Gold (I)-Catalyzed Cyclization of (*E*)-Ketene-N,O-Acetals: A Synthetic Route to Spiro-Oxazole-γ-Lactone

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SUPPORTING INFORMATION

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General Experimental Information

All the reactions were performed in oven-dried Schlenk flasks and sealed tubes. Commercial grade solvents were distilled prior to use. Column chromatography was performed using silica gel (100–200 Mesh) eluting with hexanes and ethyl acetate mixture. Thin layer chromatography (TLC) was performed on silica gel GF254 plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. Proton, carbon and fluorine nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded based on 400 MHz (^{1}H NMR, 400 MHz; ^{13}C NMR, 101 MHz; ^{19}F NMR, 376 MHz) spectrometer and 500 MHz (^{1}H NMR, 500 MHz; ^{13}C NMR, 126 MHz; ^{19}F NMR, 471 MHz) spectrometer having solvent resonance as internal standard (^{1}H NMR, $CHCl_3$ at 7.26 ppm; ^{13}C NMR, $CDCl_3$ at 77.0 ppm). Few cases tetramethylsilane (TMS) at 0.00 ppm was used as reference standard. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), the abbreviations were used to explain the multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; dd = doublets of doublet; m = multiplet; br = broad; dt = doublets of triplet; coupling constants *J* in Hz. ^{13}C NMR, ^{19}F NMR were reported in terms of chemical shift (ppm). IR spectra were recorded on FT/IR spectrometer and reported in cm^{-1}. High resolution mass spectra (HRMS) were obtained in ESI mode. Melting points were determined by electro-thermal heating and are uncorrected. LC-MS spectra were obtained with a Shimadzu 2010A (EI-positive/ negative mode) with ionization voltage of 70ev; data was reported in the form of m/z (intensity relative to base peak = 100). X–ray data was collected at 298K on a Bruker D8 Quest CCD diffractometer using Mo-Kα radiation (0.71073 Å).

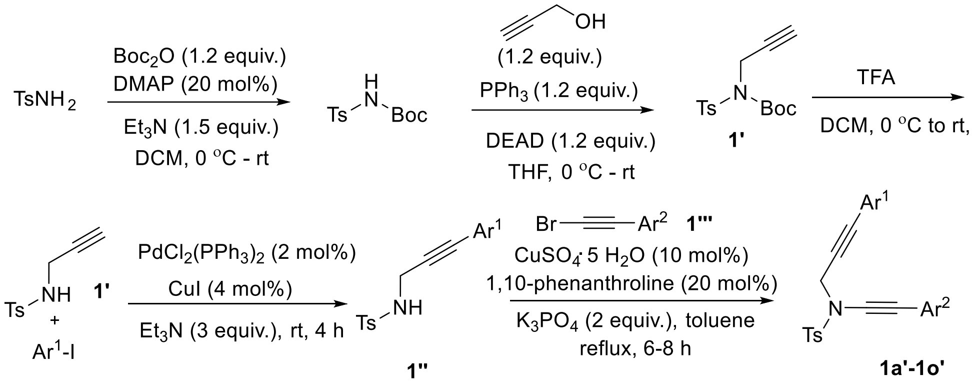
Materials

Unless otherwise noted, all the reagents and intermediates were obtained commercially and used without purification. 1,4-dioxane, dichloromethane (DCM), toluene, acetonitrile (CH_3CN), 1,2-dichloroethane (DCE) and acetone were distilled over CaH_2. THF was freshly distilled over sodium/benzophenone ketyl under dry nitrogen. Catalyst PPh_3AuCl, Jhonphos gold(I)-SbF_6 (catalyst A), CyJohnPhosAu-SbF_6 (catalyst **B**), XphosAu-NTf_2 (catalyst **C**), Brettphosgold-NTf_2 (catalyst **D),** NHC-Au catalysts (**E** and **F**), $In(OTf)_2$, $Pd(OAc)_2$, $PdCl_2(PPh_3)_2$, $Sc(OTf)_3$ and $Cu(OTf)_2$ were purchased from Sigma Aldrich Ltd. and used as received. Silver salts such as $AgSbF_6$, $AgNTf_2$ and $AgBF_4$ were purchased from Aldrich Ltd. and used as received. PTSA·H_2O,

$PhB(OH)_2$ and phenyl acetylene were purchased from Aldrich Ltd. and used as received. PPh_3, DEAD, $CuSO_4{\cdot}5H_2O$, 1, 10-phenanthroline, K_3PO_4, Na_2CO_3 were purchased from Merck. The aryl iodides were purchased from Aldrich and used. Analytical and spectral data of all those known compounds are exactly matching with the reported values.

Experimental Procedures

Scheme S1: General procedures for the synthesis of starting precursors



Compound **1'** was prepared using two known synthetic steps from the commercially available tosyl amine. The first step involves N–Boc protection of tosylamide. Mitsunobu reaction between N-Boc protected tosylamine and propargyl alcohol in the presence of triphenyl phosphine (Ph_3P) and diethyl azodicarboxylate (DEAD) in THF delivers **1**'. Following the reported procedures, substrate **1a'-1o'** were prepared from **1′** in two simple synthetic steps. Sonogashira reaction between **1'** and aryl iodides provides **1''** in good to excellent yields. Finally, Cu-catalyzed C-N bond formation between **1''** and 1-bromo-2-arylacetylene (**1'''**) affords precursor **1a'-1o'** in overall good yield. Physical and spectroscopic data of compound **1a**'**-1o'** are concurrently matching with the reported values.

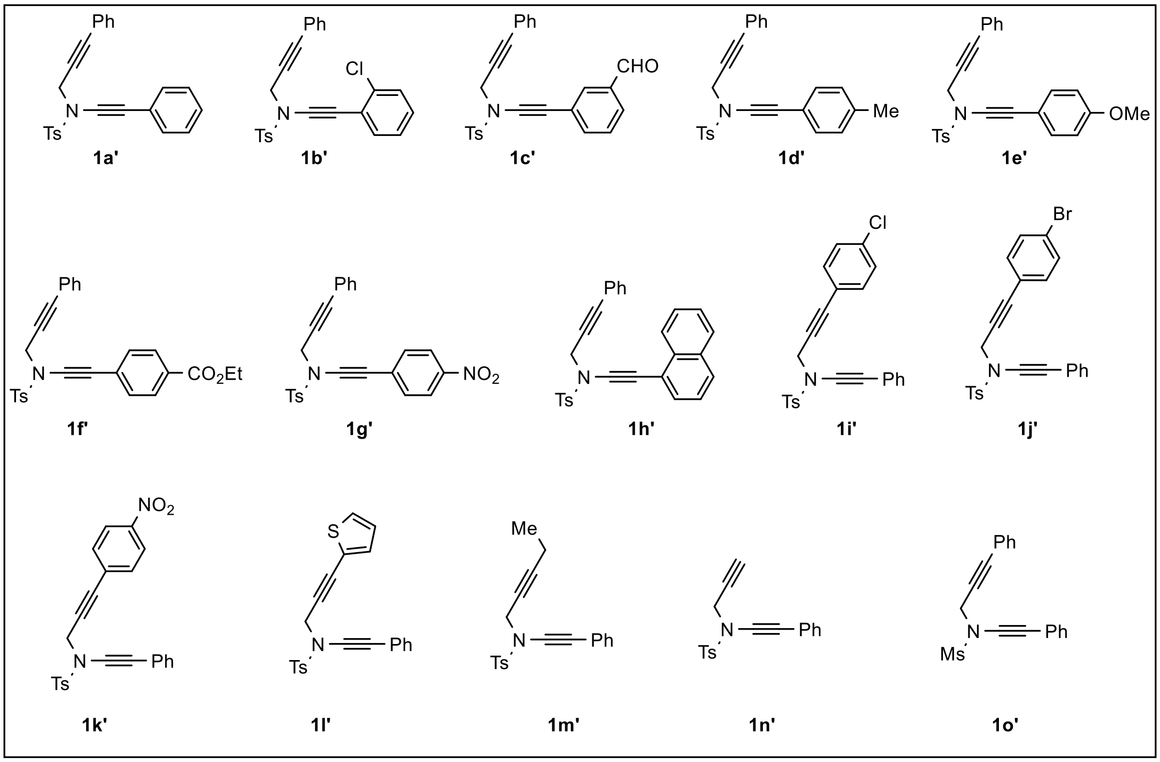
General Procedure for the Synthesis of 1″ (GP–1):[1]

To a solution of terminal alkyne **1′** (1.0 mmol), $PdCl_2(PPh_3)_2$ (0.02 mmol), and CuI (0.04 mmol) in THF (5.0 mL) were added aryl iodide (1.3 mmol) and Et_3N (3.0 mmol) successively under an argon atmosphere. The resulting mixture was stirred at room temperature for 4-6 h. The crude reaction mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified using column chromatography on silica gel to afford **1″**.

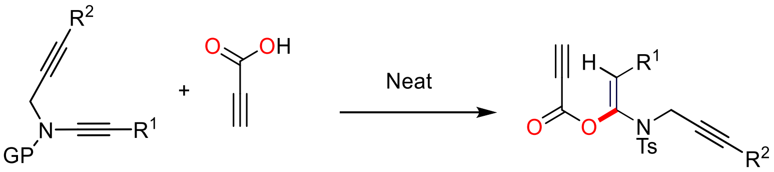
General Procedure for the Synthesis of 1 (GP–2):[2]

A solution of **1″** (1.0 mmol), $CuSO_4\cdot 5H_2O$ (0.10 mmol), 1,10-phenanthroline (0.20 mmol), and K_3PO_4 (2.0 mmol) in dry toluene (5.0 mL) was stirred in a Schlenck tube at rt. 1-Bromo-2-arylacetylene (**1‴**) was subsequently introduced into the Schlenck tube at rt. The reaction mixture was next heated at 70-80 ^{o}C in an oil bath under inert atmosphere. Progress of the reaction was monitored periodically by TLC. Upon completion, the reaction mixture was cooled to room temperature and diluted with dichloromethane (10 mL). The crude mixture was filtered through a small pad of Celite and concentrated under the reduced pressure. The crude residue was purified using column chromatography on silica gel to provide **1a'-1o'** (**Table S1**). Compounds **1a′-1o′** are known; analytical data of these compounds are concurrently matching with the reported values.[3]

Table S1: List of the propargyl-tethered ynamides (**1a′-1o′**)



General procedure for the chemo-, regio-, and stereoselective hydropropioloxylation of ynamide 1 with terminal propiolic acid 2a (GP-3)[3, 4]:



1a'-1o' **1b** **1**

The ynamide **1a′** (0.3 mmol) was taken in an RB flask and then propiolic acid **1b** (0.36 mmol) was introduced dropwise. The reaction mixture was stirred at RT. The progress of the reaction was periodically monitored by TLC. After the complete consumption of ynamide **1a′**, the reaction mixture was diluted with EtOAc and neutralized with saturated $NaHCO_3$ solution. The organic layer was further extracted with EtOAc (10 mL) and dried over anhydrous Na_2SO_4. After evaporation of the solvent under reduced pressure, the residue was purified by flash chromatography on silica gel (hexane/EtOAc) to afford the expected product **1**.

Table S2: List of the N, O acetalas (1a-1o)

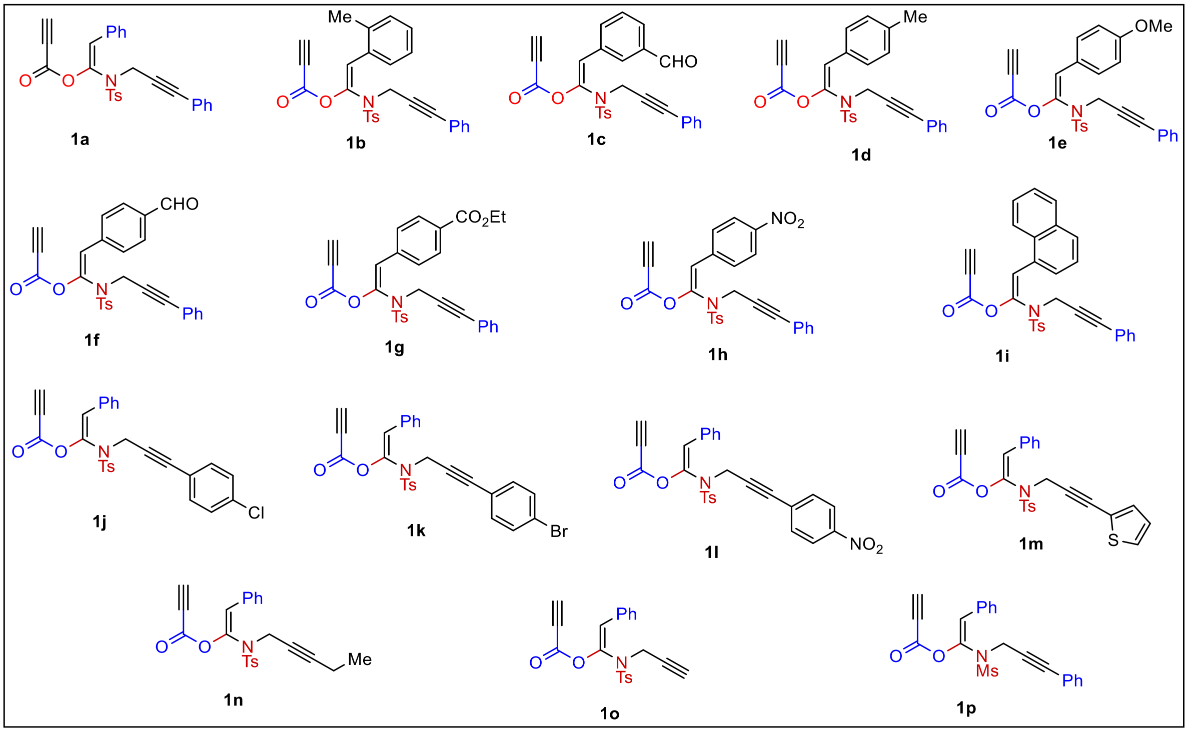
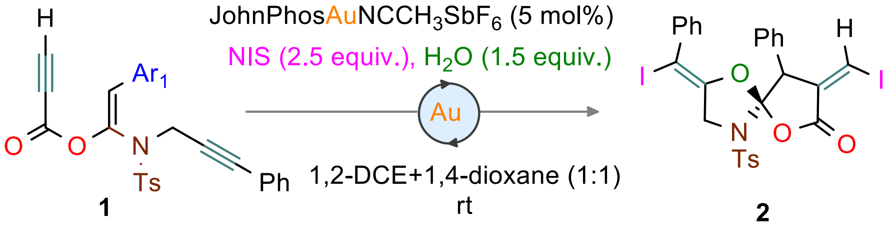


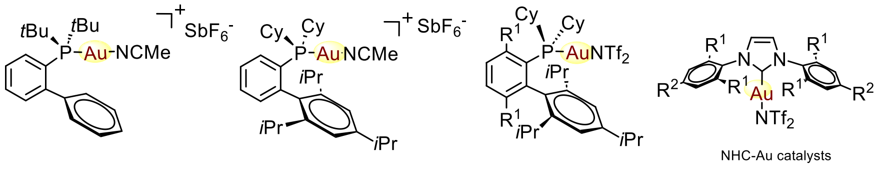
Table 3. Optimization of regioselective spiro cyclization [a,b]

Entry	Catalyst	X- source	H_2O equiv	Solvent	2a[b] yield
1	PPh_3AuCl /$AgSbF_6$	NIS (2)	2	1,2-DCE	38
2	PPh_3AuCl / $AgNTf_2$	NIS (2)	2	1,2-DCE	26
3	**A**	NIS (2)	2	1,2-DCE	55
4	**B**	NIS (2)	2	1,2-DCE	39
5	**C**	NIS (2)	2	1,2-DCE	25
6	**D**	NIS (2)	2	1,2-DCE	16
7	**E**	NIS (2)	2	1,2-DCE	complex
8	**F**	NIS (2)	2	1,2-DCE	complex
9	**A**	NIS (2)	2	DCM	48
10	**A**	NIS (2)	2	THF	31
11	**A**	NIS (2)	2	CH_3NO_2	24
12	**A**	NIS (2)	2	1,4-Dioxane	57
13	**A**	NIS (2)	2	DCE/Dioxane (1.1)	69
14	**A**	NIS (2.5)	2	DCE/Dioxane (1.1)	77
15	**A**	NIS (2.5)	1.5	DCE/Dioxane (1.1)	79

[a]**Reaction conditions**: **1** (0.25 mmol), Au(I) (5.0 mol %) in 1,2-DCE: 1,4-dioxane (1:1, 0.05 M). at RT for 6 h; [b]isolated yield of the compounds.

General Procedure for the Au-Catalyzed Cascade Double 5-*exo*-dig Cyclization of 1: (GP−4):





Jhonphos Au(I)-SbF6
(catalyst **A**)

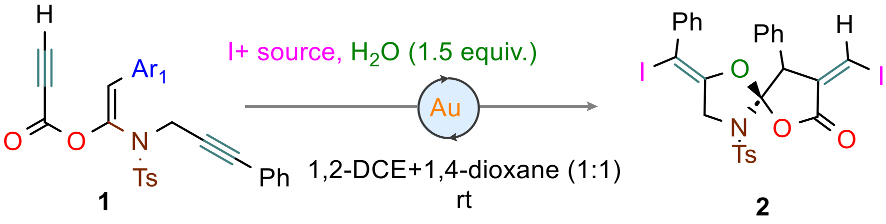
CyJohnPhosAu-SbF$_6$
(catalyst **B**)

C: R^1 = H, CyJohnPhosAu-NTf$_2$
D: R^1 = OMe, BrettPhosAu-NTf$_2$

E: R^1= ^{i}Pr, R^2 = H
F: R^1, R^2 = Me

A solution of **1** (0.25 mmol) in 1,4-dioxane (3.0 mL), was added NIS (2.5 equiv.) in RB flask under an argon atmosphere. The catalyst JohnphosAuSbF$_6$ (**A**; 7.6 mg, 5 mol%) in DCE (3.0 mL) was next introduced along with 1.5 equiv. of H_2O. The reaction mixture was stirred for the 6-8 h. The progress of the reaction was periodically monitored by TLC. After 6 h, the reaction mixture was quenched with saturated sodium thiosulfate solution and extracted with ethyl acetate (3 x 5 mL). The combined organic layers were dried over $MgSO_4$. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel to afford product **2a–2i & 3a–3g**.

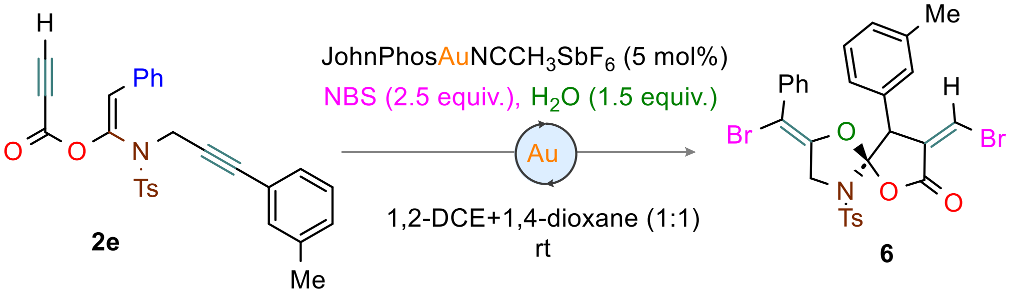
Screening of I+ sources:



Entry	I+ sources	Yield of 2 (%)
1	I_2	0
2	ICl	0

3	NIS	0

Screening NBS for Spirolactonisation:



calculate M+H$^+$ = 643.9736 ; observed M+H$^+$ = 643.9709

A solution of **2e** (0.25 mmol) in 1,4-dioxane (3.0 mL), was added NBS (2.5 equiv.) in RB flask under an argon atmosphere. The catalyst JohnphosAuSbF_6 (**A**; 7.6 mg, 5 mol%) in DCE (3.0 mL) was next introduced along with 1.5 equiv. of H_2O. The reaction mixture was stirred for the 6-8 h. The progress of the reaction was periodically monitored by TLC. After 6 h, the reaction mixture was quenched with saturated sodium thiosulfate solution and extracted with ethyl acetate (3 x 5 mL). The combined organic layers were dried over $MgSO_4$. The reaction profile was complex; purification of the crude mixture was found cumbersome. Thus, the crude mixture was subjected to HRMS study; a peak at 643.9709 was detected indicating the formation of **6**.

