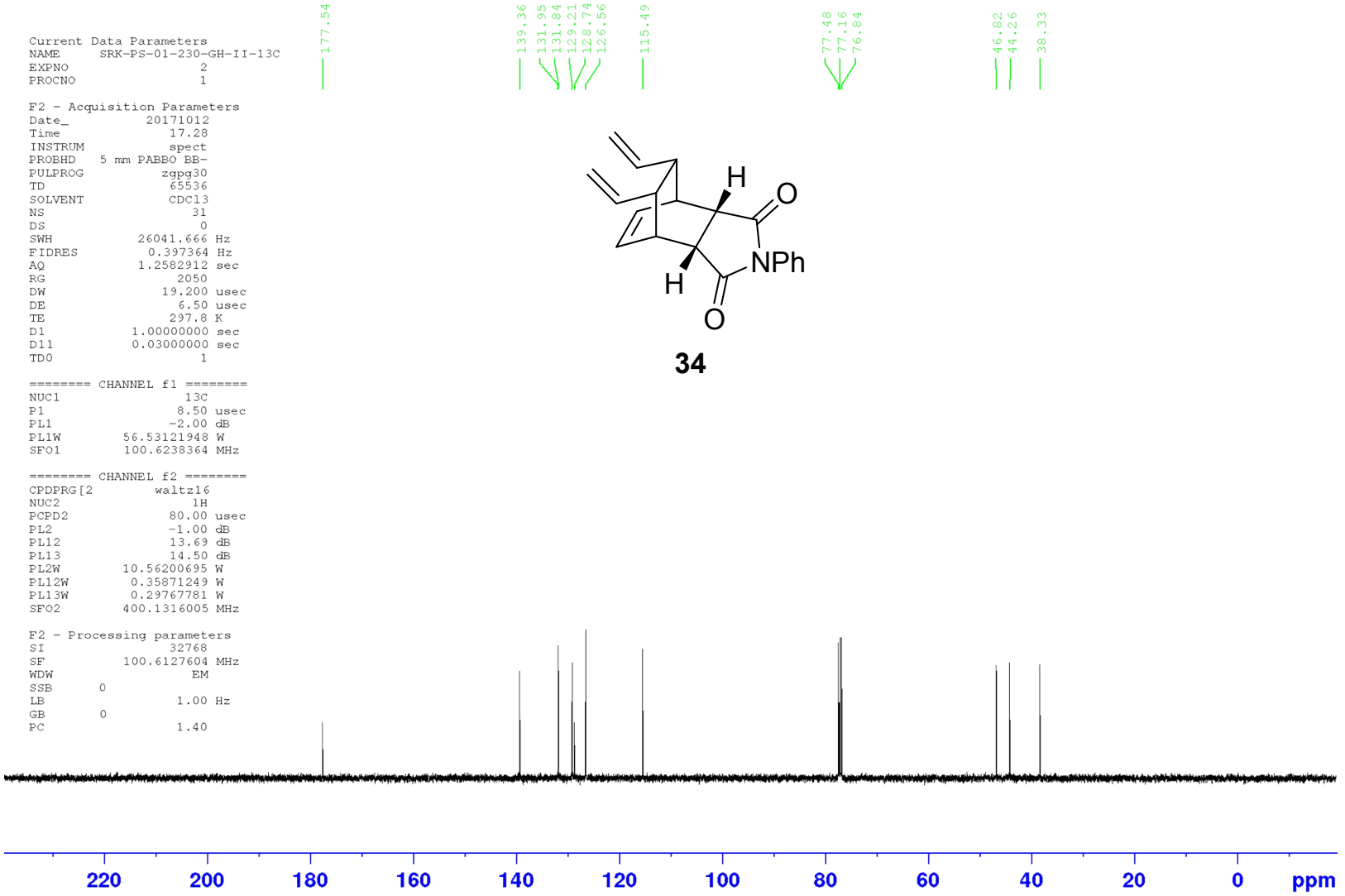
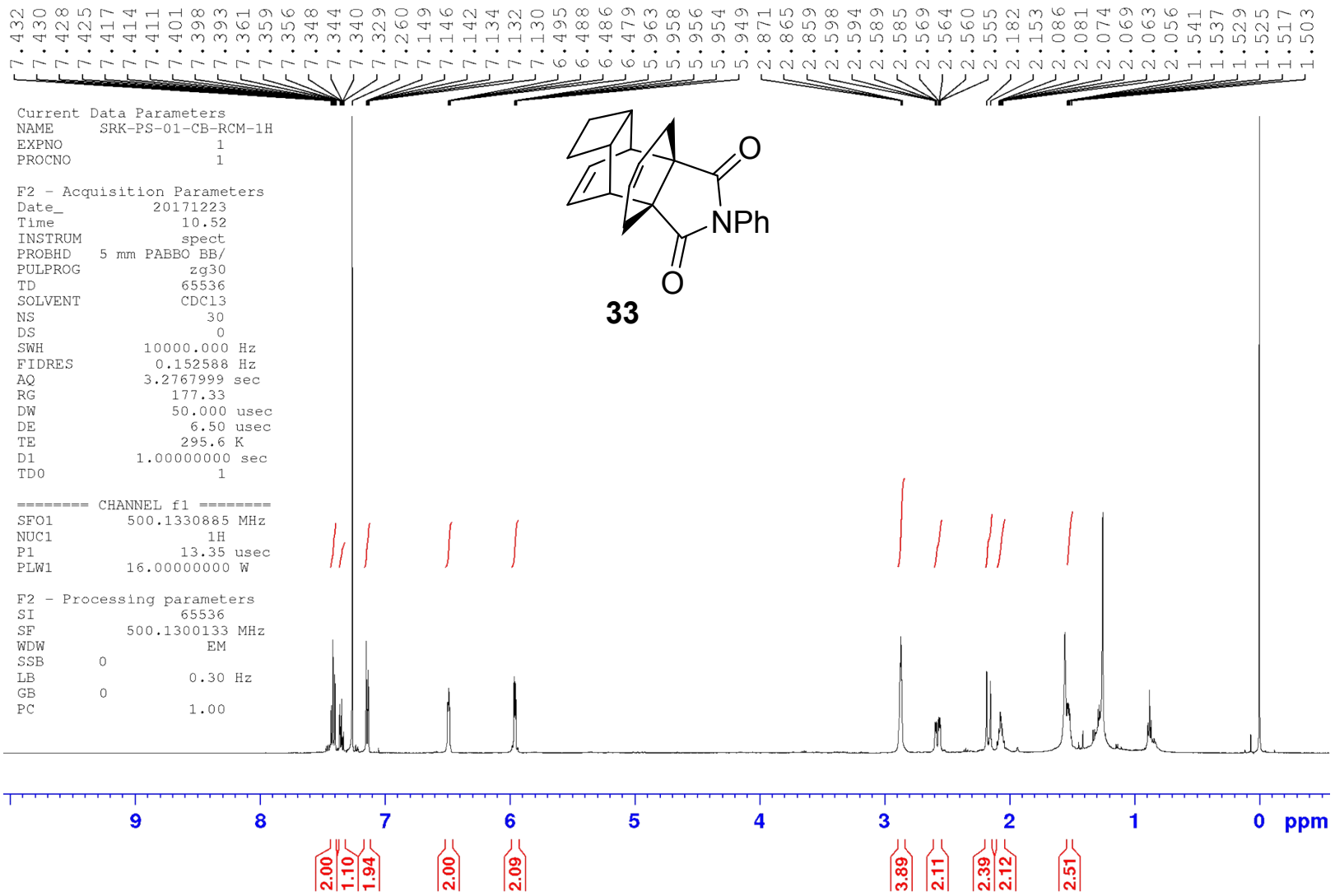
^{1}H NMR of the compound **34**



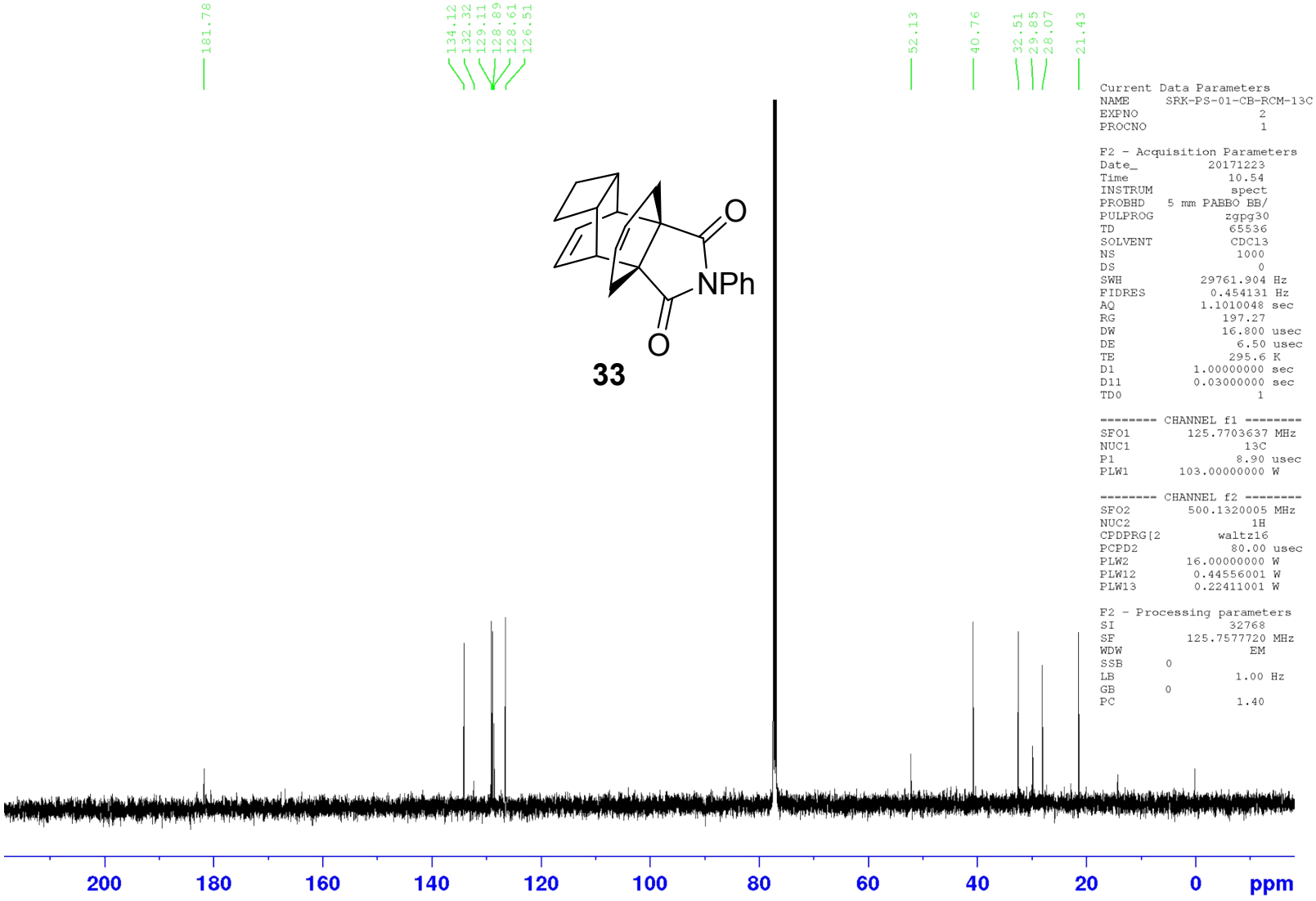
^{13}C NMR of the compound **34**



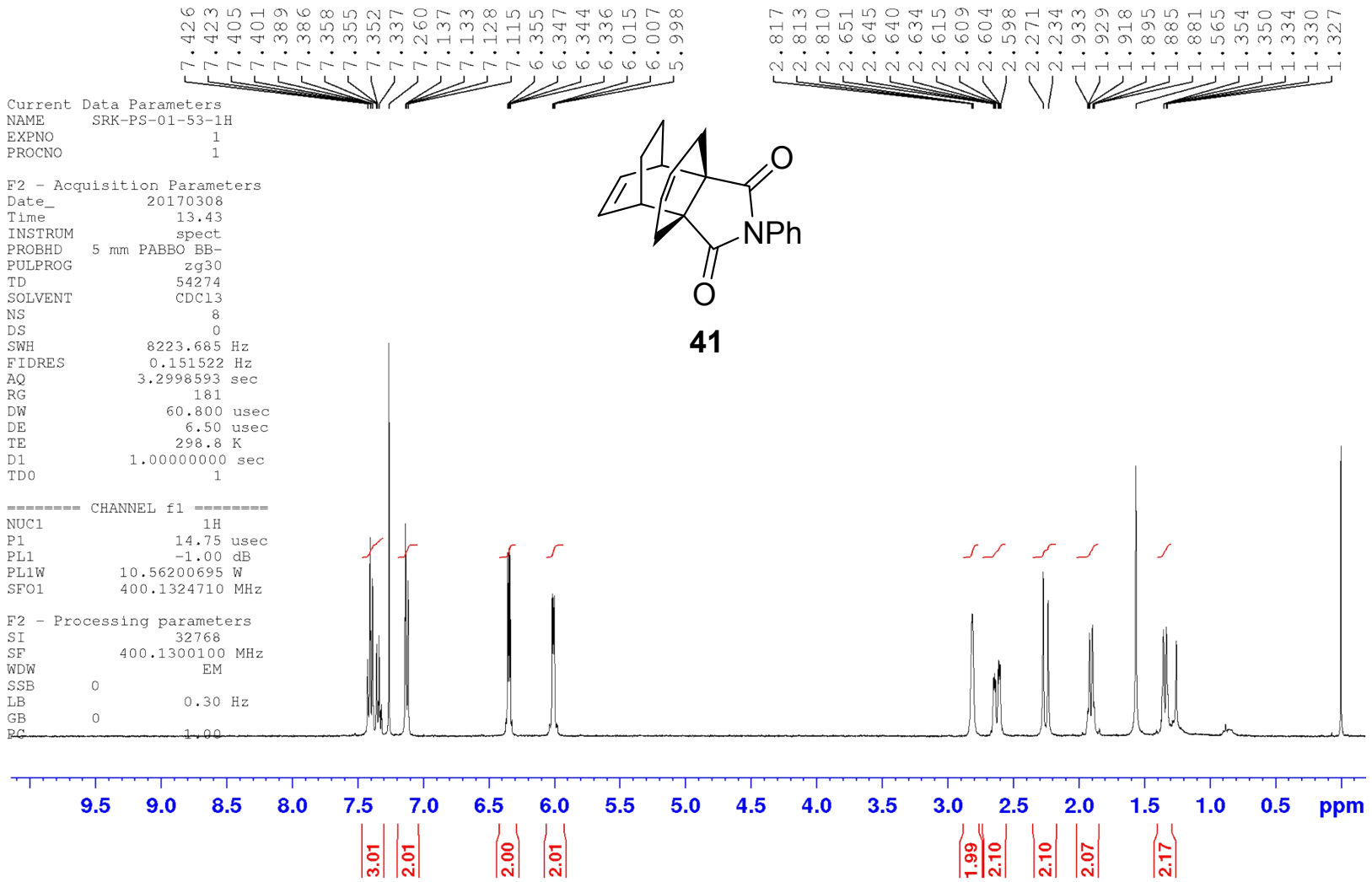
[1]H NMR of the compound **33**