Display Report

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Sample Name SV-4B
Comment

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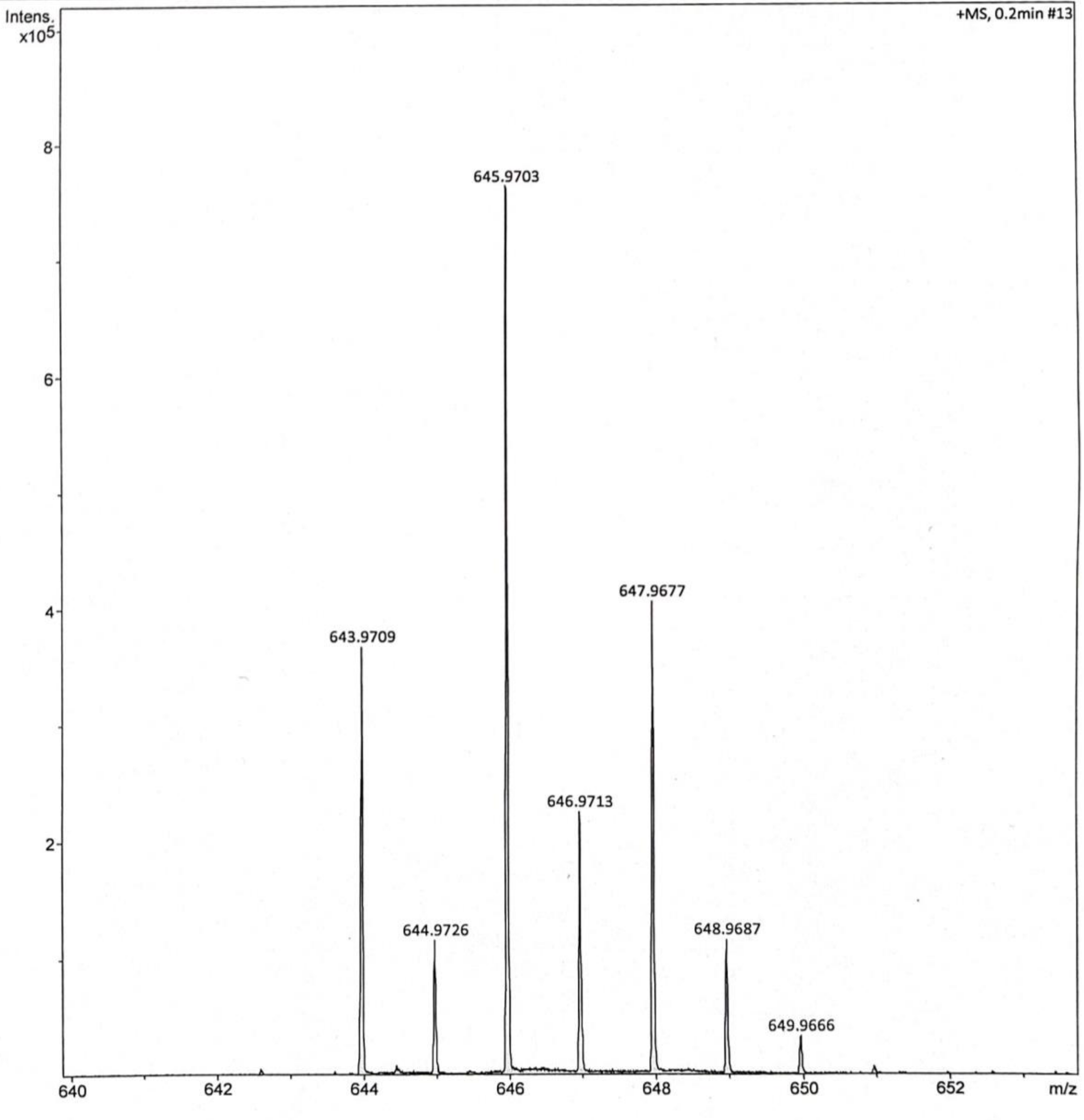

SV-4B.d
Bruker Compass DataAnalysis 4.2 printed: 30-04-2024 12:01:43 by: UOH Page 1 of 1

X-ray crystallography:

X-ray reflections for **2a** were collected on Bruker D8 Quest CCD diffractometer using Mo-Kα, radiation. Data reduction was performed using CrysAlisPro (version 1.171.33.55). Apex 2 and SHELX-TL 97 program were used to solve and refine the data. All non-hydrogen atoms were refined anisotropically and C−H hydrogens were fixed.[5, 6]

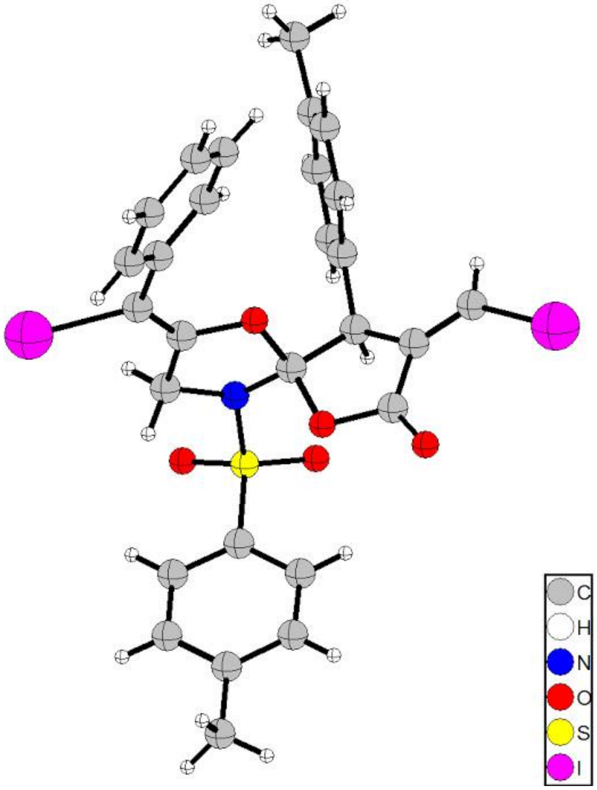

Figure 1. Molecular structures of compounds **2d;** thermal ellipsoids are set at 50% probability**.** Oxygen (red), nitrogen (blue), and sulfur (yellow).

Table 1. Crystallographic Data for Compound **2d**

Compound	**2d**
formula	$C_{28}H_{23}NI_2O_5S$
Formula weight	739.33
crystal system	Monoclinic

space group	P 21/n
T [K]	293(2) K
a [Å]	12.2400 (3)
b [Å]	9.6340 (3)
c [Å]	24.0129 (5)
α [°]	90
β [°]	92.000 (2)
γ [°]	90
V [Å^3]	2829.88 (13)
Z	4
ρ_{calcd} [g cm^{-3}]	1.735
μ [mm^{-1}]	2.334
total reflns	6178
unique reflns	4539
observed	5920
$R_1[I>2\sigma(I)]$	0.0434
wR2 [all]	0.1689
GOF	1.213
Diffractometer	Bruker D8 Quest CCD
CCDC Number	2120442

References

(1) (a) R. Shintani, H. Nakatsu, K. Takatsu, T. Hayashi, *Chem. –Euro. J.* 2009, **15**, 8692; (b)K. Sonogashira, Y. Tohda, N. Hagihara, *Tetrahedron Lett.* 1975, **16**, 4467.

(2). (a) X. Zhang, Y. Zhang, J. Huang, R. P. Hsung, K. C. M. Kurtz, J. Oppenheimer, M. E. Petersen, I. K. Sagamanova, L. Shen, M. R. Tracey, M. R. *J. Org. Chem*. 2006, **71**, 4170. (b) R. Liu, G. N WMcYang, Z-Y.; Zhou, X.; Song, W.; Guzei, I. A.; Xu, X.; Tang, W. *J. Am. Chem.Soc.* 2013, **135**, 8201.

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13981.

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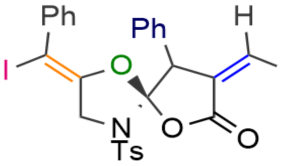
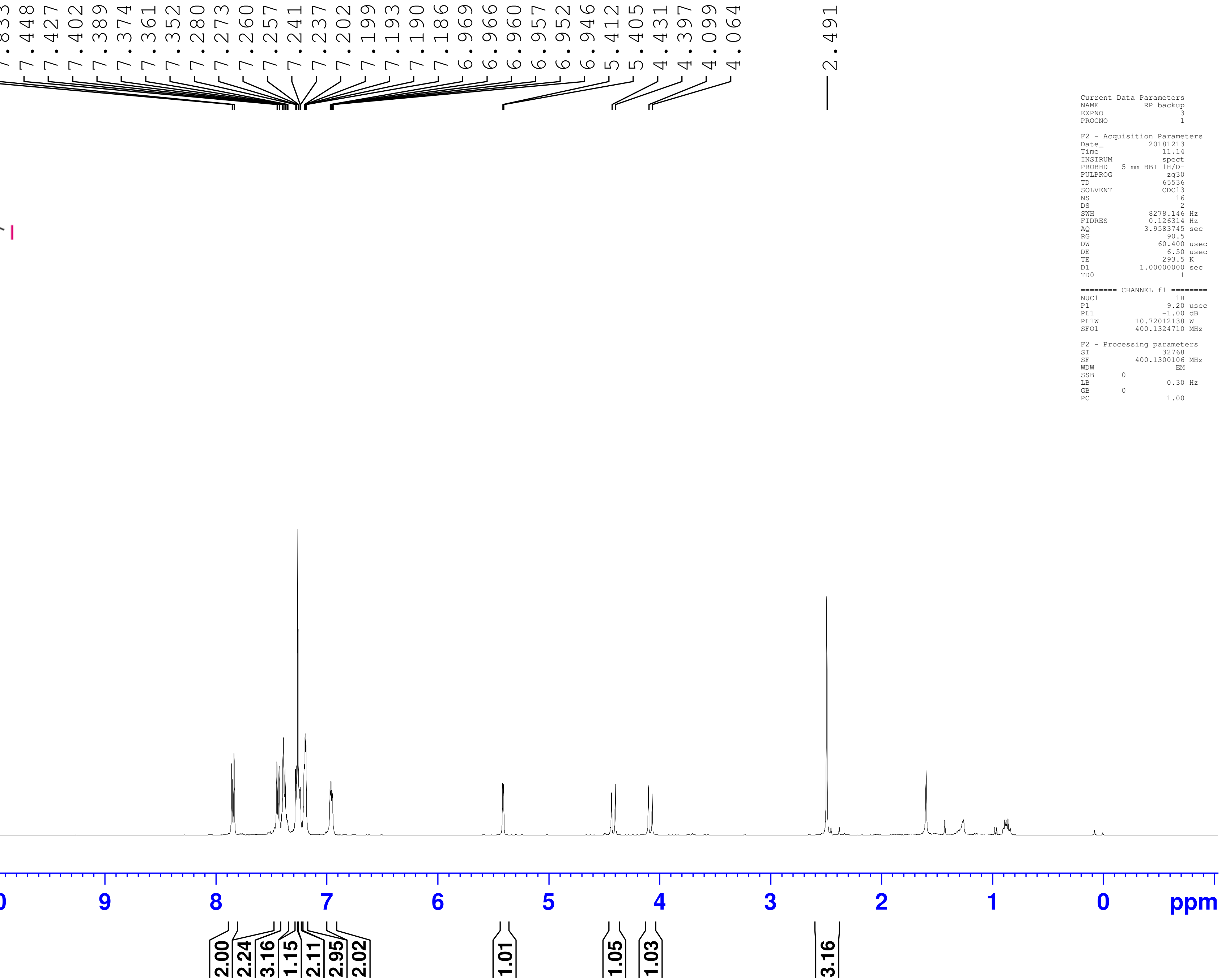
(6). (a) M. A. Spackman, J. J. McKinnon, CrystEngComm., 2002, 4, 378. (b) M.A. Spackman, D. Jayatilake, CrystEngComm., 2009, 11, 19. (c) C. Zhang, X. Xue, Y. Cao, Y. Zhou, H. Li, J. Zhou, T. Gao, CrystEngComm., 2013, 15, 6837. (d) M. J. Turner, M. J. J. McKinnon, S. K. Wolff, D. J. Grimwood, P. R. Spackman, D. Jayatilaka, M. A. Spackman, Crystal Explorer 17 University of Western Australia: Pert, Australia, 2017.



2a



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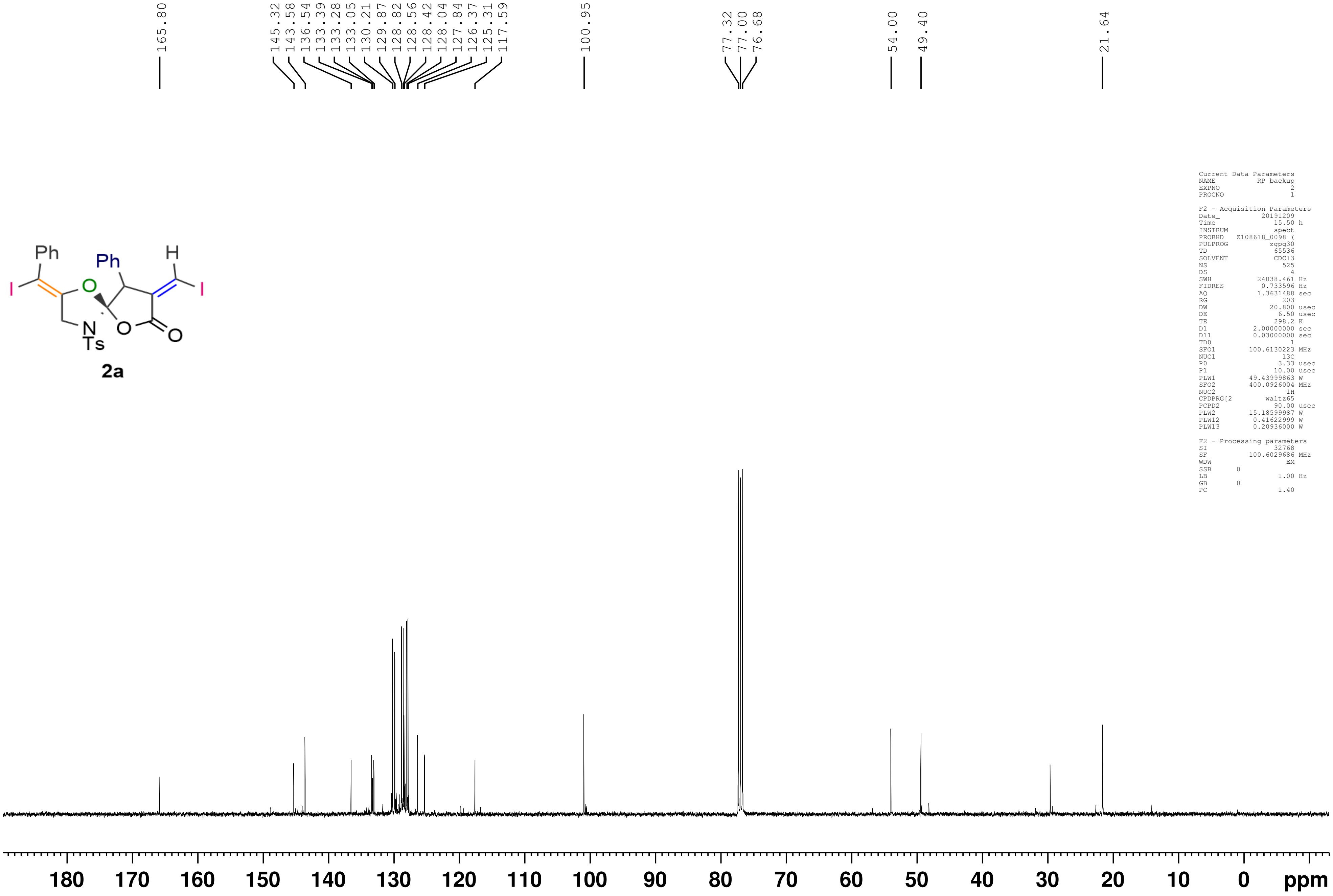

2a

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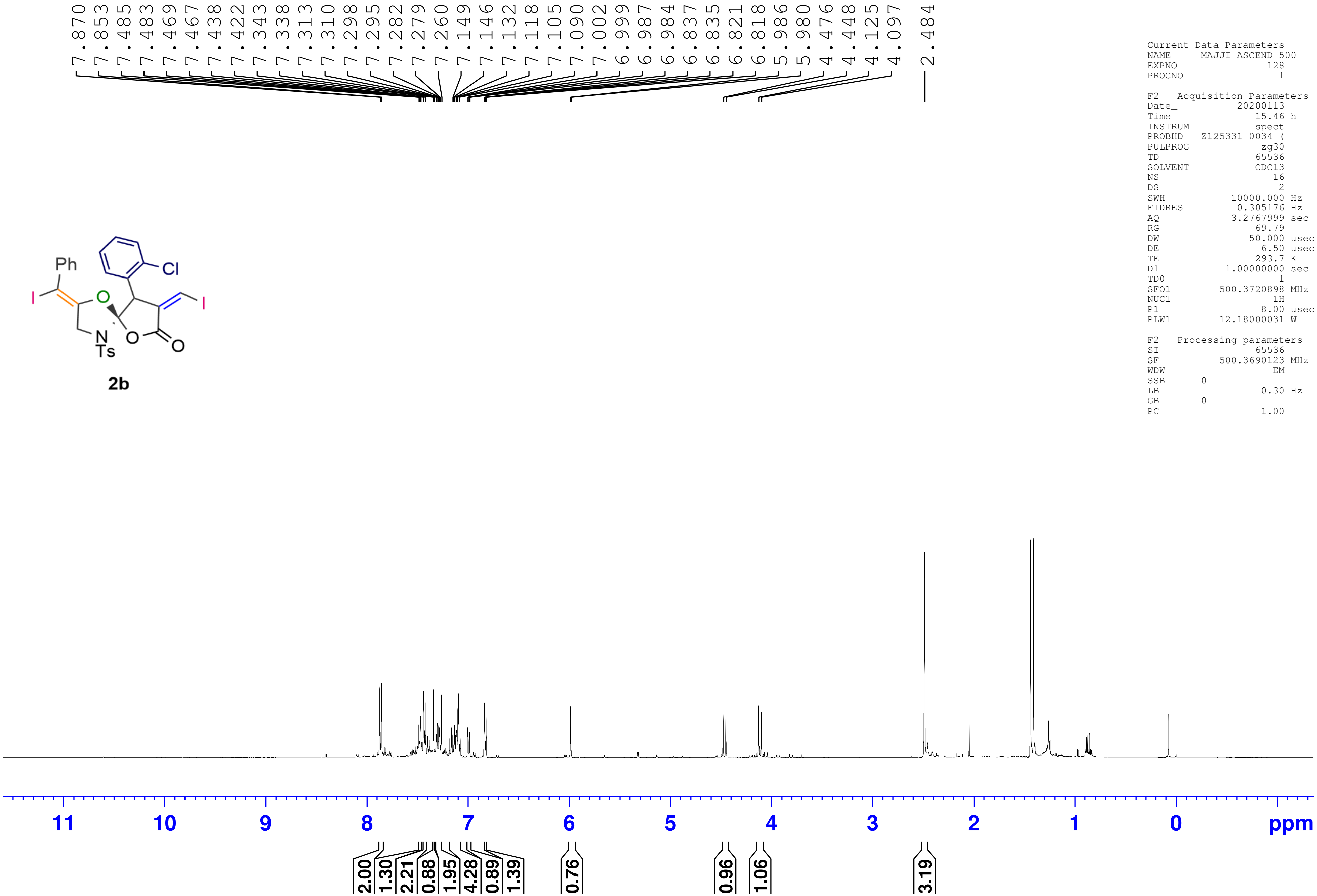

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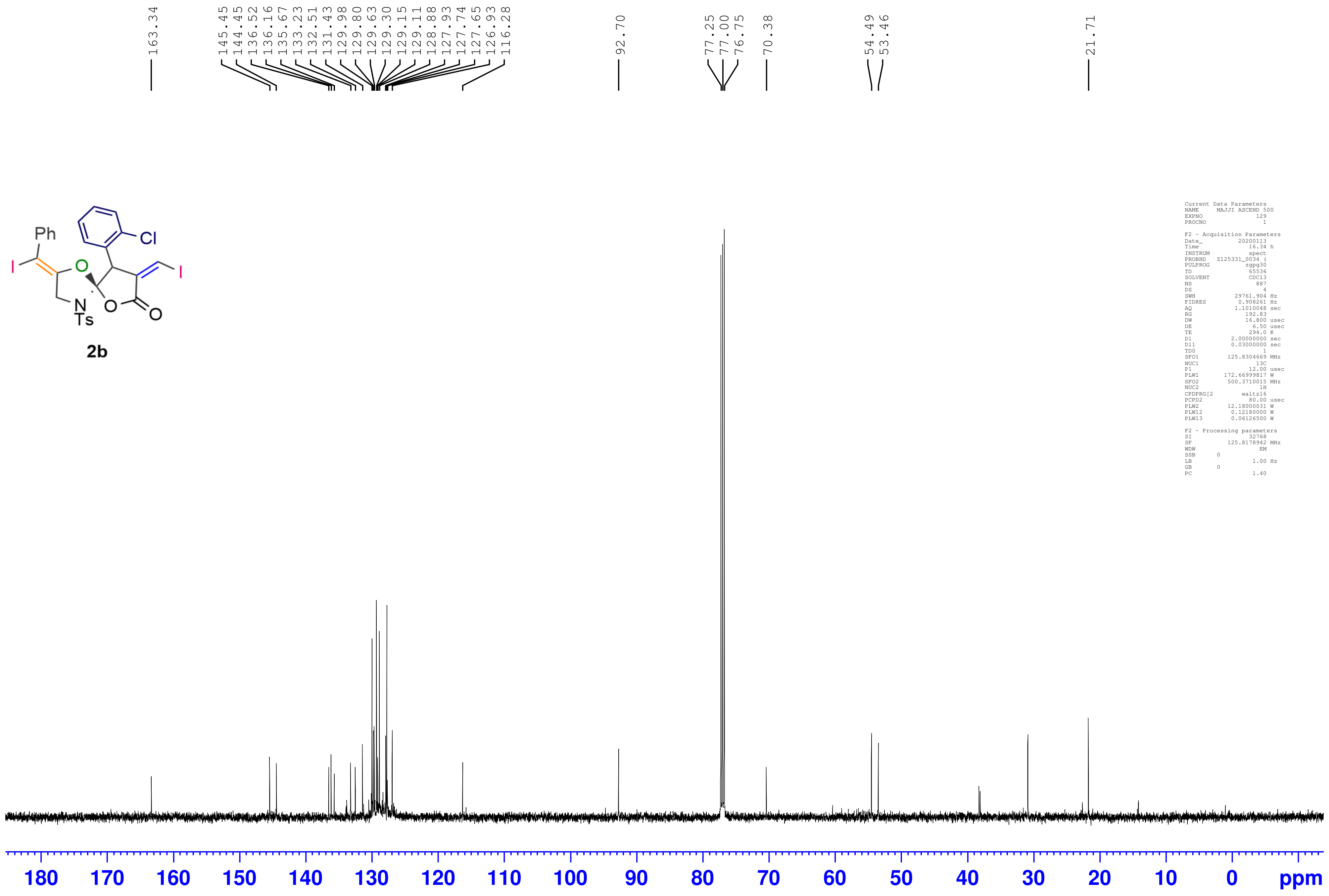

2b

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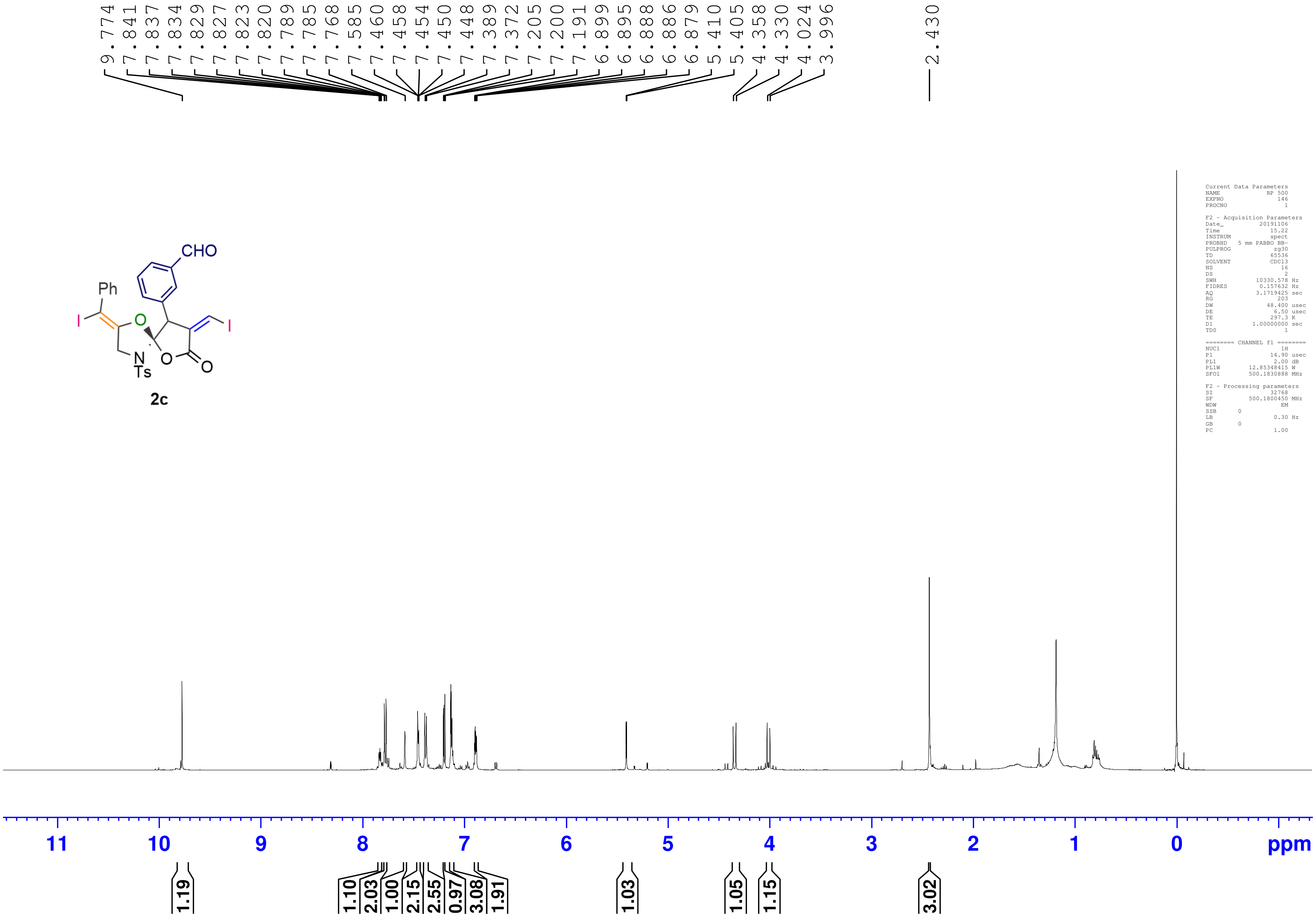

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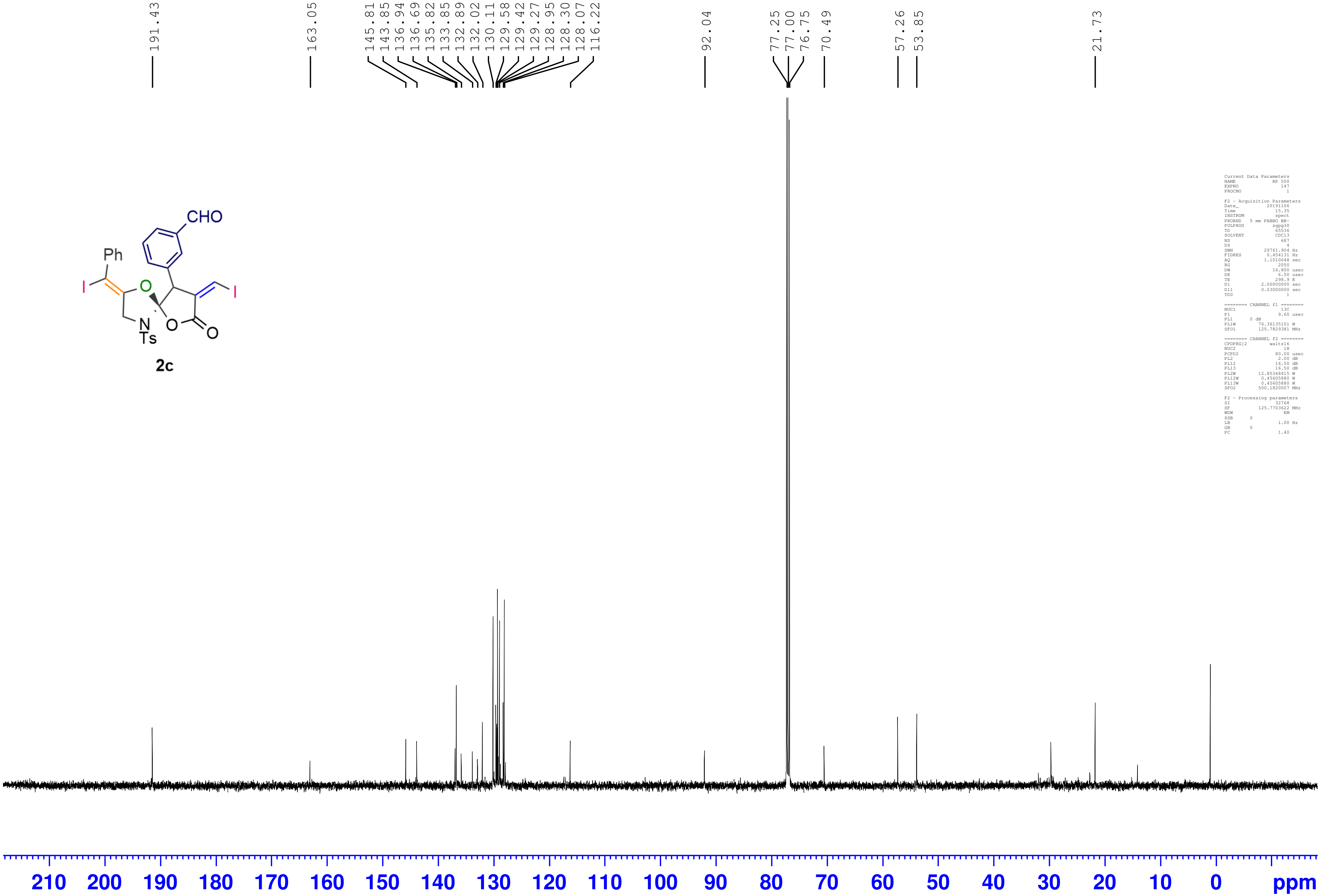

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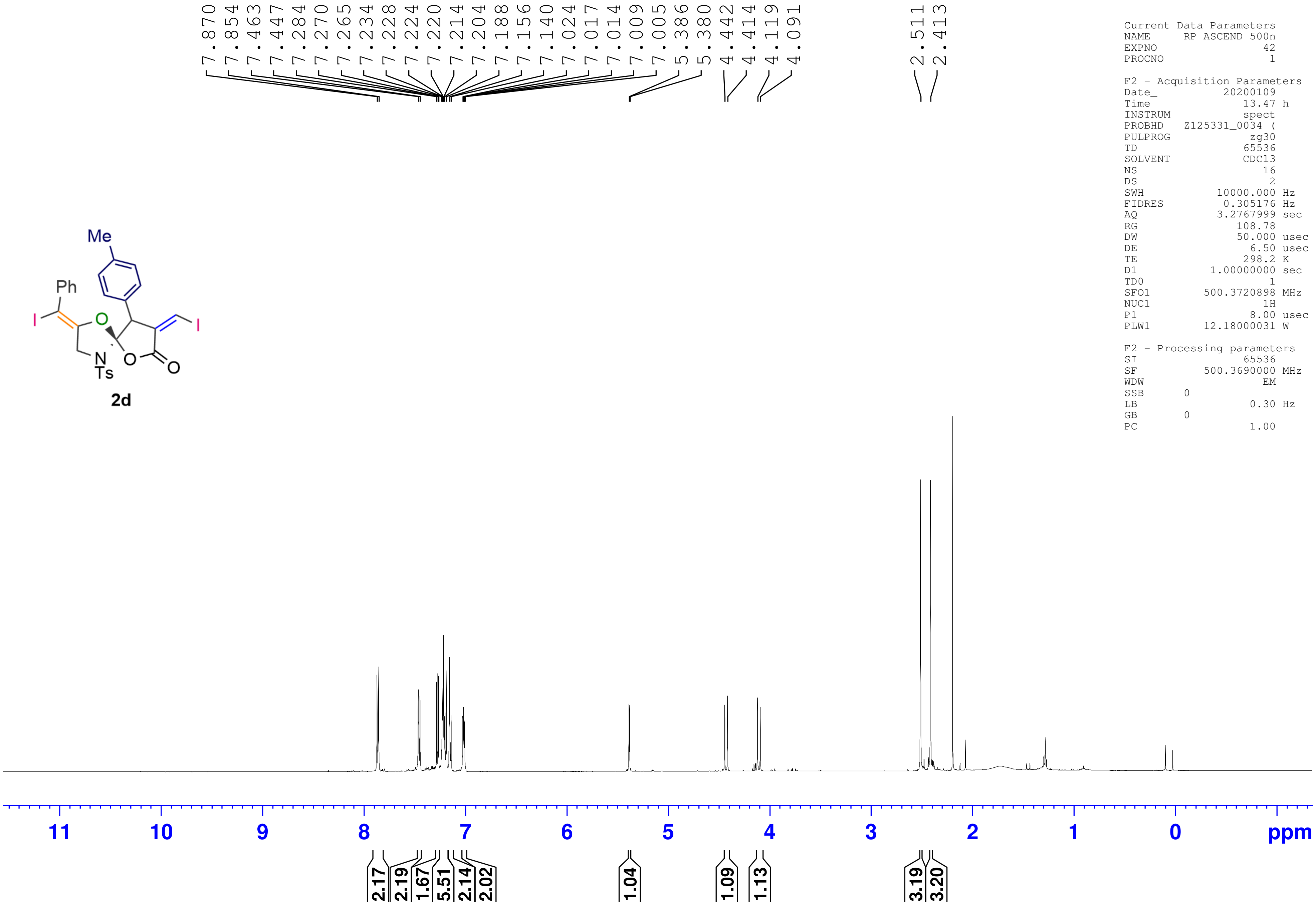
DW                 16.800 usec
DE                   6.50 usec
TE                  298.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.60 usec
PL1      0 dB
PL1W          76.36135101 W
SFO1          125.7829381 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                16.50 dB
PL13                16.50 dB
PL2W          12.85348415 W
PL12W          0.45605880 W
PL13W          0.45605880 W
SFO2          500.1820007 MHz

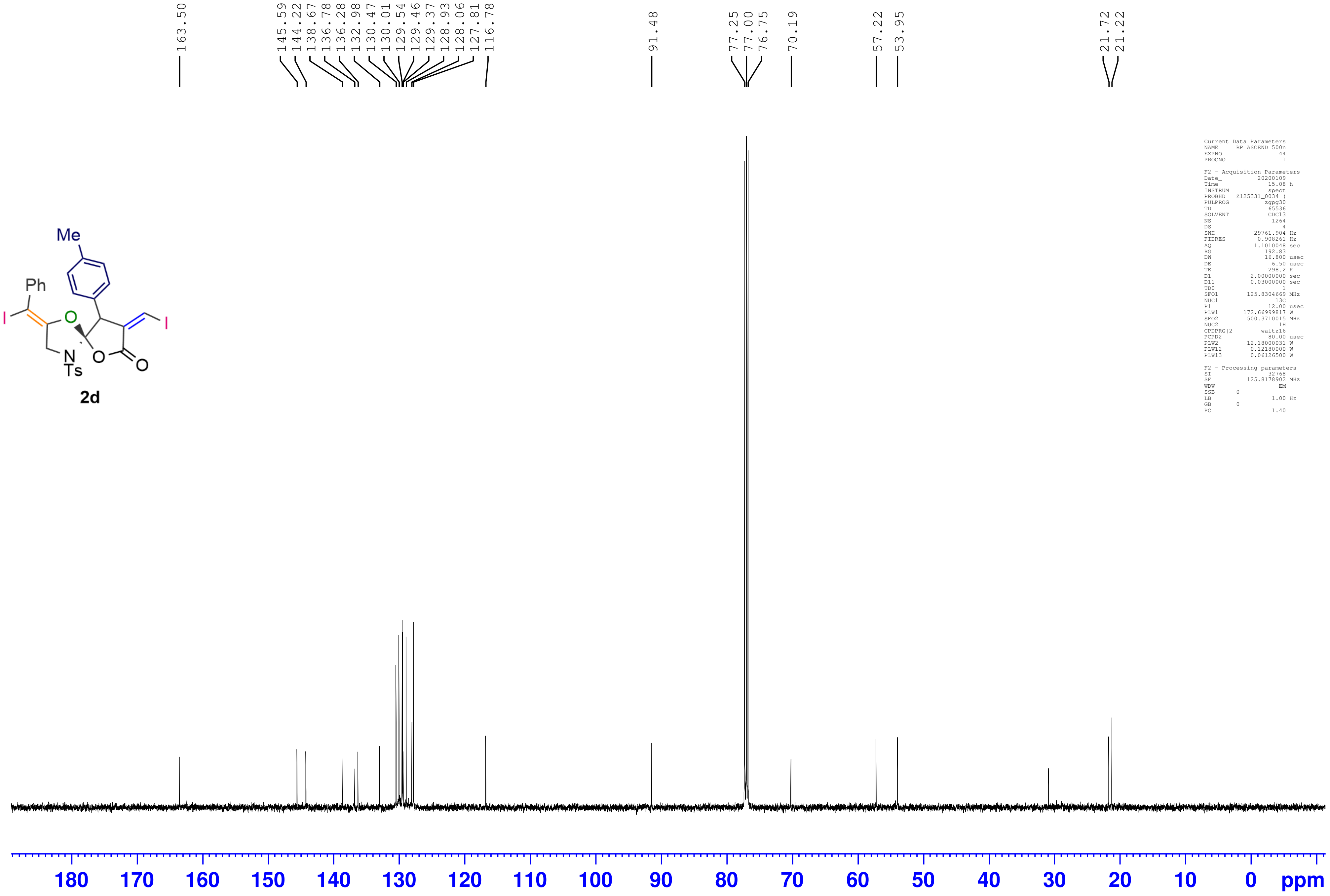
F2 - Processing parameters
SI                  32768
SF            125.7703622 MHz
WDW                    EM
SSB      0
LB                   1.00 Hz
GB       0
PC                   1.40
```



```
Current Data Parameters
NAME        RP ASCEND 500n
EXPNO                   42
PROCNO                   1

F2 - Acquisition Parameters
Date_             20200109
Time                 13.47 h
INSTRUM              spect
PROBHD    Z125331_0034 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES            0.305176 Hz
AQ               3.2767999 sec
RG                  108.78
DW                  50.000 usec
DE                    6.50 usec
TE                   298.2 K
D1              1.00000000 sec
TD0                      1
SFO1           500.3720898 MHz
NUC1                    1H
P1                    8.00 usec
PLW1           12.18000031 W

F2 - Processing parameters
SI                   65536
SF             500.3690000 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