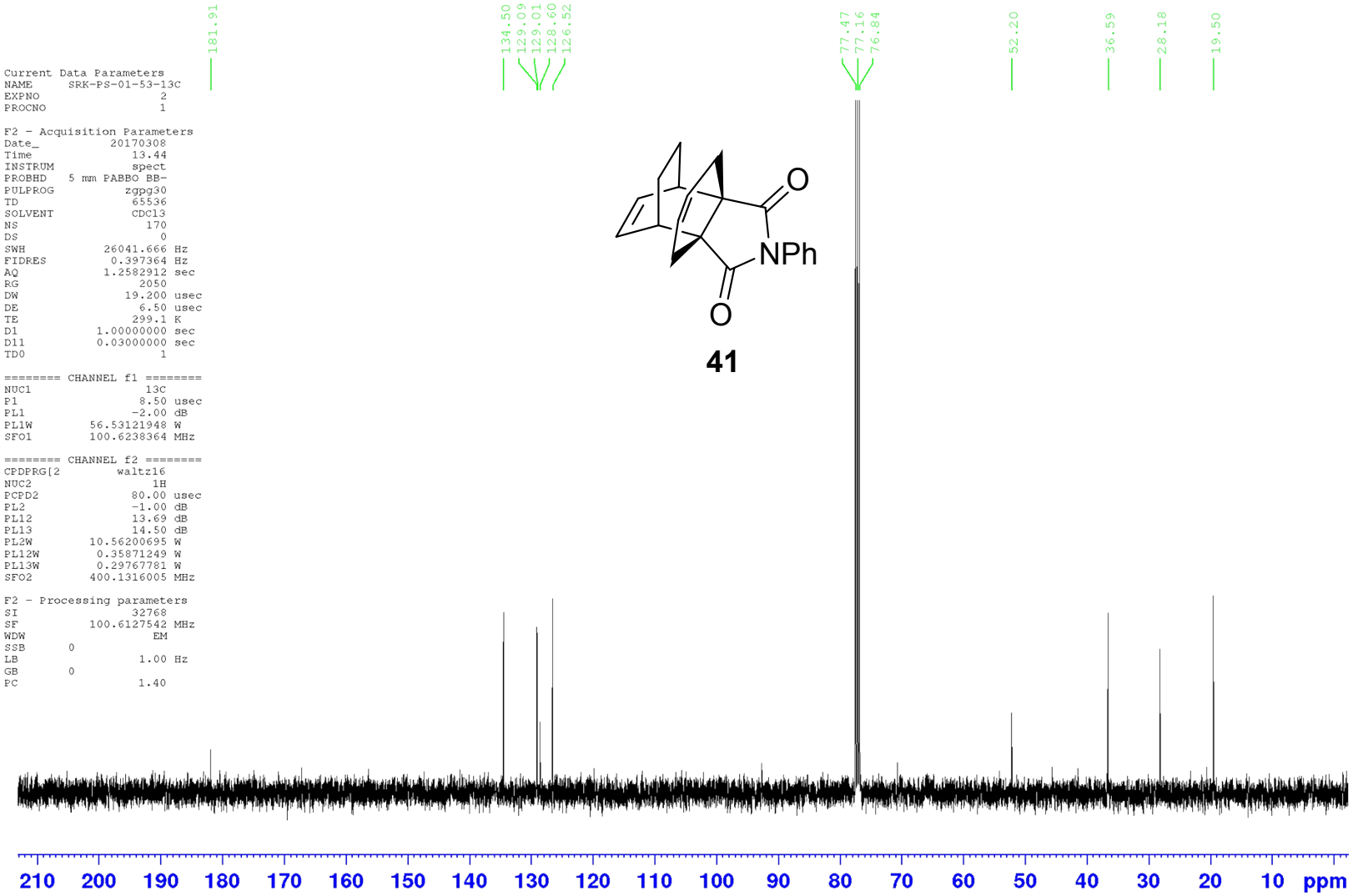
^{13}C NMR of the compound **33**



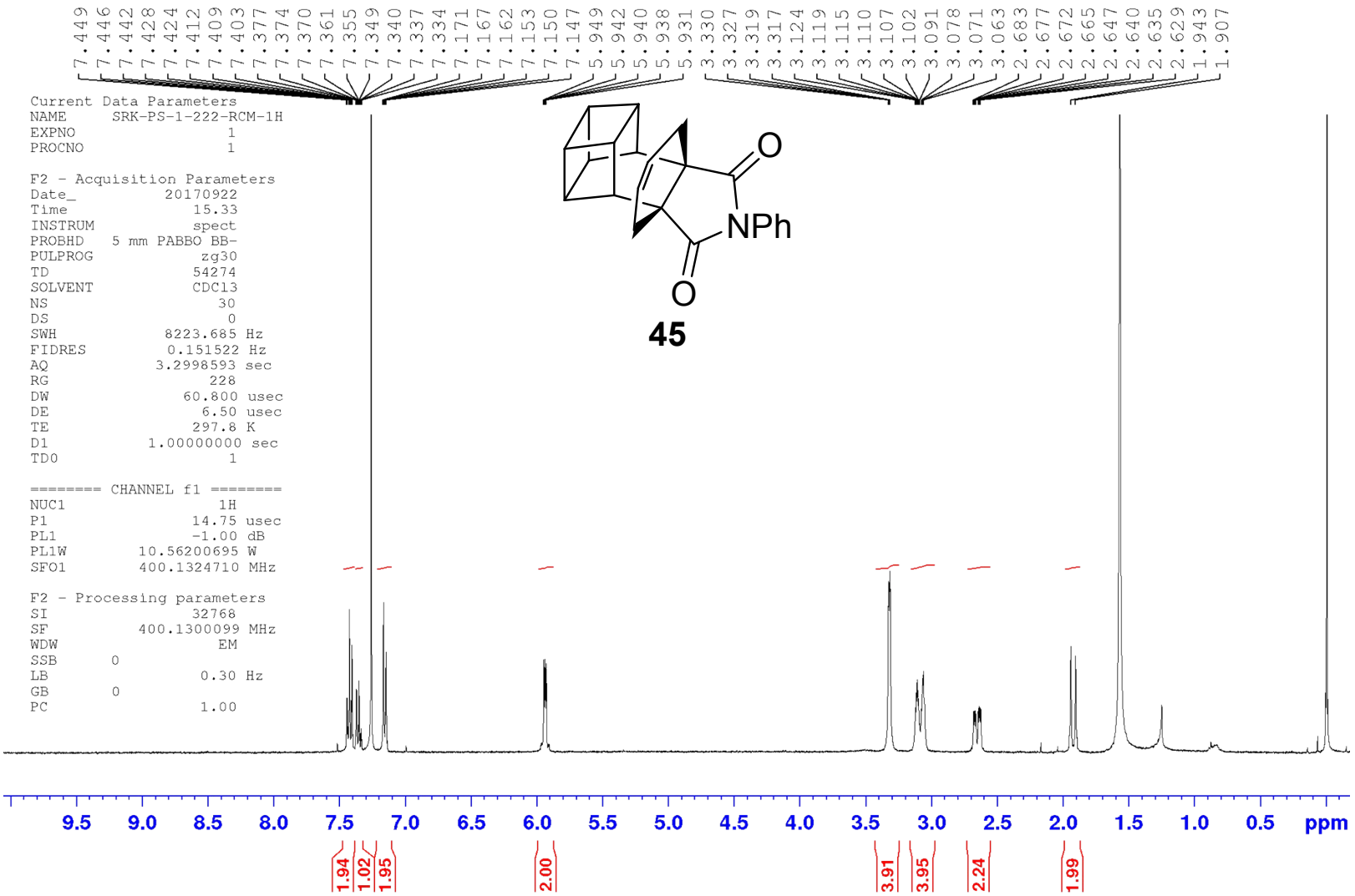