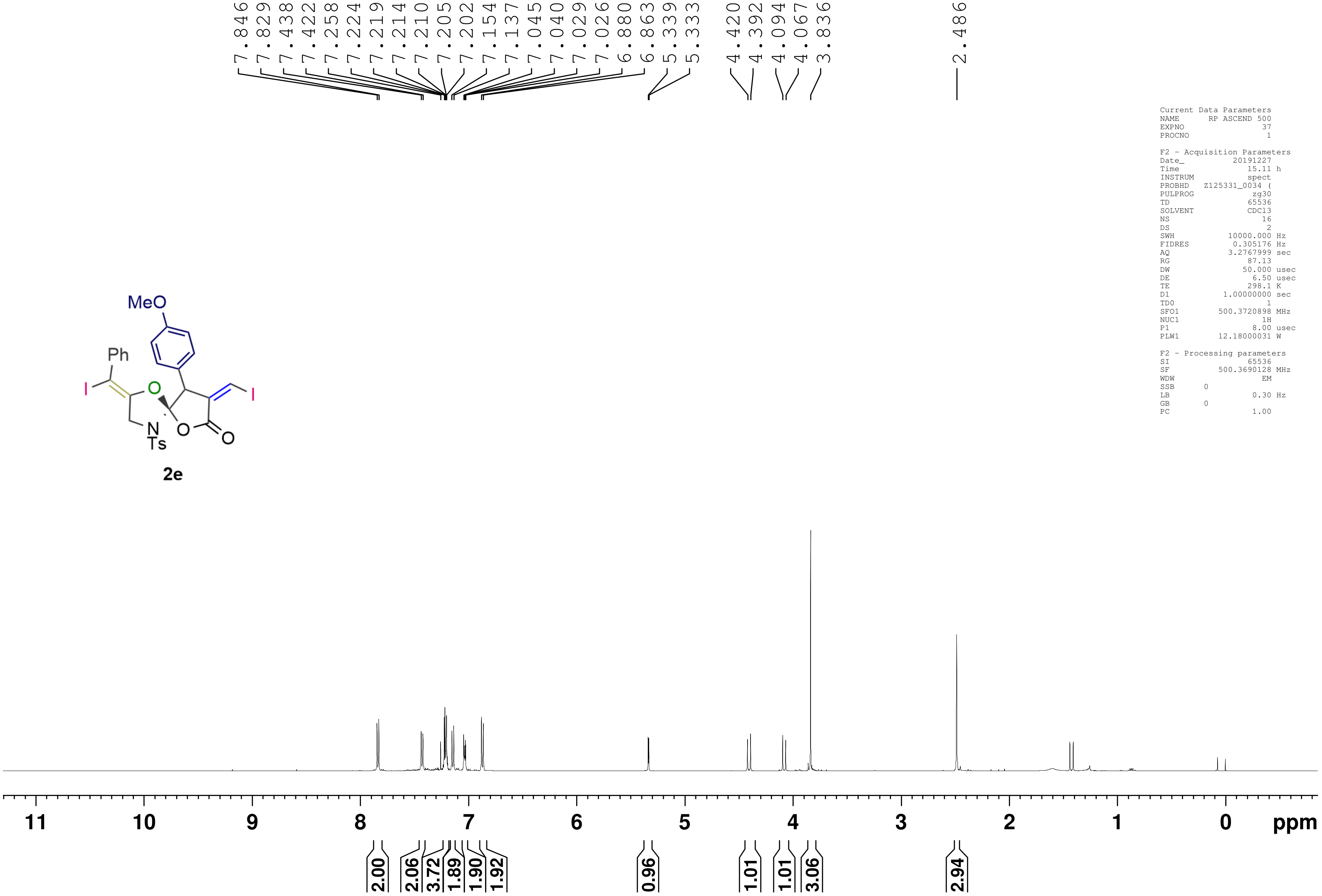


2d

```
Current Data Parameters
NAME     RP ASCEND 500n
EXPNO                44
PROCNO                1

F2 - Acquisition Parameters
Date_          20200109
Time              15.08 h
INSTRUM           spect
PROBHD   Z125331_0034 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1264
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               192.83
DW               16.800 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.8304669 MHz
NUC1                13C
P1                12.00 usec
PLW1       172.66999817 W
SFO2        500.3710015 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        12.18000031 W
PLW12        0.12180000 W
PLW13        0.06126500 W

F2 - Processing parameters
SI                32768
SF          125.8178902 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

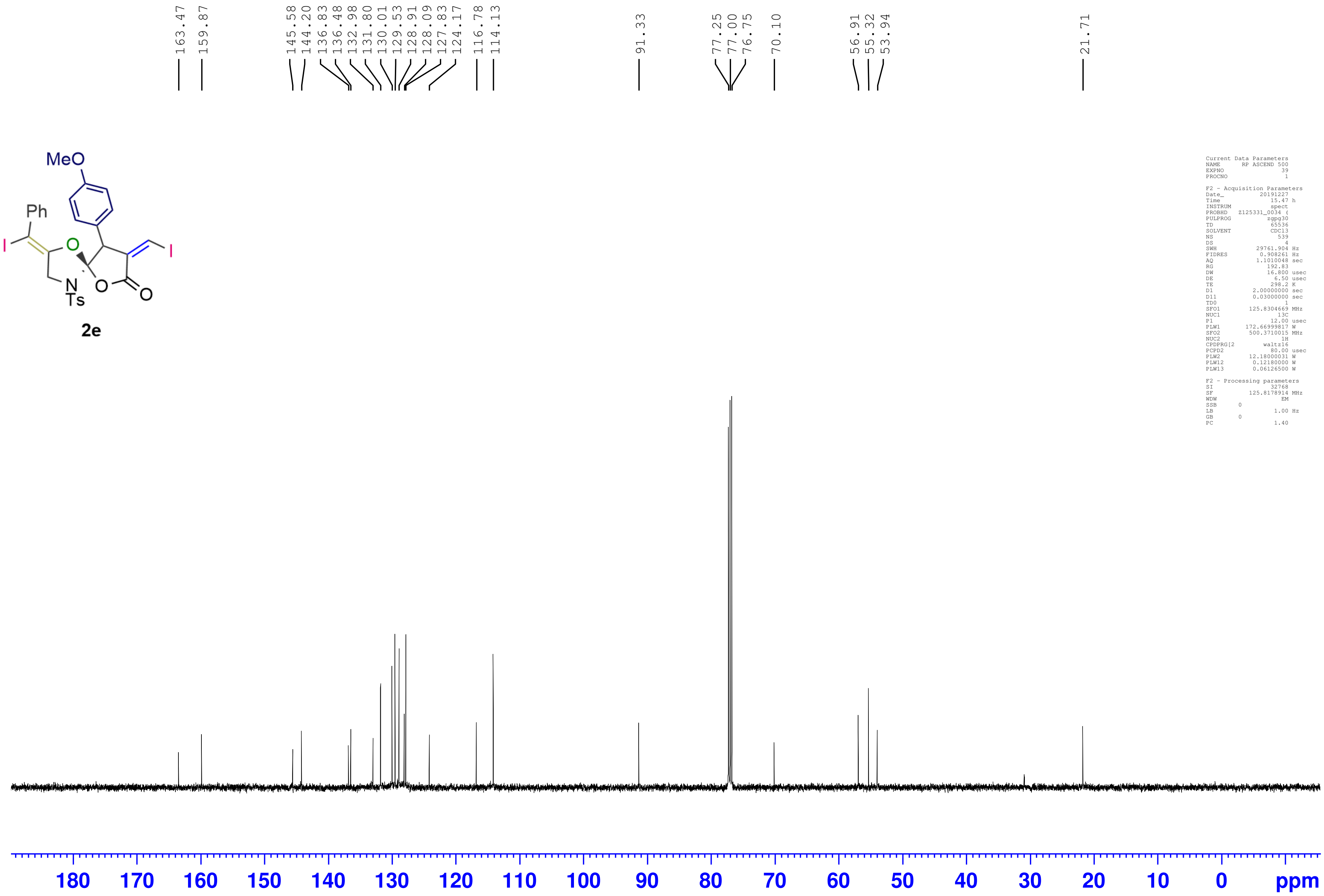


2e

```
Current Data Parameters
NAME       RP ASCEND 500
EXPNO                 37
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191227
Time               15.11 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ             3.2767999 sec
RG                 87.13
DW                50.000 usec
DE                  6.50 usec
TE                 298.1 K
D1            1.00000000 sec
TD0                    1
SFO1         500.3720898 MHz
NUC1                  1H
P1                  8.00 usec
PLW1         12.18000031 W

F2 - Processing parameters
SI                 65536
SF           500.3690128 MHz
WDW                   EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```

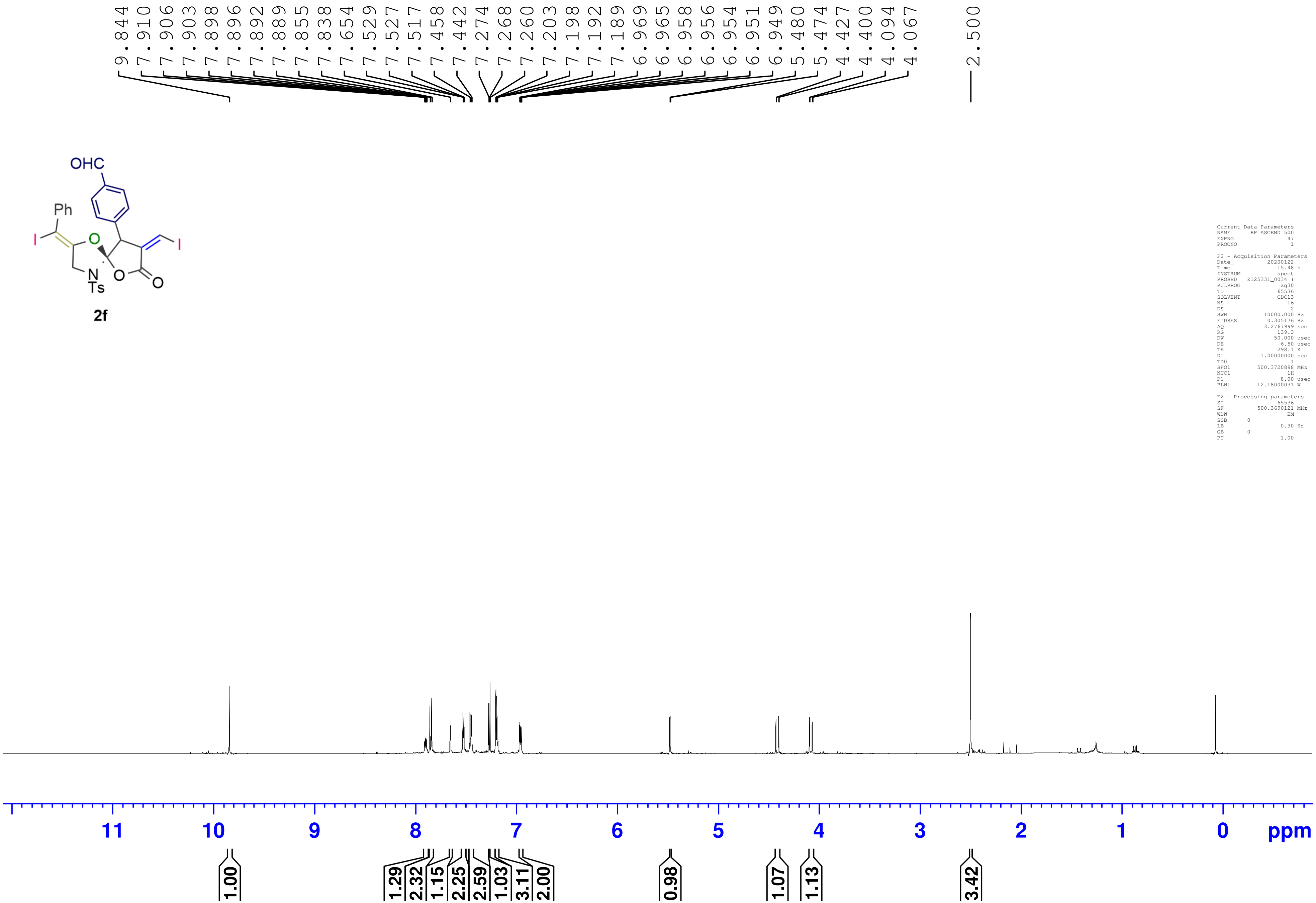


2e

```
Current Data Parameters
NAME       RP ASCEND 500
EXPNO                 39
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191227
Time               15.47 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   539
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                192.83
DW                16.800 usec
DE                  6.50 usec
TE                 298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.8304669 MHz
NUC1                 13C
P1                 12.00 usec
PLW1        172.66999817 W
SFO2         500.3710015 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         12.18000031 W
PLW12         0.12180000 W
PLW13         0.06126500 W

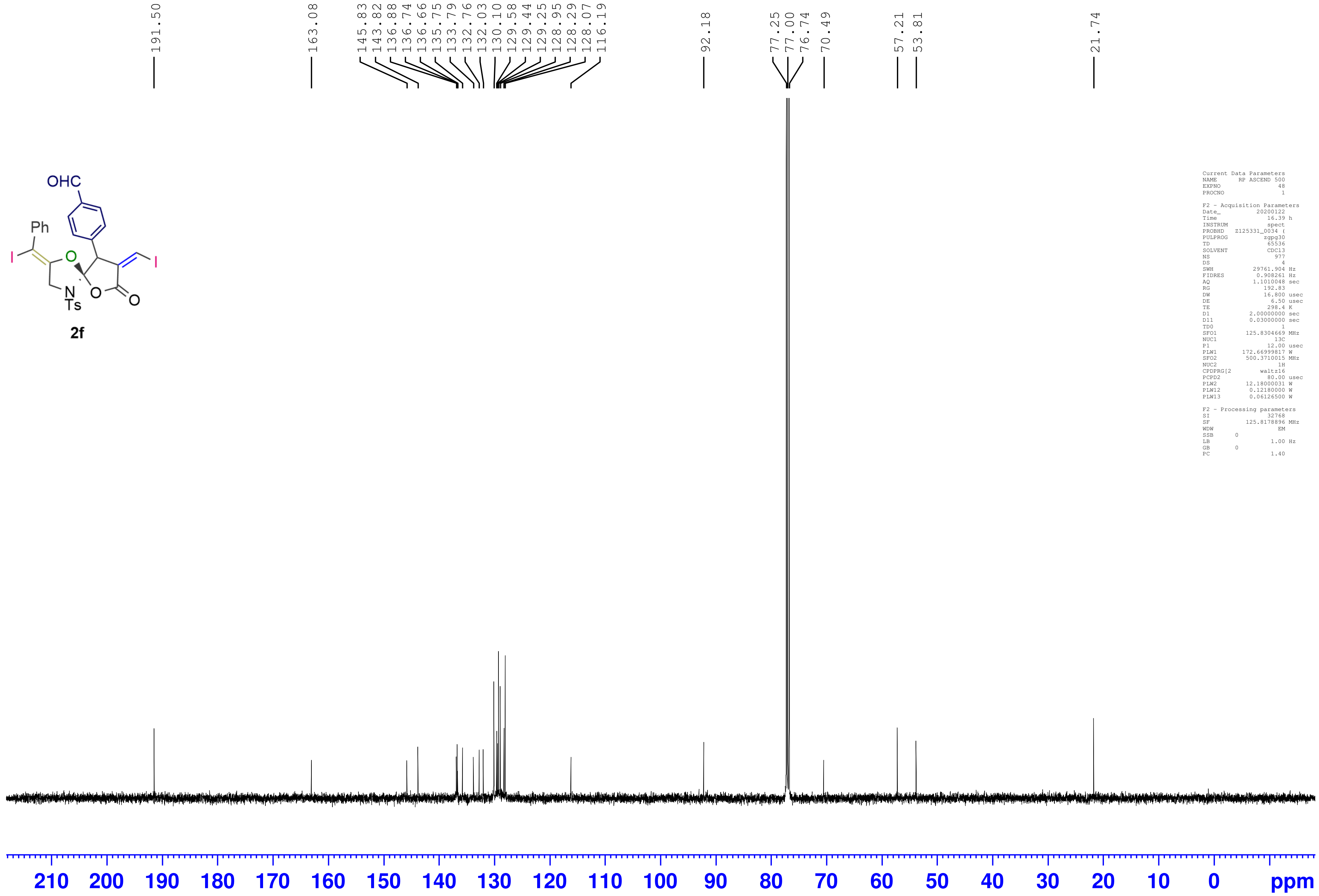
F2 - Processing parameters
SI                 32768
SF           125.8178914 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```



```
Current Data Parameters
NAME      RP ASCEND 500
EXPNO                47
PROCNO                1

F2 - Acquisition Parameters
Date_          20200122
Time              15.48 h
INSTRUM           spect
PROBHD   Z125331_0034 (
PULPROG           zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            3.2767999 sec
RG                139.3
DW               50.000 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                   1
SFO1        500.3720898 MHz
NUC1                 1H
P1                 8.00 usec
PLW1        12.18000031 W

F2 - Processing parameters
SI                65536
SF          500.3690121 MHz
WDW                  EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

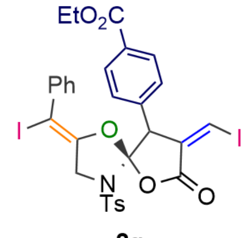


2f

```
Current Data Parameters
NAME       RP ASCEND 500
EXPNO                 48
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200122
Time               16.39 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   977
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                192.83
DW                16.800 usec
DE                  6.50 usec
TE                 298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.8304669 MHz
NUC1                 13C
P1                 12.00 usec
PLW1        172.66999817 W
SFO2         500.3710015 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         12.18000031 W
PLW12         0.12180000 W
PLW13         0.06126500 W

F2 - Processing parameters
SI                 32768
SF           125.8178896 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

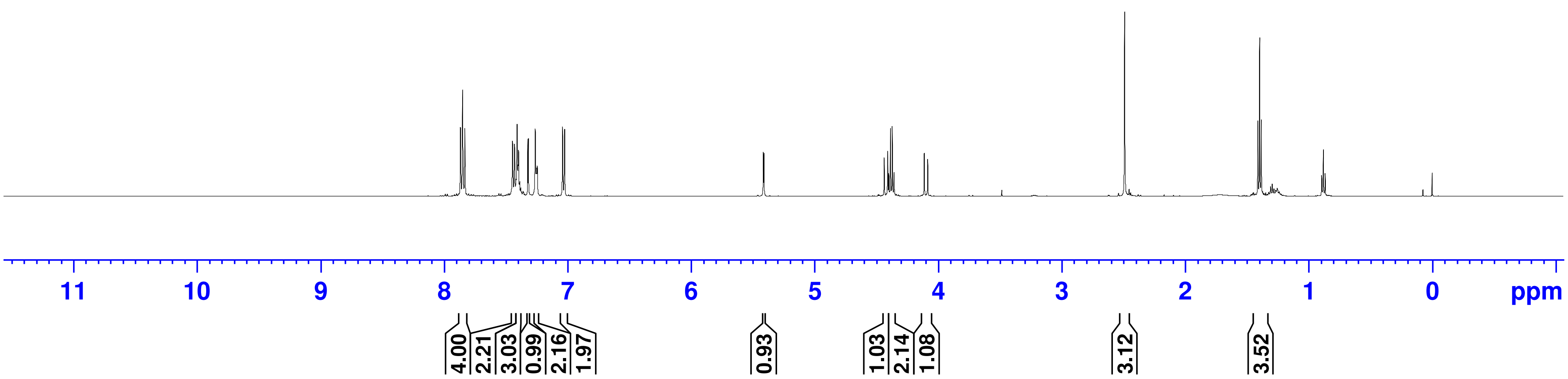


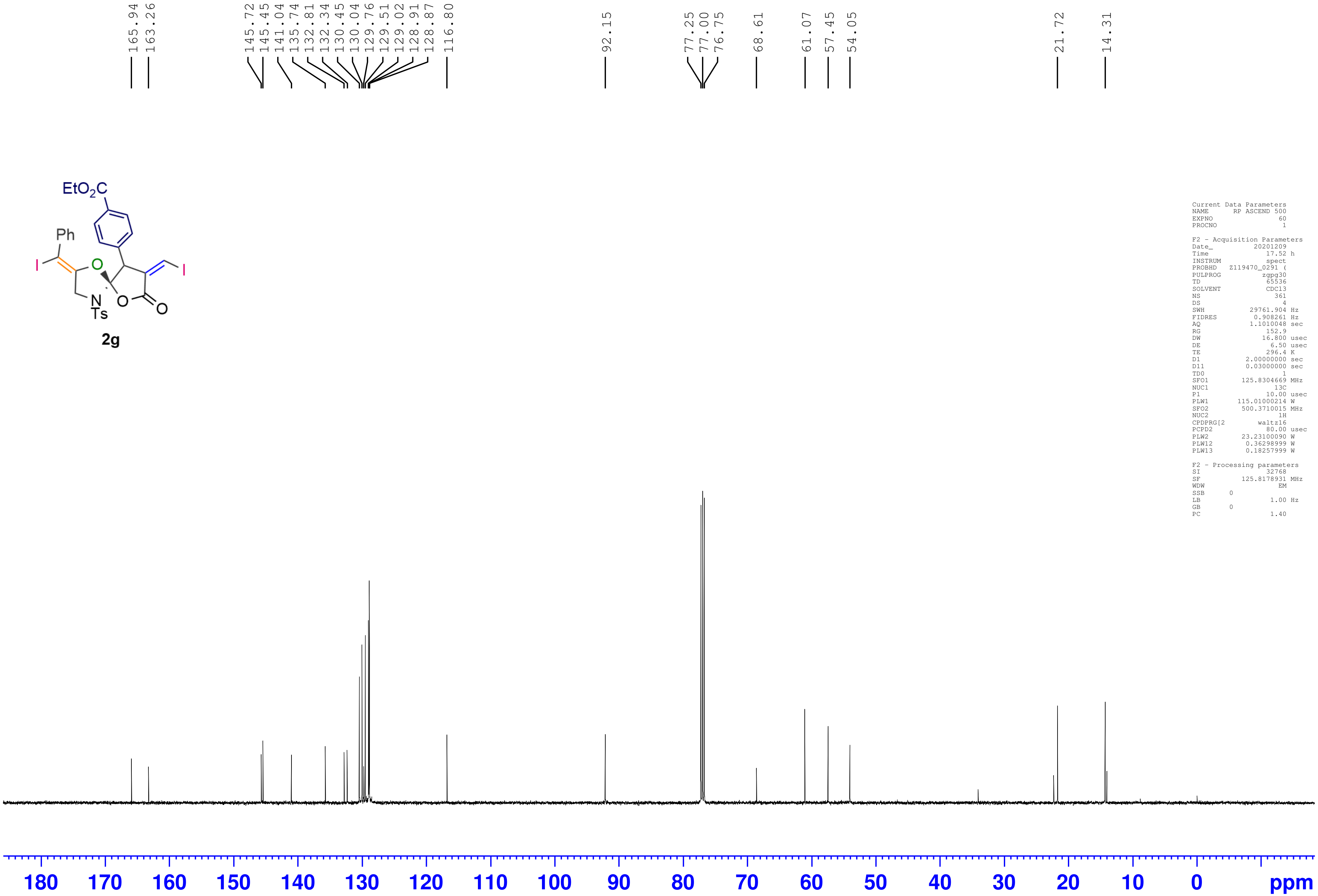
2g

```
Current Data Parameters
NAME      RP ASCEND 500
EXPNO                59
PROCNO                1

F2 - Acquisition Parameters
Date_          20201209
Time              17.31 h
INSTRUM           spect
PROBHD   Z119470_0291 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            3.2767999 sec
RG                62.04
DW               50.000 usec
DE                 6.50 usec
TE                295.8 K
D1           1.00000000 sec
TD0                   1
SFO1        500.3720898 MHz
NUC1                 1H
P1                10.00 usec
PLW1        23.23100090 W

F2 - Processing parameters
SI                65536
SF          500.3690105 MHz
WDW                  EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```



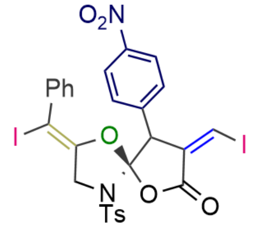


2g

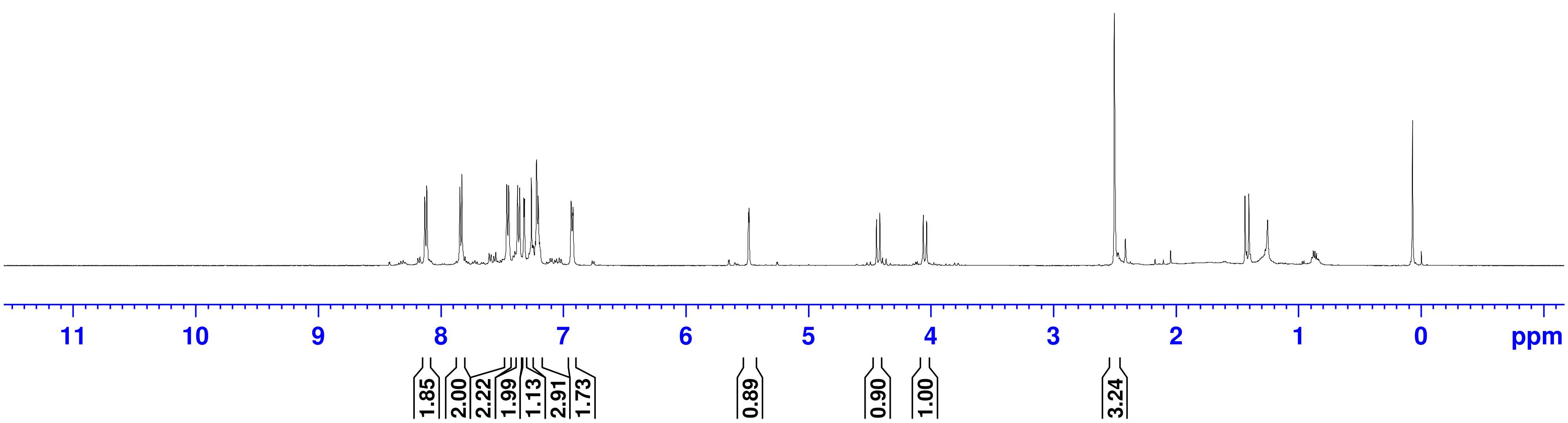
```
Current Data Parameters
NAME       RP ASCEND 500
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201209
Time               17.52 h
INSTRUM            spect
PROBHD   Z119470_0291 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   361
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                 152.9
DW                16.800 usec
DE                  6.50 usec
TE                 296.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.8304669 MHz
NUC1                 13C
P1                 10.00 usec
PLW1        115.01000214 W
SFO2         500.3710015 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         23.23100090 W
PLW12         0.36298999 W
PLW13         0.18257999 W

F2 - Processing parameters
SI                 32768
SF           125.8178931 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```



2h

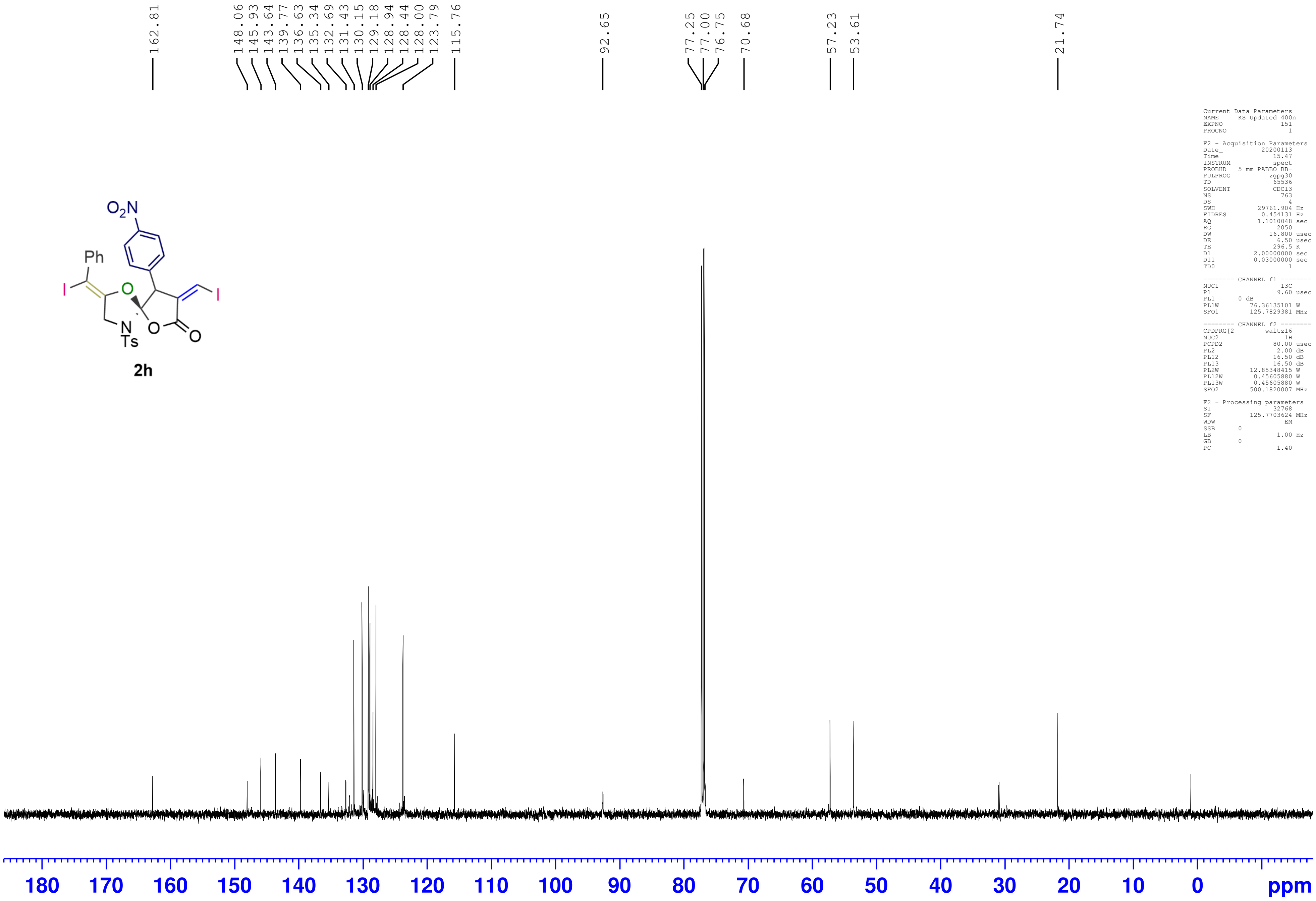


```
Current Data Parameters
NAME     KS Updated 400n
EXPNO                150
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200113
Time               15.46
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719425 sec
RG                   228
DW                48.400 usec
DE                  6.50 usec
TE                 296.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.90 usec
PL1                 2.00 dB
PL1W         12.85348415 W
SFO1         500.1830888 MHz

F2 - Processing parameters
SI                 32768
SF           500.1800098 MHz
WDW                   EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```



2h

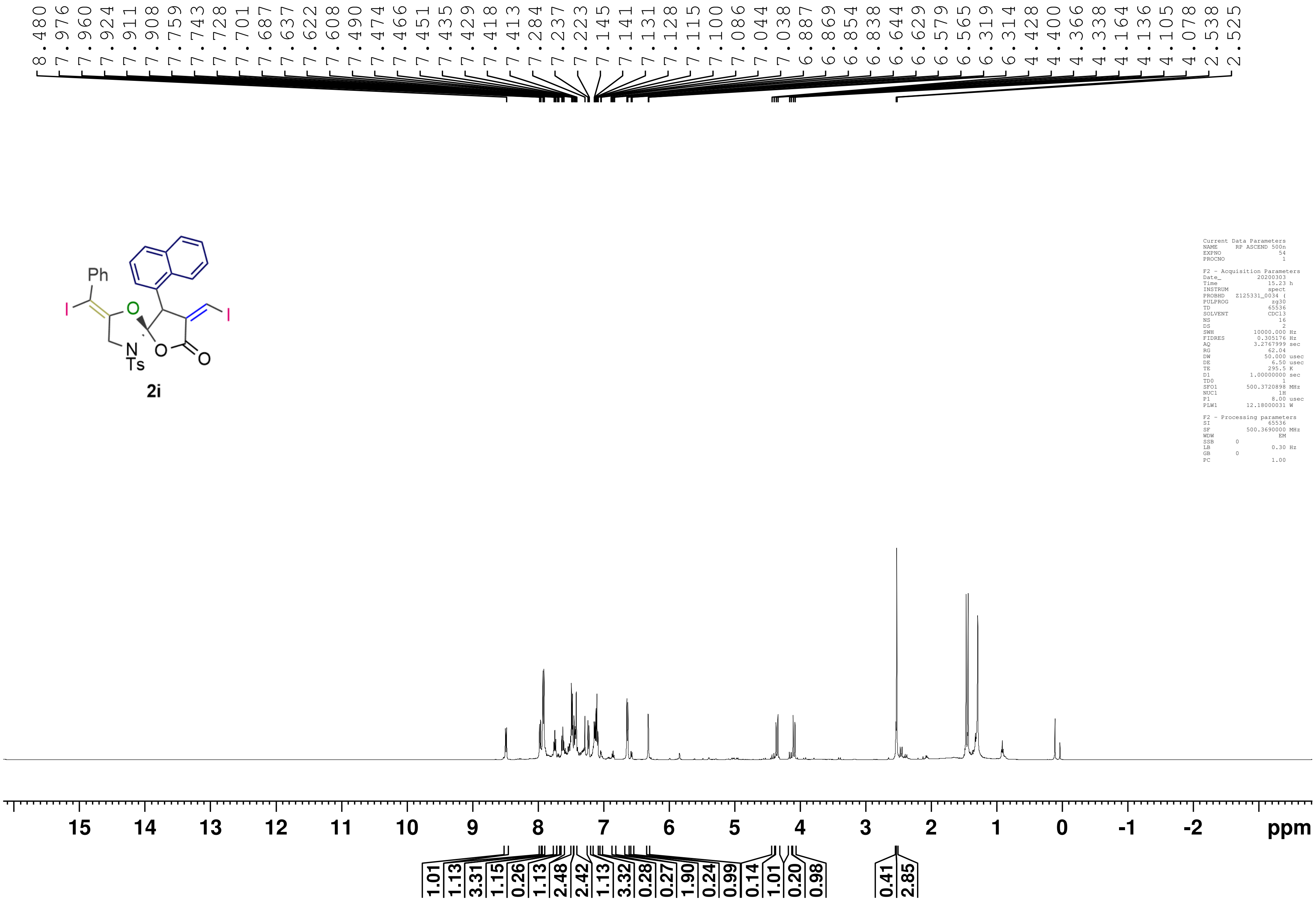
```
Current Data Parameters
NAME     KS Updated 400n
EXPNO                151
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200113
Time               15.47
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   763
DS                     4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG                  2050
DW              16.800 usec
DE                6.50 usec
TE               296.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.60 usec
PL1      0 dB
PL1W        76.36135101 W
SFO1        125.7829381 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 2.00 dB
PL12               16.50 dB
PL13               16.50 dB
PL2W         12.85348415 W
PL12W         0.45605880 W
PL13W         0.45605880 W
SFO2         500.1820007 MHz

F2 - Processing parameters
SI                 32768
SF           125.7703624 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```

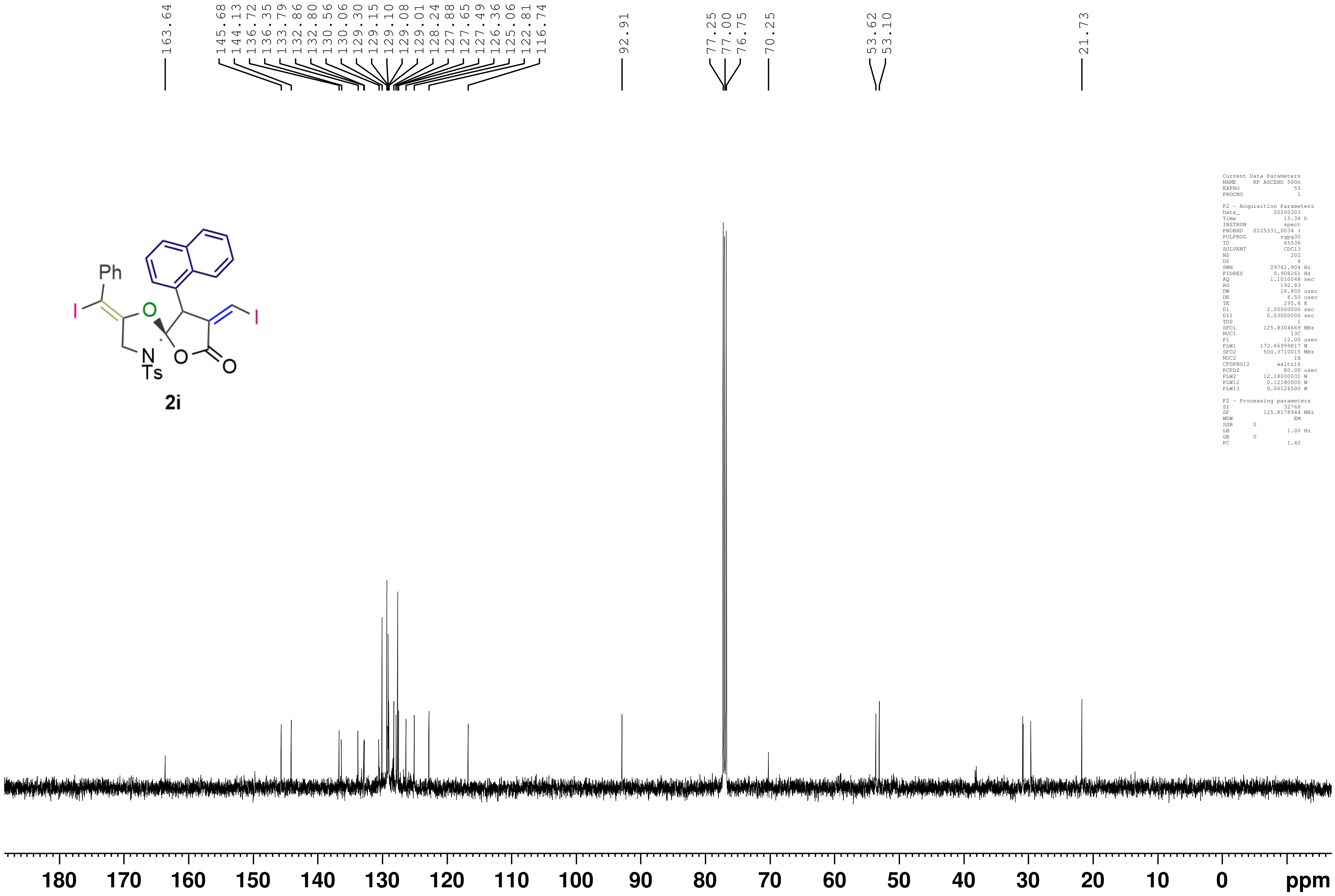


2i

```
Current Data Parameters
NAME      RP ASCEND 500n
EXPNO                 54
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200303
Time               15.23 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ             3.2767999 sec
RG                 62.04
DW                50.000 usec
DE                  6.50 usec
TE                 295.5 K
D1            1.00000000 sec
TD0                    1
SFO1         500.3720898 MHz
NUC1                  1H
P1                  8.00 usec
PLW1         12.18000031 W

F2 - Processing parameters
SI                 65536
SF           500.3690000 MHz
WDW                   EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```