^{1}H NMR of the compound **41**



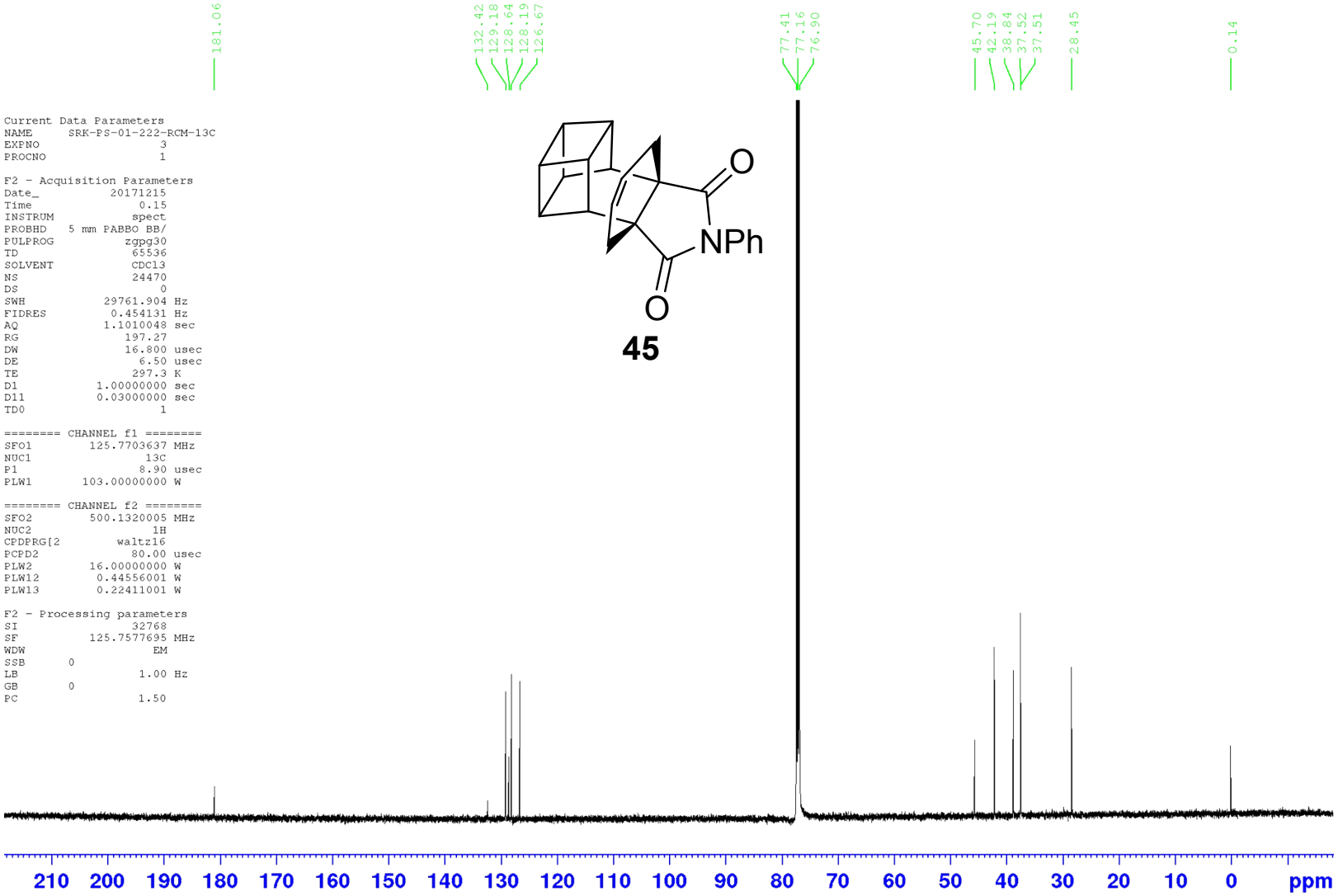
^{13}C NMR of the compound **41**



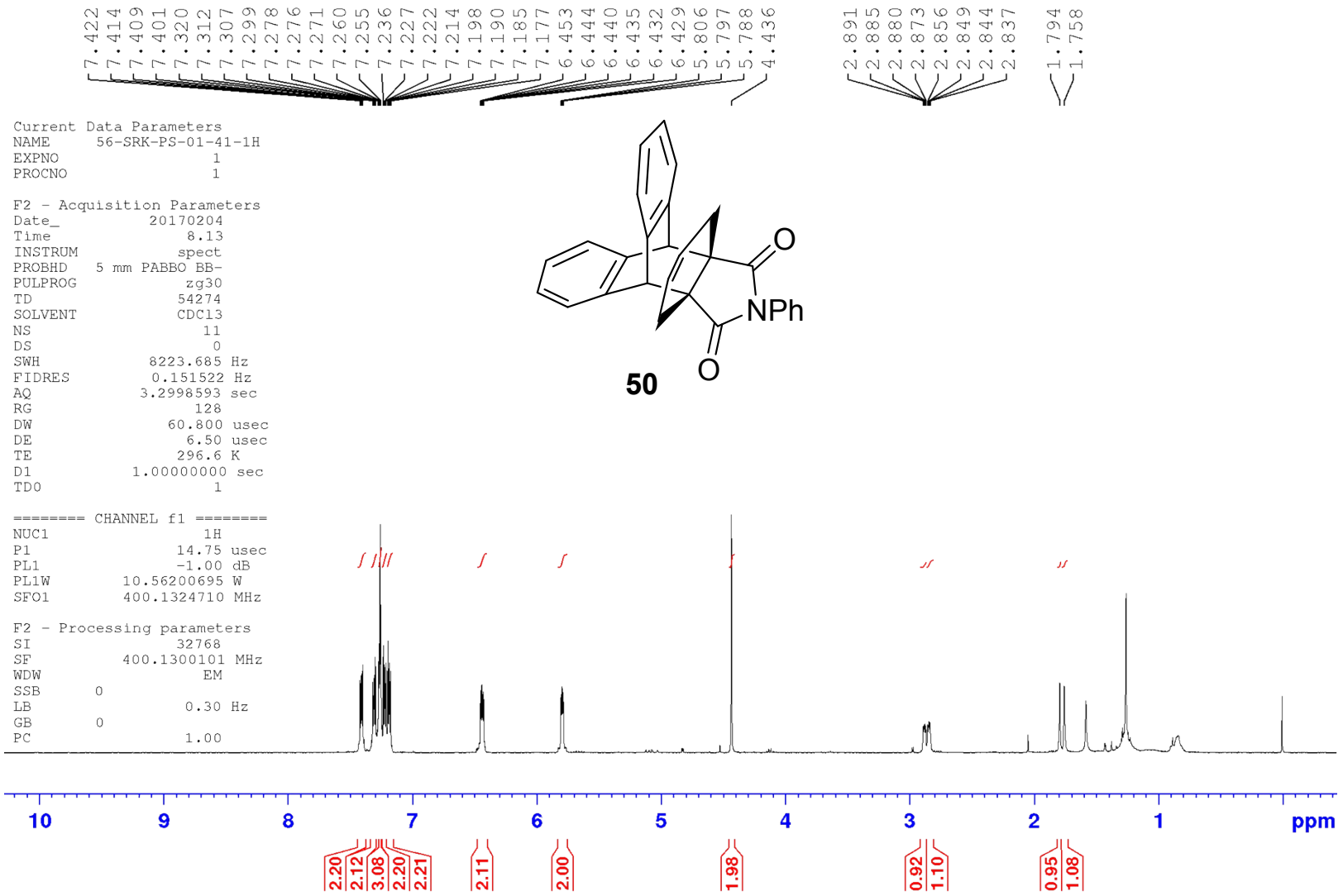