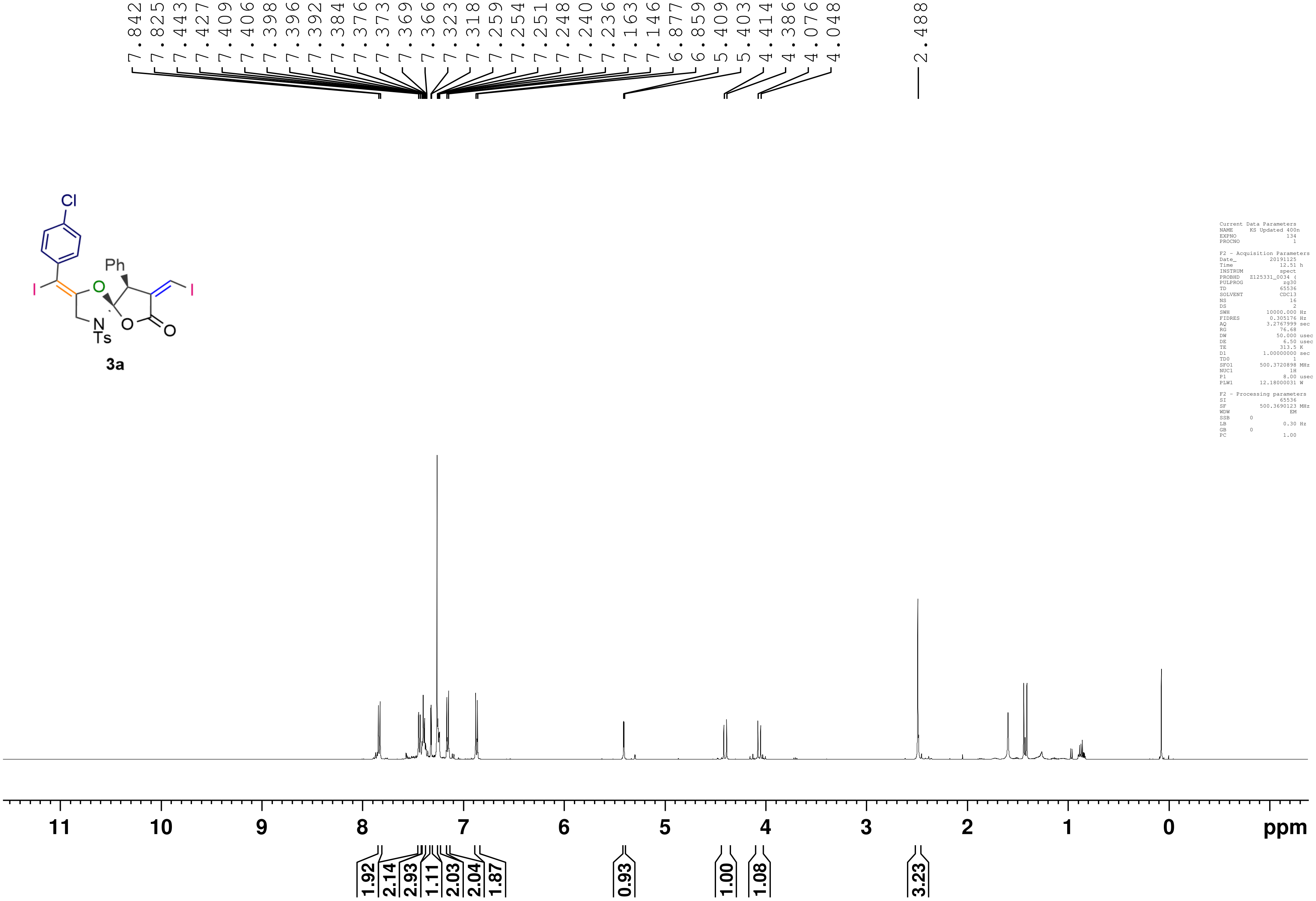


2i

```
Current Data Parameters
NAME     RP ASCEND 500n
EXPNO                55
PROCNO                1

F2 - Acquisition Parameters
Date_          20200303
Time              15.34 h
INSTRUM           spect
PROBHD   Z125331_0034 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  202
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               192.83
DW               16.800 usec
DE                 6.50 usec
TE                295.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.8304669 MHz
NUC1                13C
P1                12.00 usec
PLW1       172.66999817 W
SFO2        500.3710015 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        12.18000031 W
PLW12        0.12180000 W
PLW13        0.06126500 W

F2 - Processing parameters
SI                32768
SF          125.8178944 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

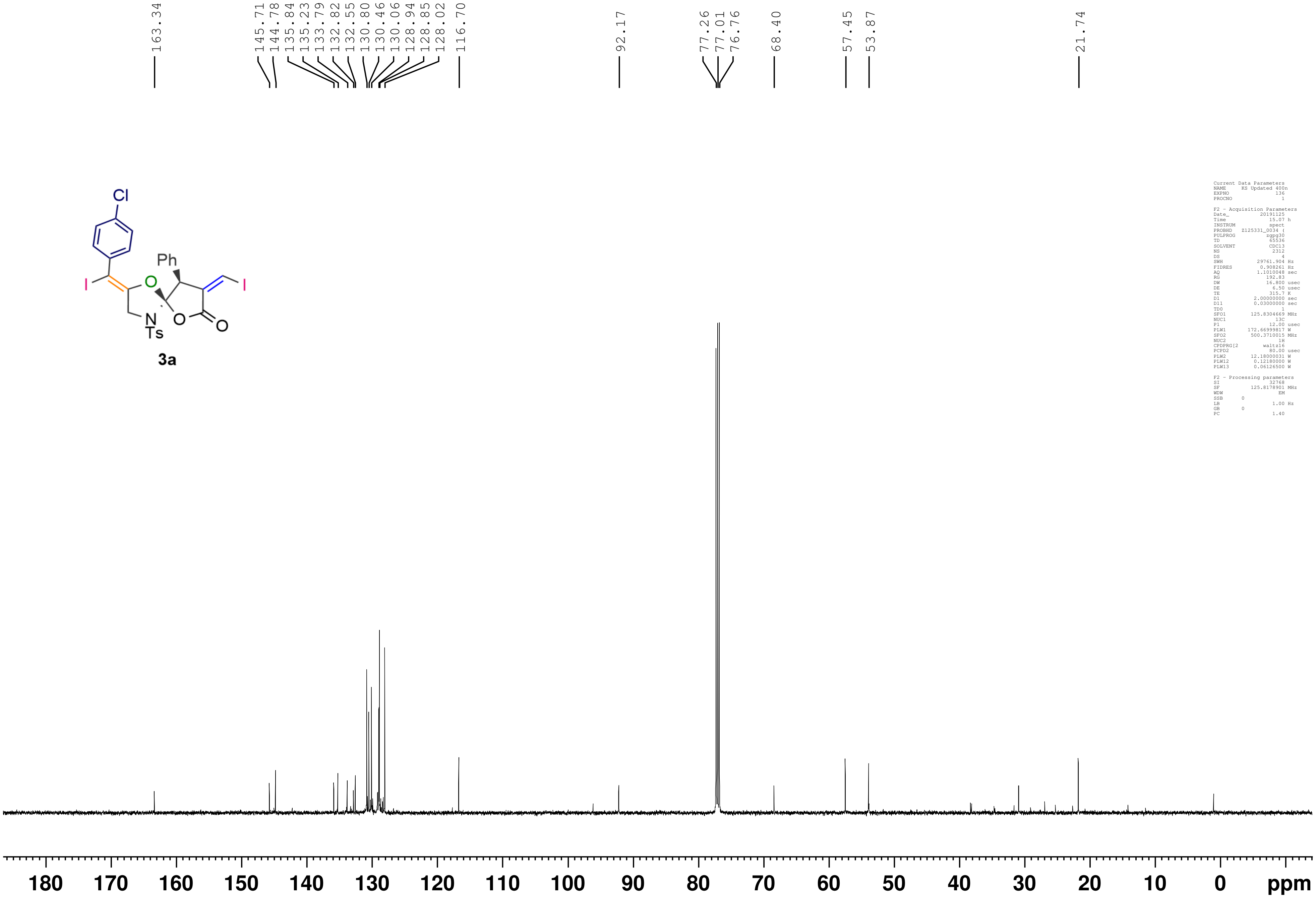


3a

```
Current Data Parameters
NAME     KS Updated 400n
EXPNO                134
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time               12.51 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ             3.2767999 sec
RG                 76.68
DW                50.000 usec
DE                  6.50 usec
TE                 313.5 K
D1            1.00000000 sec
TD0                    1
SFO1         500.3720898 MHz
NUC1                  1H
P1                  8.00 usec
PLW1         12.18000031 W

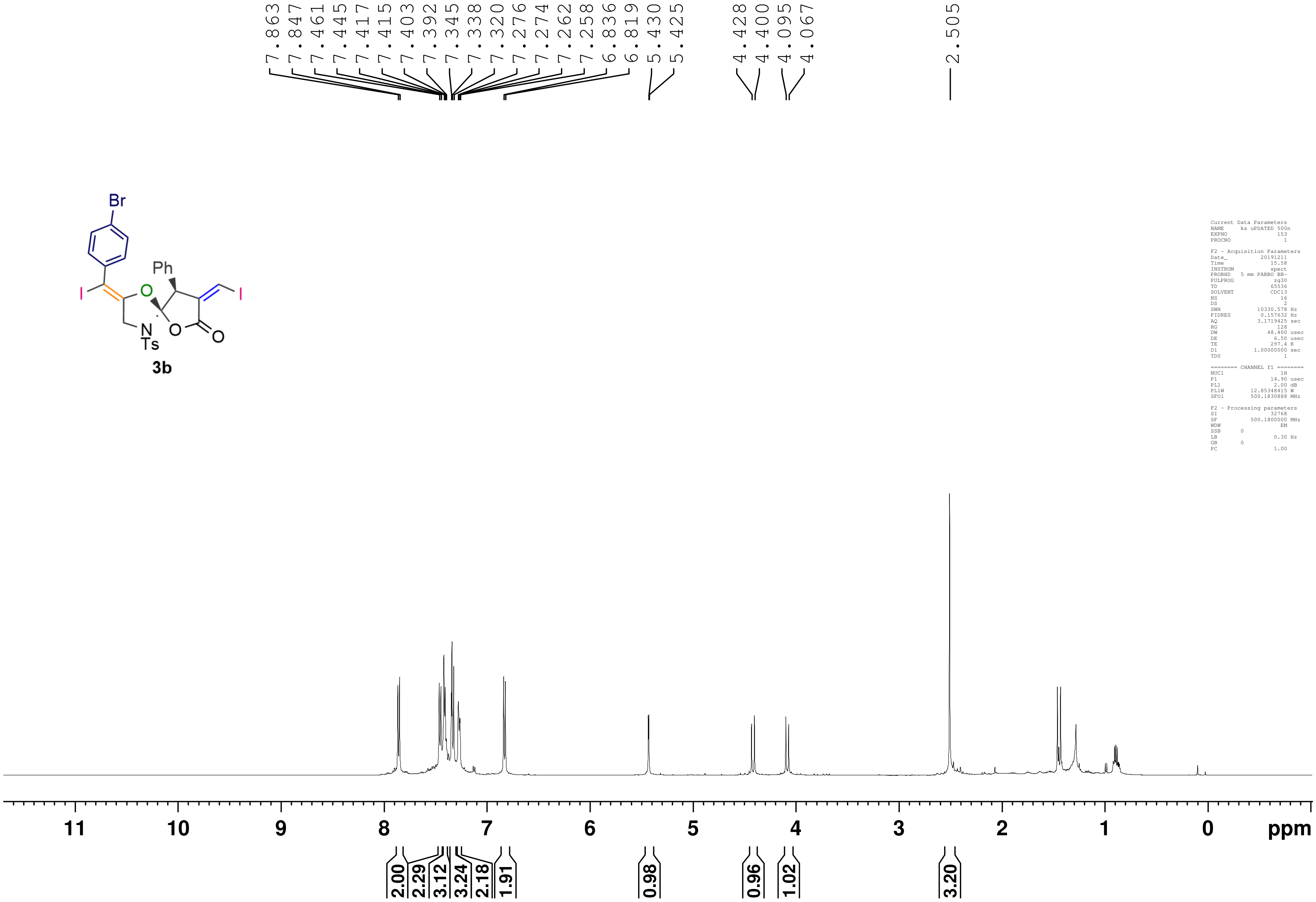
F2 - Processing parameters
SI                 65536
SF           500.3690123 MHz
WDW                   EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```



```
Current Data Parameters
NAME     KS Updated 400n
EXPNO                136
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time               15.07 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2312
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                192.83
DW                16.800 usec
DE                  6.50 usec
TE                 315.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.8304669 MHz
NUC1                 13C
P1                 12.00 usec
PLW1        172.66999817 W
SFO2         500.3710015 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         12.18000031 W
PLW12         0.12180000 W
PLW13         0.06126500 W

F2 - Processing parameters
SI                 32768
SF           125.8178901 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```



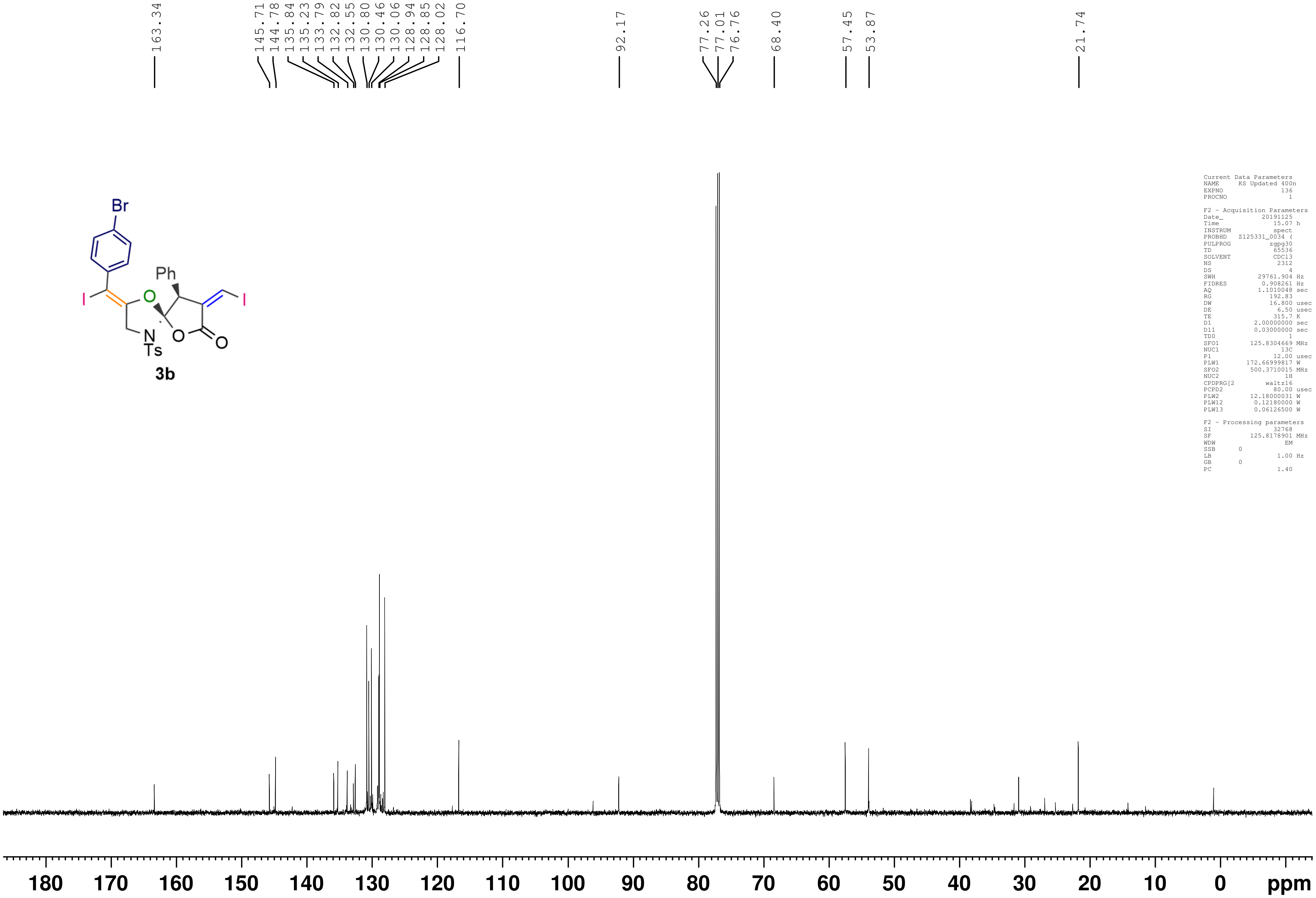
3b

```
Current Data Parameters
NAME     ks uPDATED 500n
EXPNO                153
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191211
Time               15.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                   128
DW                48.400 usec
DE                  6.50 usec
TE                 297.4 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.90 usec
PL1                 2.00 dB
PL1W         12.85348415 W
SFO1         500.1830888 MHz

F2 - Processing parameters
SI                 32768
SF           500.1800000 MHz
WDW                   EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```

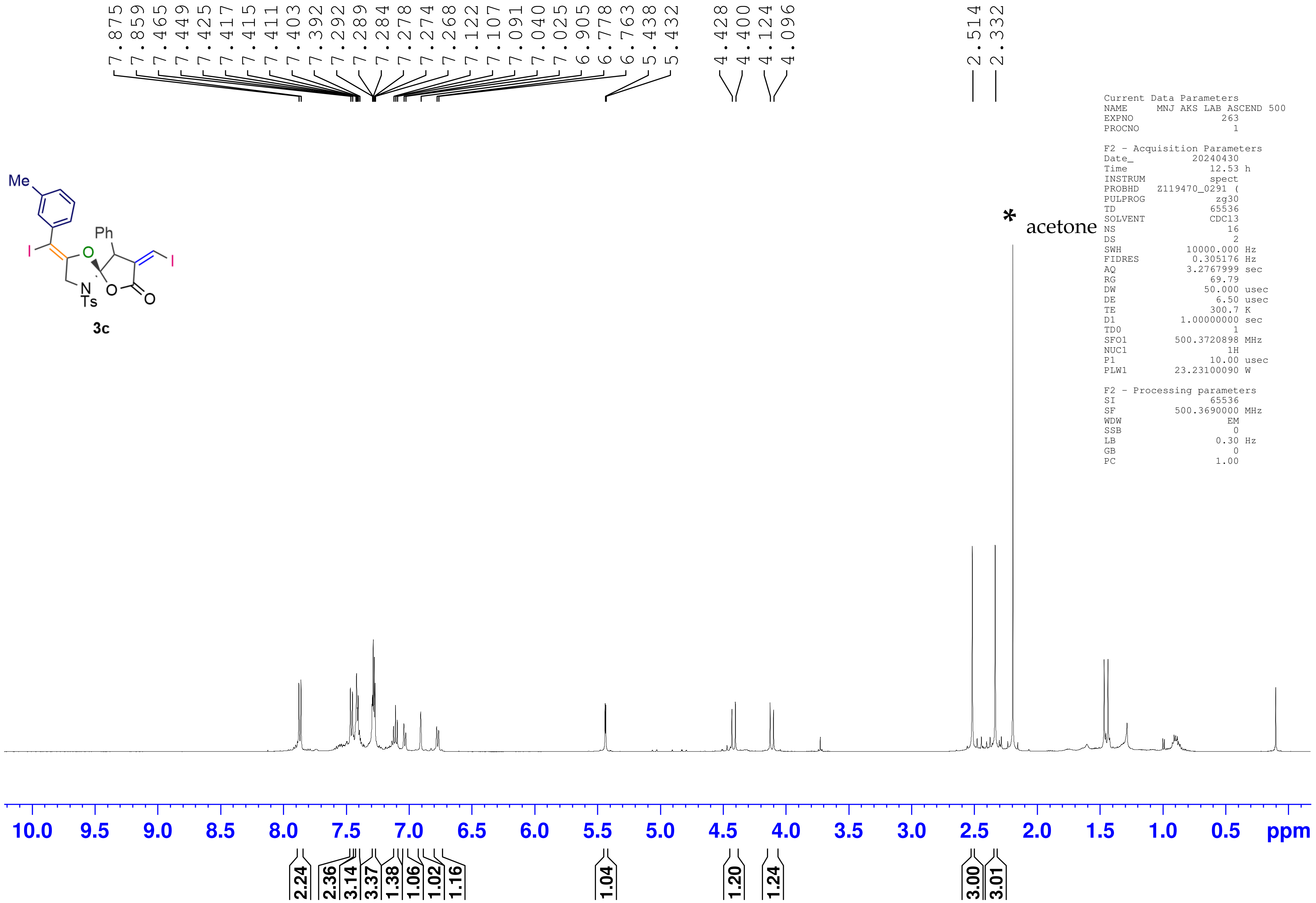


3b

```
Current Data Parameters
NAME     KS Updated 400n
EXPNO                136
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time               15.07 h
INSTRUM            spect
PROBHD   Z125331_0034 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2312
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                192.83
DW                16.800 usec
DE                  6.50 usec
TE                 315.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.8304669 MHz
NUC1                 13C
P1                 12.00 usec
PLW1        172.66999817 W
SFO2         500.3710015 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         12.18000031 W
PLW12         0.12180000 W
PLW13         0.06126500 W

F2 - Processing parameters
SI                 32768
SF           125.8178901 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```

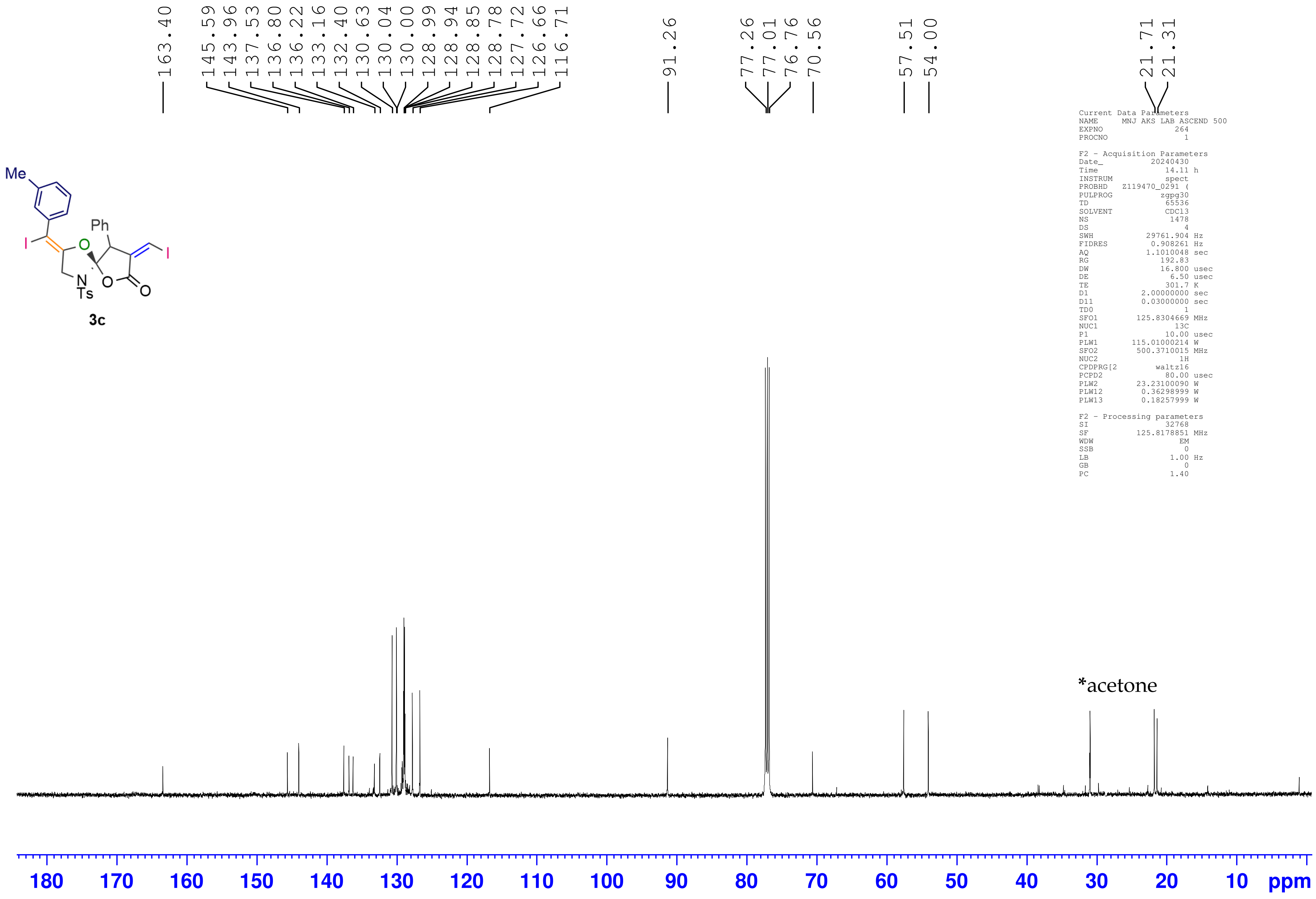


3c

```
Current Data Parameters
NAME     MNJ AKS LAB ASCEND 500
EXPNO                 263
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240430
Time                12.53 h
INSTRUM             spect
PROBHD   Z119470_0291 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES           0.305176 Hz
AQ              3.2767999 sec
RG                  69.79
DW                 50.000 usec
DE                   6.50 usec
TE                  300.7 K
D1         1.00000000 sec
TD0                     1
SFO1        500.3720898 MHz
NUC1                   1H
P1                  10.00 usec
PLW1         23.23100090 W

F2 - Processing parameters
SI                  65536
SF          500.3690000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

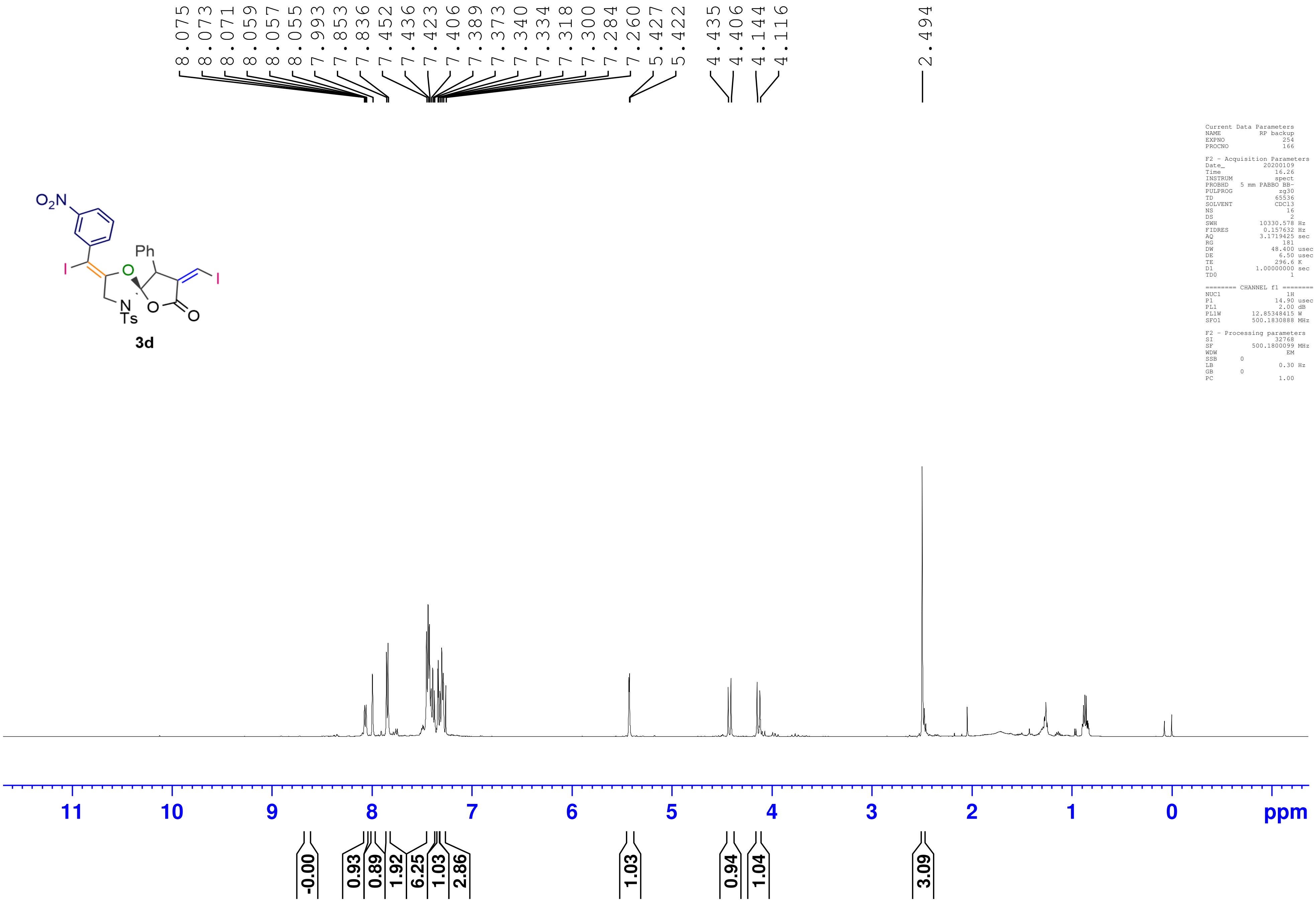


3c

```
Current Data Parameters
NAME      MNJ AKS LAB ASCEND 500
EXPNO                    264
PROCNO                     1

F2 - Acquisition Parameters
Date_              20240430
Time                  14.11 h
INSTRUM               spect
PROBHD    Z119470_0291 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1478
DS                        4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                1.1010048 sec
RG                   192.83
DW                   16.800 usec
DE                     6.50 usec
TE                    301.7 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1
SFO1            125.8304669 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           115.01000214 W
SFO2            500.3710015 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2            23.23100090 W
PLW12            0.36298999 W
PLW13            0.18257999 W

F2 - Processing parameters
SI                    32768
SF              125.8178851 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



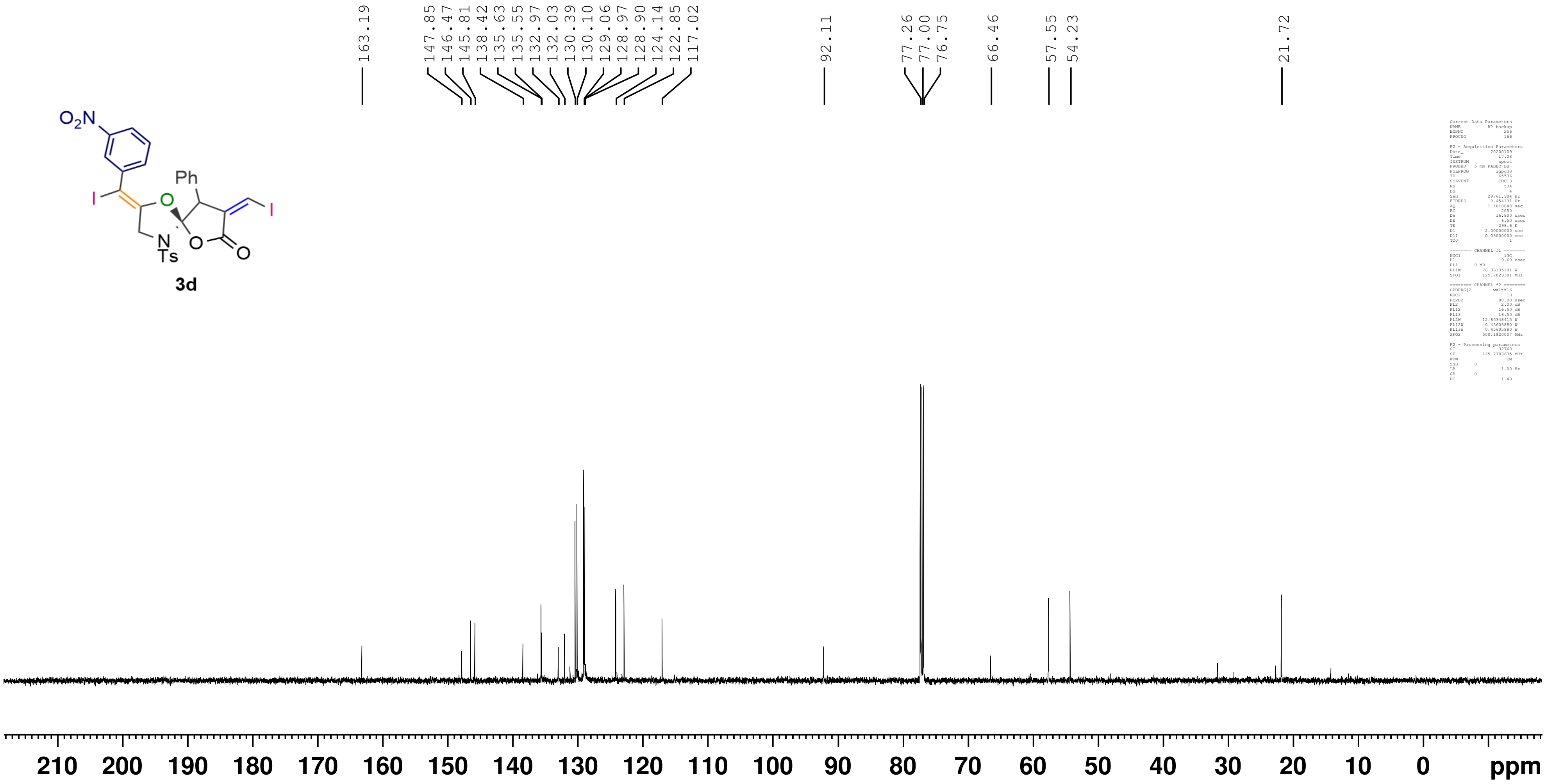
3d

```
Current Data Parameters
NAME          RP backup
EXPNO               254
PROCNO              166

F2 - Acquisition Parameters
Date_          20200109
Time              16.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH          10330.578 Hz
FIDRES        0.157632 Hz
AQ           3.1719425 sec
RG                  181
DW               48.400 usec
DE                 6.50 usec
TE                296.6 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.90 usec
PL1                2.00 dB
PL1W        12.85348415 W
SFO1        500.1830888 MHz

F2 - Processing parameters
SI                32768
SF          500.1800099 MHz
WDW                  EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```



3d

```
Current Data Parameters
NAME          RP backup
EXPNO               256
PROCNO              166

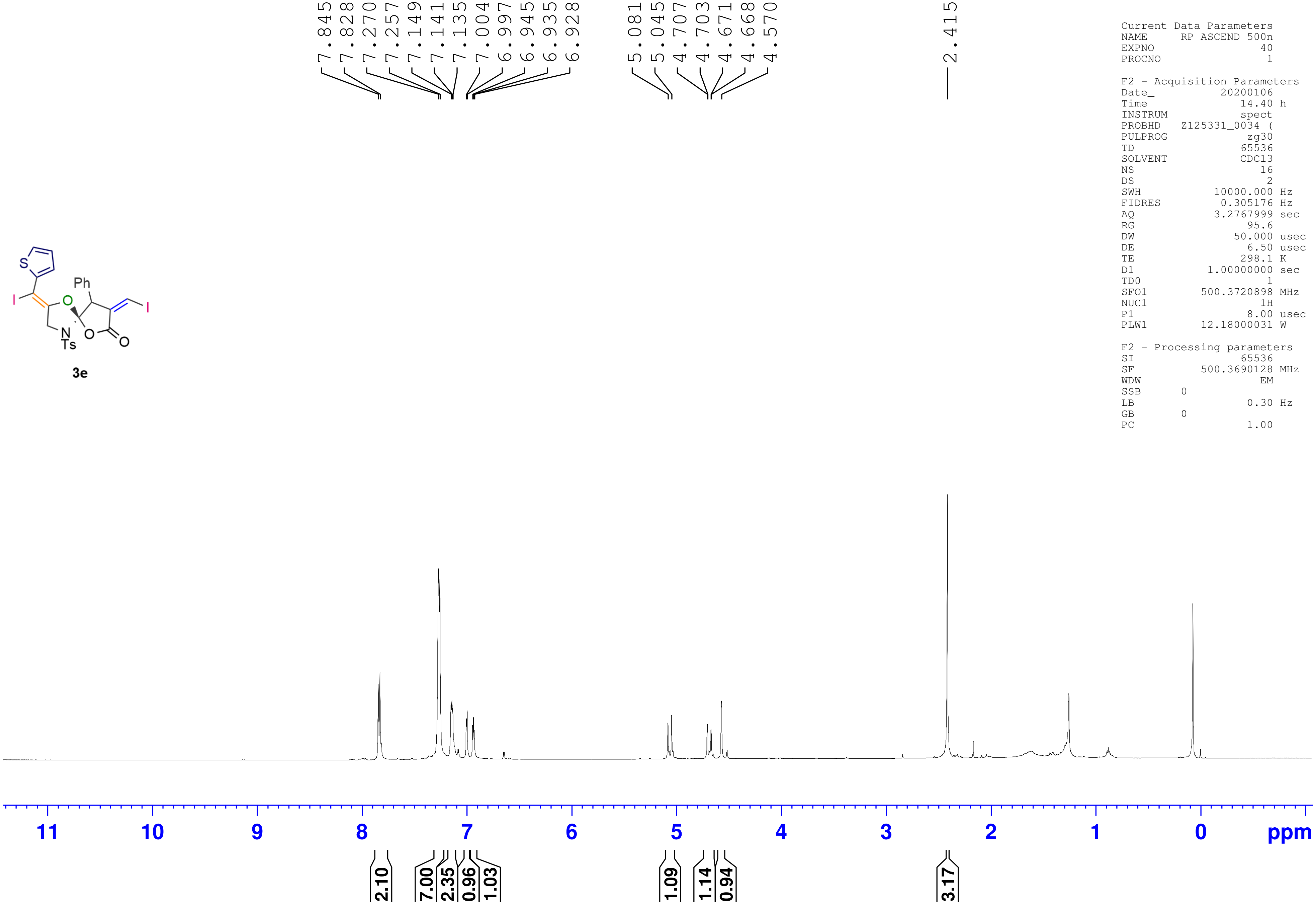
F2 - Acquisition Parameters
Date_          20200109
Time              17.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  534
DS                    4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG                 2050
DW               16.800 usec
DE                 6.50 usec
TE                298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.60 usec
PL1      0 dB
PL1W        76.36135101 W
SFO1        125.7829381 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.00 dB
PL12              16.50 dB
PL13              16.50 dB
PL2W        12.85348415 W
PL12W        0.45605880 W
PL13W        0.45605880 W
SFO2        500.1820007 MHz

F2 - Processing parameters
SI                32768
SF          125.7703635 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

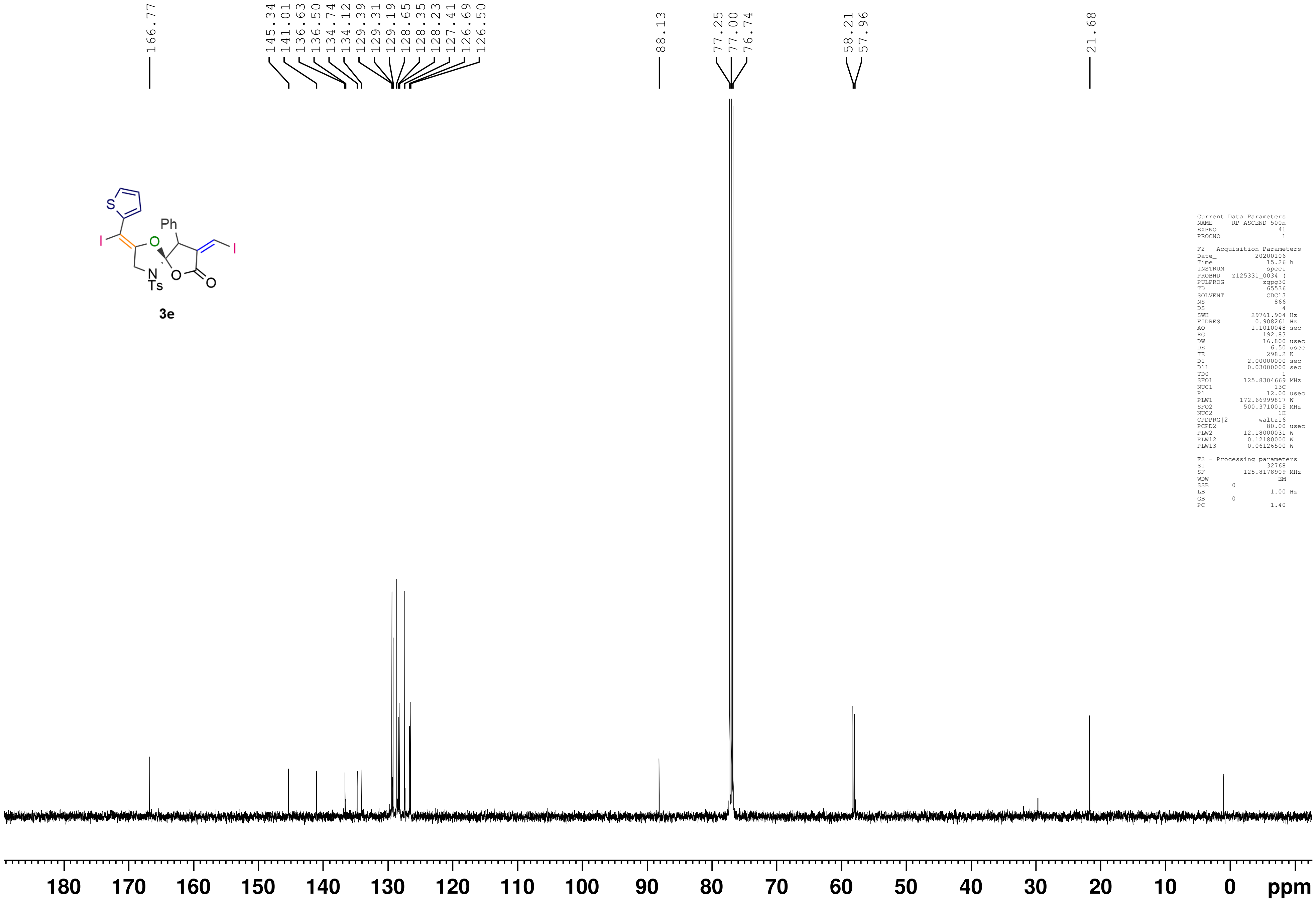
3e



```
Current Data Parameters
NAME     RP ASCEND 500n
EXPNO              40
PROCNO              1

F2 - Acquisition Parameters
Date_          20200106
Time              14.40 h
INSTRUM           spect
PROBHD   Z125331_0034 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            3.2767999 sec
RG                 95.6
DW               50.000 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                   1
SFO1        500.3720898 MHz
NUC1                 1H
P1                 8.00 usec
PLW1        12.18000031 W

F2 - Processing parameters
SI                65536
SF          500.3690128 MHz
WDW                  EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