^{1}H NMR of the compound **45**



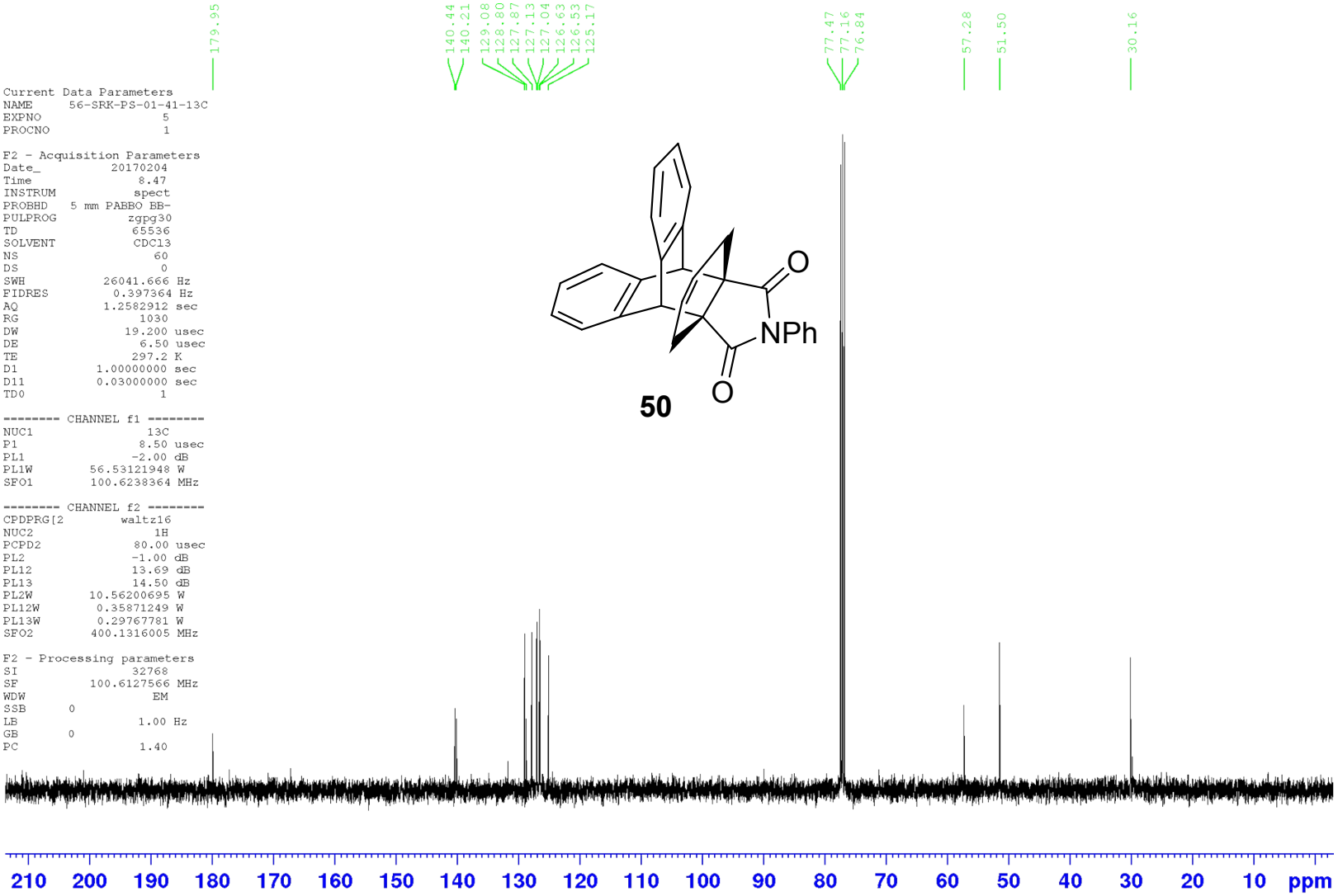
^{13}C NMR of the compound **45**



^{1}H NMR of the compound **50**



^{13}C NMR of the compound **50**



Energies and cartesian coordinates of optimized geometries of 30, 33, 41 and 45.

Compound **30**

Zero-point correction= 0.417491 (Hartree/Particle)
Thermal correction to Energy= 0.438881
Thermal correction to Enthalpy= 0.439825
Thermal correction to Gibbs Free Energy= 0.367218
Sum of electronic and zero-point Energies= -1132.698142
Sum of electronic and thermal Energies= -1132.676752
Sum of electronic and thermal Enthalpies= -1132.675808
Sum of electronic and thermal Free Energies= -1132.748415

0 1

O	1.35978200	0.11559000	2.28264600
N	1.68144200	0.05645500	-0.00000200
C	-0.72205400	2.05411500	1.40341600
H	-1.79056200	2.29966000	1.36148000
H	-0.44164000	2.00226700	2.45900700
C	0.05742400	3.11446800	0.66649100
H	0.59830400	3.86665500	1.23269400
C	-1.03632800	-1.74630100	0.66809400
H	-0.76089800	-2.60152000	1.27665400
C	-3.87326800	-1.09001100	1.40494400
H	-3.69712900	-2.14796900	1.21229900
C	0.93932100	0.25260600	1.16054500
C	-0.48144200	0.66683900	0.77416300
C	-2.89807600	-0.12532200	0.78574200
H	-3.18537200	0.87477400	1.12656600
C	5.38081800	0.21411500	0.00003200
H	6.16844400	0.96031100	0.00004500
C	3.04922700	-0.35193400	0.00000600
C	-1.45684400	-0.43189600	1.28719600
H	-1.42817300	-0.45748700	2.37981600

C	4.04875800	0.61396100	0.00002200
H	3.77103200	1.66303400	0.00002800
C	3.35764100	-1.70767400	-0.00000100
H	2.54996100	-2.43287800	-0.00001400
C	5.70134100	-1.14131200	0.00002400
H	6.74135800	-1.45114200	0.00003100
C	4.69174800	-2.10079300	0.00000800
H	4.94322100	-3.15617600	0.00000200
C	-4.89170400	-0.72629800	2.17682600
H	-5.56112500	-1.45669500	2.61859000
H	-5.09443400	0.32032600	2.38992000
O	1.35978000	0.11548500	-2.28265300
C	-0.72205800	2.05405200	-1.40350700
H	-1.79056600	2.29959800	-1.36157800
H	-0.44164700	2.00215700	-2.45909700
C	0.05742200	3.11443800	-0.66663100
H	0.59830100	3.86659900	-1.23287000
C	-1.03632800	-1.74633200	-0.66801400
H	-0.76089800	-2.60157900	-1.27653500
C	-3.87326800	-1.09007600	-1.40489400
H	-3.69712500	-2.14802600	-1.21220700
C	0.93932200	0.25255700	-1.16055800
C	-0.48144300	0.66680500	-0.77419300
C	-2.89807600	-0.12535800	-0.78573600
H	-3.18537200	0.87472200	-1.12660700
C	-1.45684400	-0.43195500	-1.28717600
H	-1.42817200	-0.45759600	-2.37979500
C	-4.89171000	-0.72639700	-2.17678500
H	-5.56113100	-1.45681400	-2.61851500
H	-5.09444400	0.32021800	-2.38992000

Compound **33**			
Zero-point correction=	0.386314 (Hartree/Particle)		
Thermal correction to Energy=	0.405013		
Thermal correction to Enthalpy=	0.405957		
Thermal correction to Gibbs Free Energy=	0.339905		
Sum of electronic and zero-point Energies=	-1055.377781		
Sum of electronic and thermal Energies=	-1055.359082		
Sum of electronic and thermal Enthalpies=	-1055.358138		
Sum of electronic and thermal Free Energies=	-1055.424190		
0 1			
O	0.92214300	-0.43829300	2.25398600
N	1.28899000	0.07142500	0.02695100
C	-1.23887900	1.55693700	1.81588400
H	-2.31992000	1.74291300	1.81120900
H	-0.96130800	1.27413000	2.83494300
C	-0.52164900	2.80428400	1.36415300
H	-0.02356000	3.42778300	2.10023500
C	-1.33785300	-1.96713300	0.20441400
H	-1.00477900	-2.92201700	0.59820800
C	0.51723000	-0.05260100	1.18361800
C	-0.91852700	0.37046600	0.88340700
C	-3.26604400	-0.47888400	0.65849800
H	-3.67755000	0.29763400	1.30776700
C	4.88796400	0.25271800	-0.83836100
H	5.55736800	0.88995000	-1.40679400
C	2.67622000	-0.25020600	-0.04404000
C	-1.84367300	-0.86719300	1.11285100
H	-1.81094500	-1.15264600	2.16829900
C	3.53687100	0.57315800	-0.76841600
H	3.14349900	1.44404200	-1.27771600
C	3.15740400	-1.38281300	0.61088000
H	2.47652900	-2.00470700	1.17843400

C	5.38065200	-0.87247200	-0.18334200
H	6.43686100	-1.11526900	-0.23673800
C	4.51294100	-1.68485000	0.54111300
H	4.88972500	-2.56321100	1.05491800
O	0.96271900	0.69653300	-2.17648800
C	-1.23899900	2.21950300	-0.90441800
H	-2.32064300	2.37643400	-0.81127100
H	-0.96535000	2.43781500	-1.94031500
C	-0.52289100	3.12088400	0.06947400
H	-0.02678400	4.01446400	-0.29701700
C	-1.32268300	-1.65264400	-1.09370500
H	-0.97565100	-2.32242200	-1.87365400
C	0.53540900	0.51645600	-1.06169200
C	-0.90991600	0.73888000	-0.62095200
C	-3.25221900	-0.12004000	-0.85543400
H	-3.66348600	0.86378000	-1.09335300
C	-1.81847100	-0.25774700	-1.40864500
H	-1.76358200	-0.02997900	-2.47716600
C	-4.24092600	-1.27965900	-1.13649500
H	-5.20265100	-0.95574300	-1.53941600
H	-3.83951200	-2.06633100	-1.77999000
C	-4.26131400	-1.63176300	0.37232500
H	-3.87972800	-2.62736400	0.61211000
H	-5.23424000	-1.50684600	0.85195300

Compound **41**	
Zero-point correction=	0.351290 (Hartree/Particle)
Thermal correction to Energy=	0.368620
Thermal correction to Enthalpy=	0.369565
Thermal correction to Gibbs Free Energy=	0.306299
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Sum of electronic and thermal Energies=	-978.033360
Sum of electronic and thermal Enthalpies=	-978.032416

Sum of electronic and thermal Free Energies= -978.095681

0 1

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N	0.91362700	0.07305500	0.03777000
C	-1.85351900	0.90968800	1.88454700
H	-2.95068100	0.92330900	1.87086600
H	-1.54735100	0.52782200	2.86245800
C	-1.33835600	2.30556000	1.64012500
H	-0.96791300	2.88871400	2.47770000
C	0.12911700	-0.34102100	1.11590000
C	-1.34131900	-0.06789300	0.80682000
C	4.47937300	0.85830700	-0.59698100
H	5.07407300	1.66187600	-1.01887800
C	2.33334100	-0.04861800	-0.00955100
C	-2.09570000	-1.43060800	0.80503400
H	-2.08025300	-1.84643200	1.81583800
C	3.09590900	0.98771400	-0.54558900
H	2.60425300	1.87318300	-0.92879400
C	2.94233300	-1.20473200	0.47610700
H	2.33325900	-1.99571200	0.89579300
C	5.09894600	-0.28892700	-0.10925000
H	6.17925600	-0.38282600	-0.14836700
C	4.32753900	-1.31564800	0.42785400
H	4.80333300	-2.21270000	0.81025900
O	0.57443000	1.00919700	-2.05110800
C	-1.89165500	1.94912400	-0.72180200
H	-2.98723700	1.92076800	-0.66694400
H	-1.62348800	2.35376600	-1.70154800
C	-1.35947600	2.80103200	0.40291700
H	-1.00619400	3.80514300	0.18887500
C	0.14126300	0.58435500	-1.00704200
C	-1.33496400	0.51534600	-0.62502600
C	-2.03602100	-0.48564000	-1.59187800

H	-1.96625200	-0.10030300	-2.61245700
C	-3.54121500	-1.20749100	0.30075800
H	-4.07320300	-0.51639400	0.96055600
H	-4.07633200	-2.15899600	0.34966100
C	-3.50650900	-0.67111000	-1.15090000
H	-4.05846900	0.26863700	-1.23763800
H	-3.98222500	-1.37755800	-1.83557800
C	-1.36776200	-1.83411800	-1.43827800
H	-0.90944600	-2.34093500	-2.28106000
C	-1.40781600	-2.32862000	-0.19851000
H	-0.98635200	-3.28633700	0.08919300

Compound **45**			
Zero-point correction=	0.363179 (Hartree/Particle)		
Thermal correction to Energy=	0.379863		
Thermal correction to Enthalpy=	0.380807		
Thermal correction to Gibbs Free Energy=	0.318929		
Sum of electronic and zero-point Energies=	-1054.131824		
Sum of electronic and thermal Energies=	-1054.115140		
Sum of electronic and thermal Enthalpies=	-1054.114196		
Sum of electronic and thermal Free Energies=	-1054.176074		
0 1			
O	0.87098200	0.22488200	2.28371600
N	1.16928500	0.08514900	-0.00001300
C	-1.35320600	2.02977100	1.39595900
H	-2.44461200	2.15463300	1.34040900
H	-1.08164600	2.00337300	2.45485700
C	-0.67059200	3.15628700	0.66684500
H	-0.19166900	3.94840700	1.23463700
C	-1.73764800	-1.86634200	0.78425700
H	-1.04225500	-2.54441500	1.28113400
C	0.43441800	0.31373000	1.16294100
C	-0.99901600	0.66394800	0.77403100

C	-3.36334400	-0.48247000	0.78429600
H	-4.15016200	0.08889300	1.27852300
C	4.86073200	0.39608700	0.00010800
H	5.61627300	1.17483500	0.00021400
C	2.55334300	-0.26537700	-0.00002100
C	-1.91587300	-0.43082600	1.32007300
H	-1.89931300	-0.42776500	2.41491800
C	3.51324800	0.74062400	0.00010100
H	3.19302900	1.77759300	0.00019400
C	2.91898700	-1.60658300	-0.00013800
H	2.14526400	-2.36800500	-0.00024300
C	5.23741500	-0.94474300	-0.00000600
H	6.28943700	-1.21101000	0.00000300
C	4.26824300	-1.94462600	-0.00012800
H	4.56276800	-2.98882800	-0.00021900
O	0.87115500	0.22582400	-2.28371700
C	-1.35307600	2.02993900	-1.39581000
H	-2.44448200	2.15485900	-1.34038000
H	-1.08139800	2.00364400	-2.45468000
C	-0.67050900	3.15635500	-0.66649600
H	-0.19151800	3.94853400	-1.23414800
C	-1.73771800	-1.86622600	-0.78453600
H	-1.04237600	-2.54423300	-1.28157300
C	0.43431500	0.31346300	-1.16295400
C	-0.99901900	0.66402000	-0.77398700
C	-3.36339400	-0.48231900	-0.78422000
H	-4.15024200	0.08914400	-1.27828300
C	-1.91596000	-0.43063300	-1.32011900
H	-1.89945300	-0.42743000	-2.41496600
C	-3.28860100	-2.04207400	-0.77374000
H	-3.84758800	-2.69618800	-1.44112800
C	-3.28852800	-2.04221900	0.77354100
H	-3.84746100	-2.69645200	1.44085900