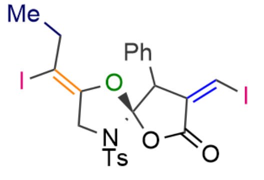


3e

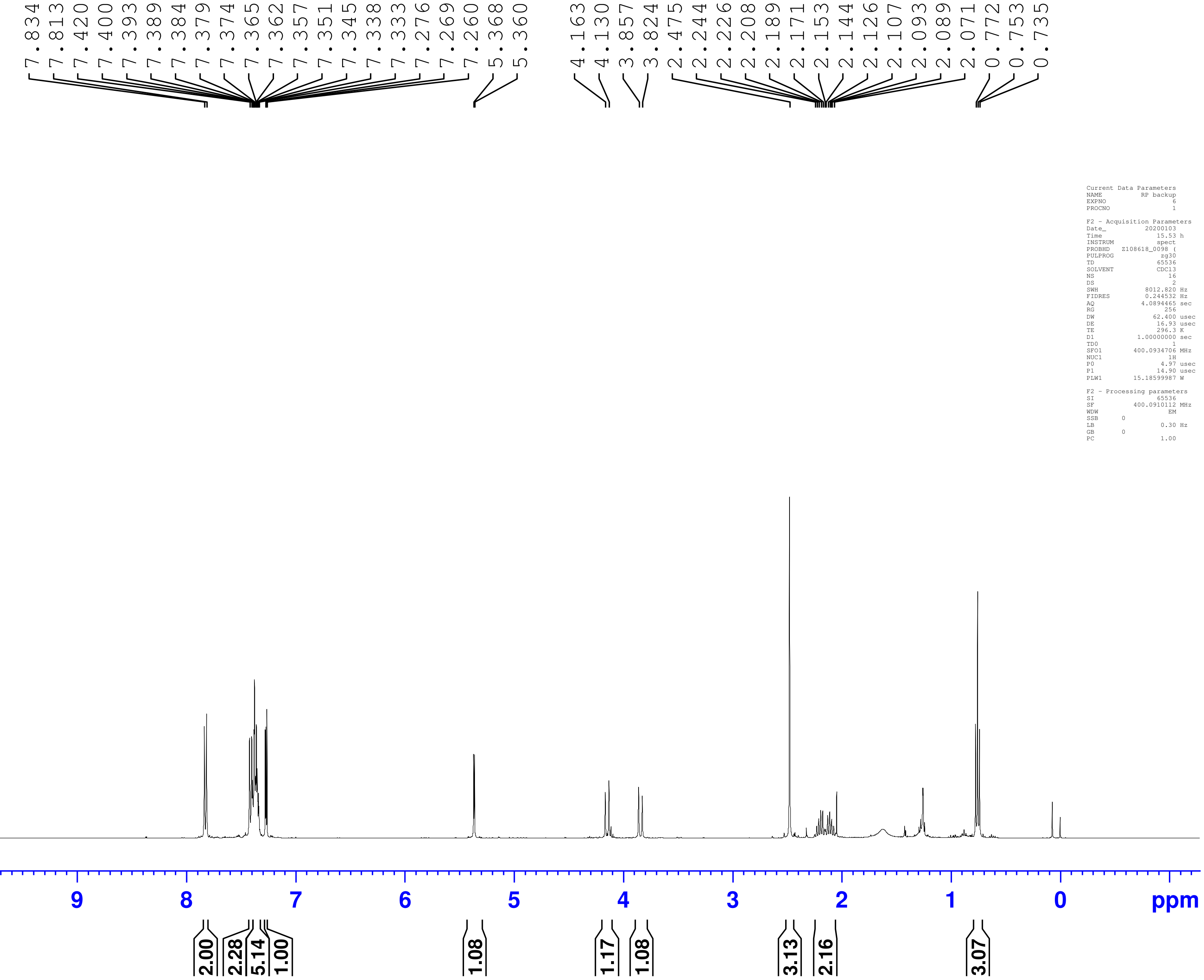
```
Current Data Parameters
NAME     RP ASCEND 500n
EXPNO                41
PROCNO                1

F2 - Acquisition Parameters
Date_          20200106
Time              15.26 h
INSTRUM           spect
PROBHD   Z125331_0034 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  866
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               192.83
DW               16.800 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.8304669 MHz
NUC1                13C
P1                12.00 usec
PLW1       172.66999817 W
SFO2        500.3710015 MHz
NUC2                 1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        12.18000031 W
PLW12        0.12180000 W
PLW13        0.06126500 W

F2 - Processing parameters
SI                32768
SF          125.8178909 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```



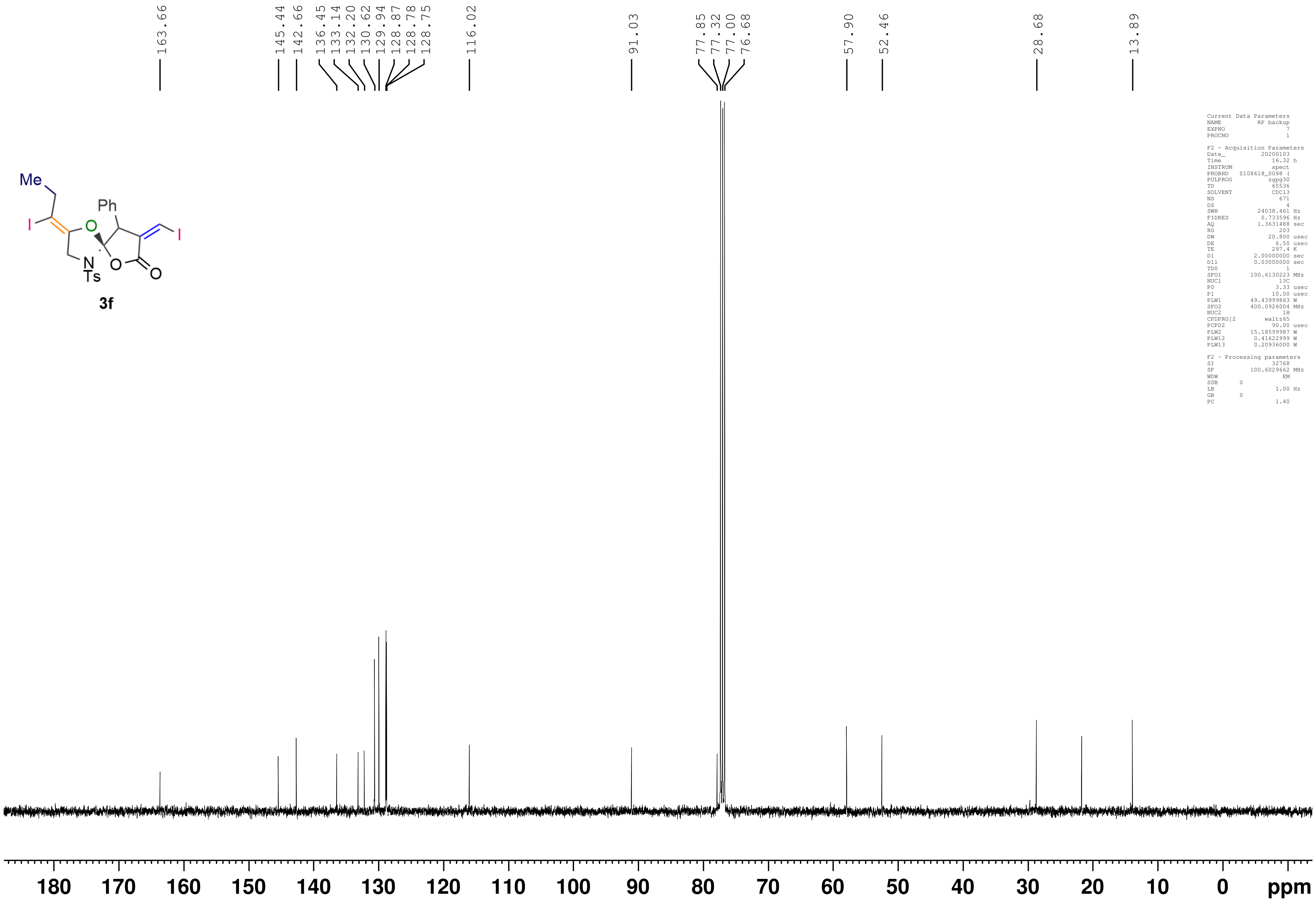
3f



```
Current Data Parameters
NAME             RP backup
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_             20200103
Time                 15.53 h
INSTRUM              spect
PROBHD   Z108618_0098 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ               4.0894465 sec
RG                     256
DW                  62.400 usec
DE                   16.93 usec
TE                   296.3 K
D1              1.00000000 sec
TD0                      1
SFO1           400.0934706 MHz
NUC1                    1H
P0                    4.97 usec
P1                   14.90 usec
PLW1           15.18599987 W

F2 - Processing parameters
SI                   65536
SF             400.0910112 MHz
WDW                     EM
SSB      0
LB                    0.30 Hz
GB       0
PC                    1.00
```

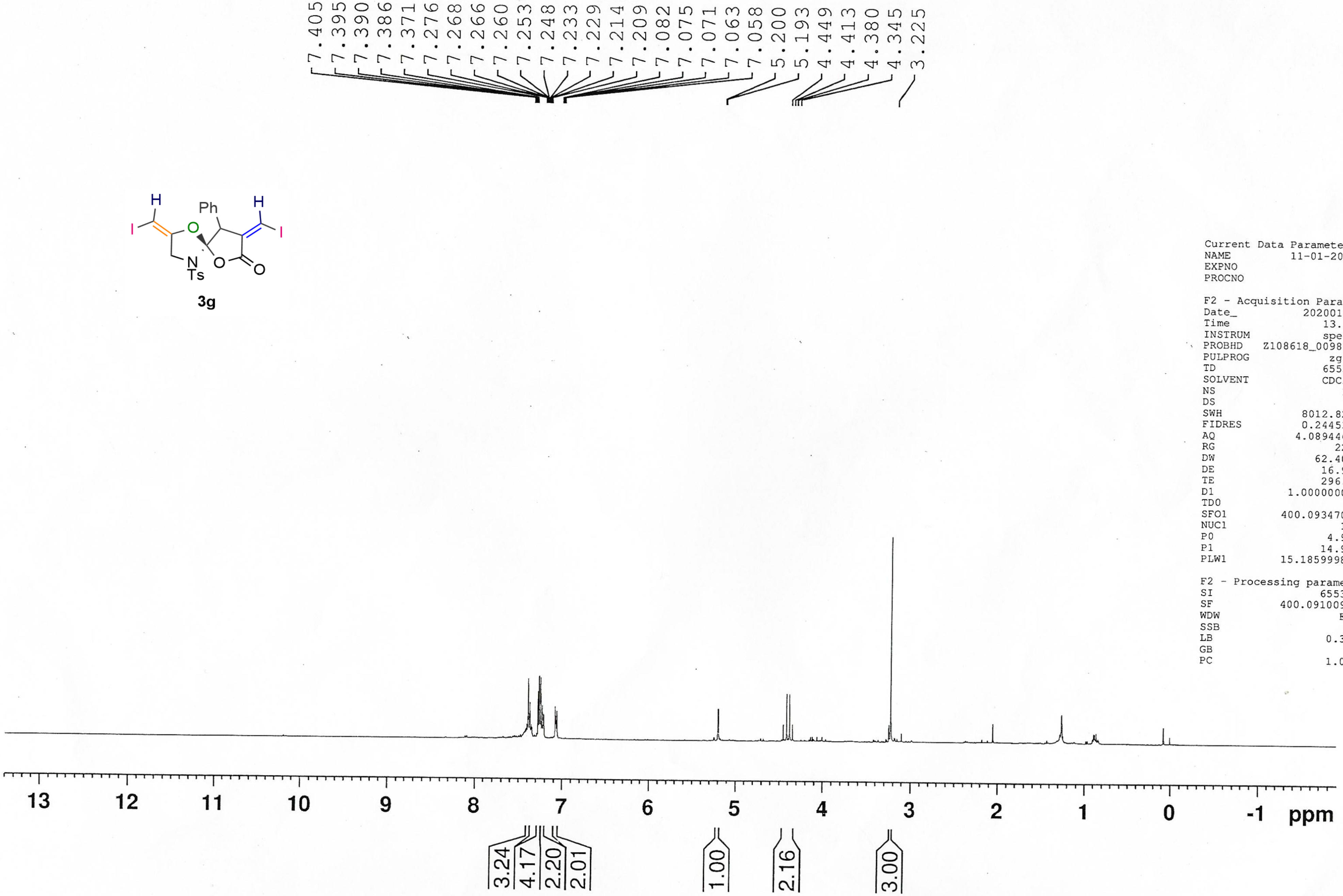


```
Current Data Parameters
NAME            RP backup
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_            20200103
Time                16.32 h
INSTRUM             spect
PROBHD   Z108618_0098 (
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    671
DS                      4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ              1.3631488 sec
RG                    203
DW                 20.800 usec
DE                   6.50 usec
TE                  297.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          100.6130223 MHz
NUC1                  13C
P0                   3.33 usec
P1                  10.00 usec
PLW1          49.43999863 W
SFO2          400.0926004 MHz
NUC2                   1H
CPDPRG[2         waltz65
PCPD2               90.00 usec
PLW2          15.18599987 W
PLW12          0.41622999 W
PLW13          0.20936000 W

F2 - Processing parameters
SI                  32768
SF            100.6029662 MHz
WDW                    EM
SSB      0
LB                   1.00 Hz
GB       0
PC                   1.40
```

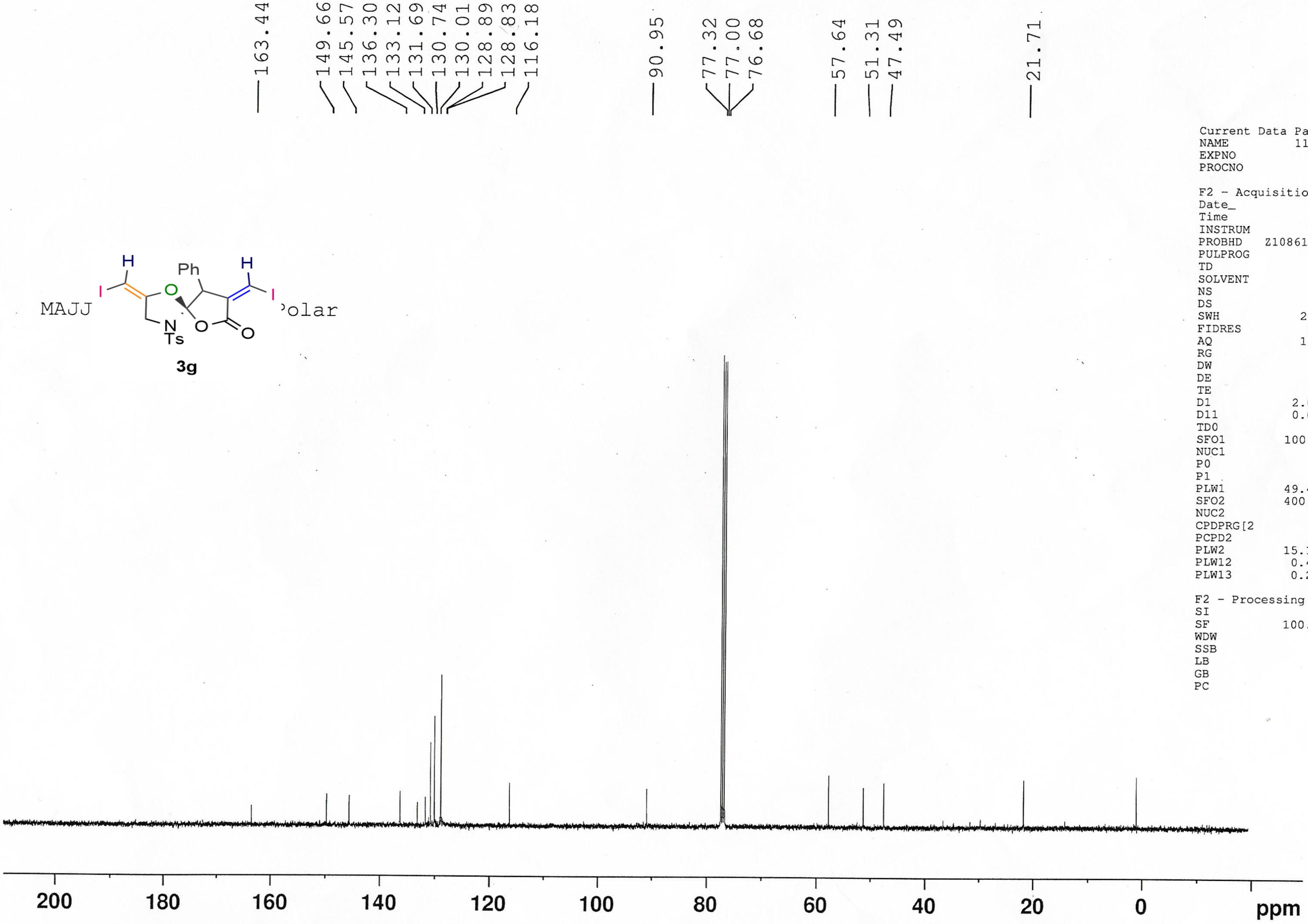
3g



```
Current Data Parameters
NAME              11-01-2020
EXPNO                      6
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200111
Time                 13.47 h
INSTRUM                spect
PROBHD       Z108618_0098 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                 4.0894465 sec
RG                       228
DW                    62.400 usec
DE                     16.93 usec
TE                     296.7 K
D1                1.00000000 sec
TD0                        1
SFO1             400.0934706 MHz
NUC1                      1H
P0                      4.97 usec
P1                     14.90 usec
PLW1             15.18599987 W

F2 - Processing parameters
SI                     65536
SF               400.0910091 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



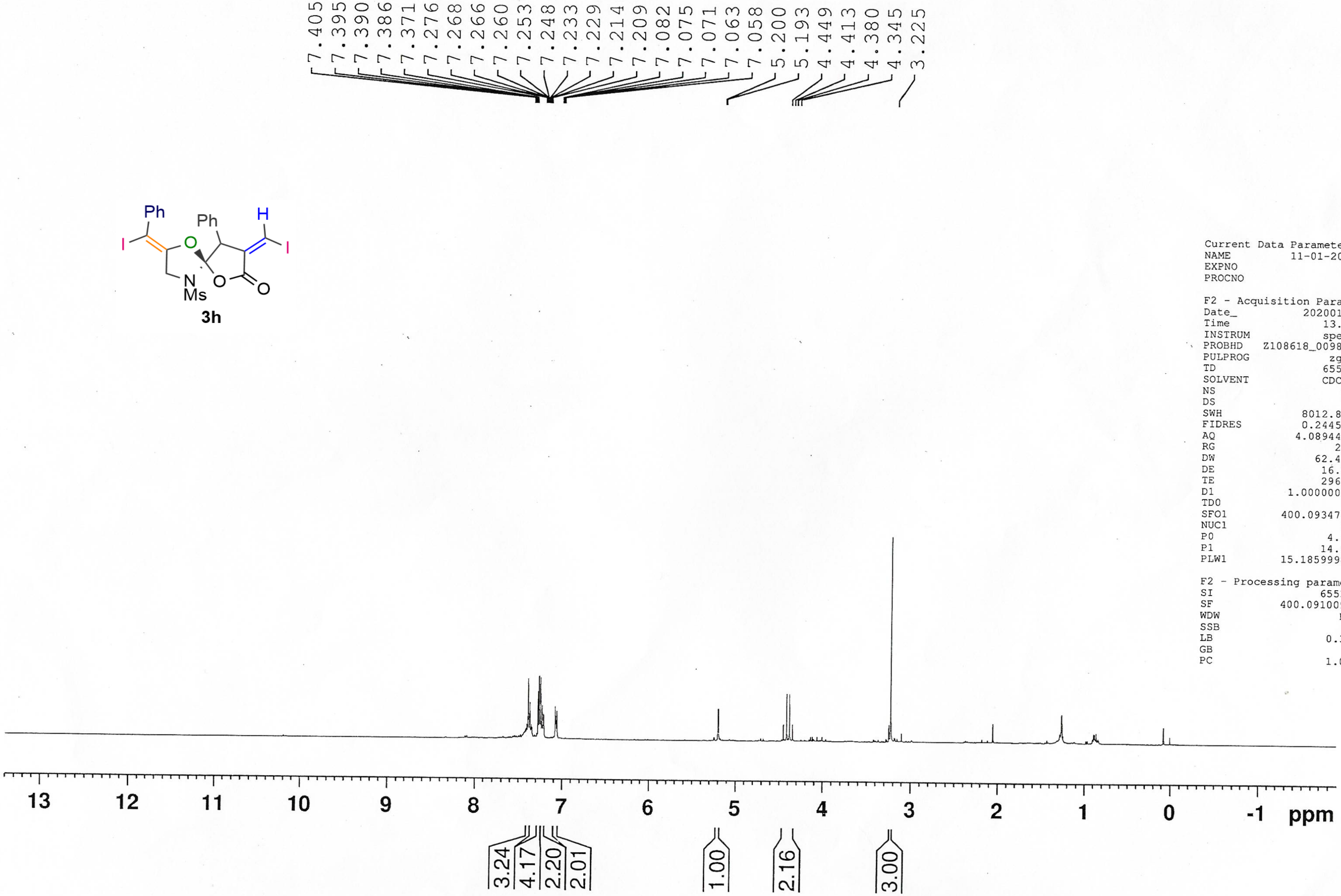
MAJJ Polar

3g

```
Current Data Parameters
NAME            11-01-2020
EXPNO                   16
PROCNO                   1

F2 - Acquisition Parameters
Date_             20200111
Time                 12.27 h
INSTRUM              spect
PROBHD     Z108618_0098 (
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     521
DS                       4
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ               1.3631488 sec
RG                     203
DW                  20.800 usec
DE                    6.50 usec
TE                   298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           100.6130223 MHz
NUC1                   13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           49.43999863 W
SFO2           400.0926004 MHz
NUC2                    1H
CPDPRG[2           waltz65
PCPD2                90.00 usec
PLW2           15.18599987 W
PLW12           0.41622999 W
PLW13           0.20936000 W

F2 - Processing parameters
SI                   32768
SF             100.6029654 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

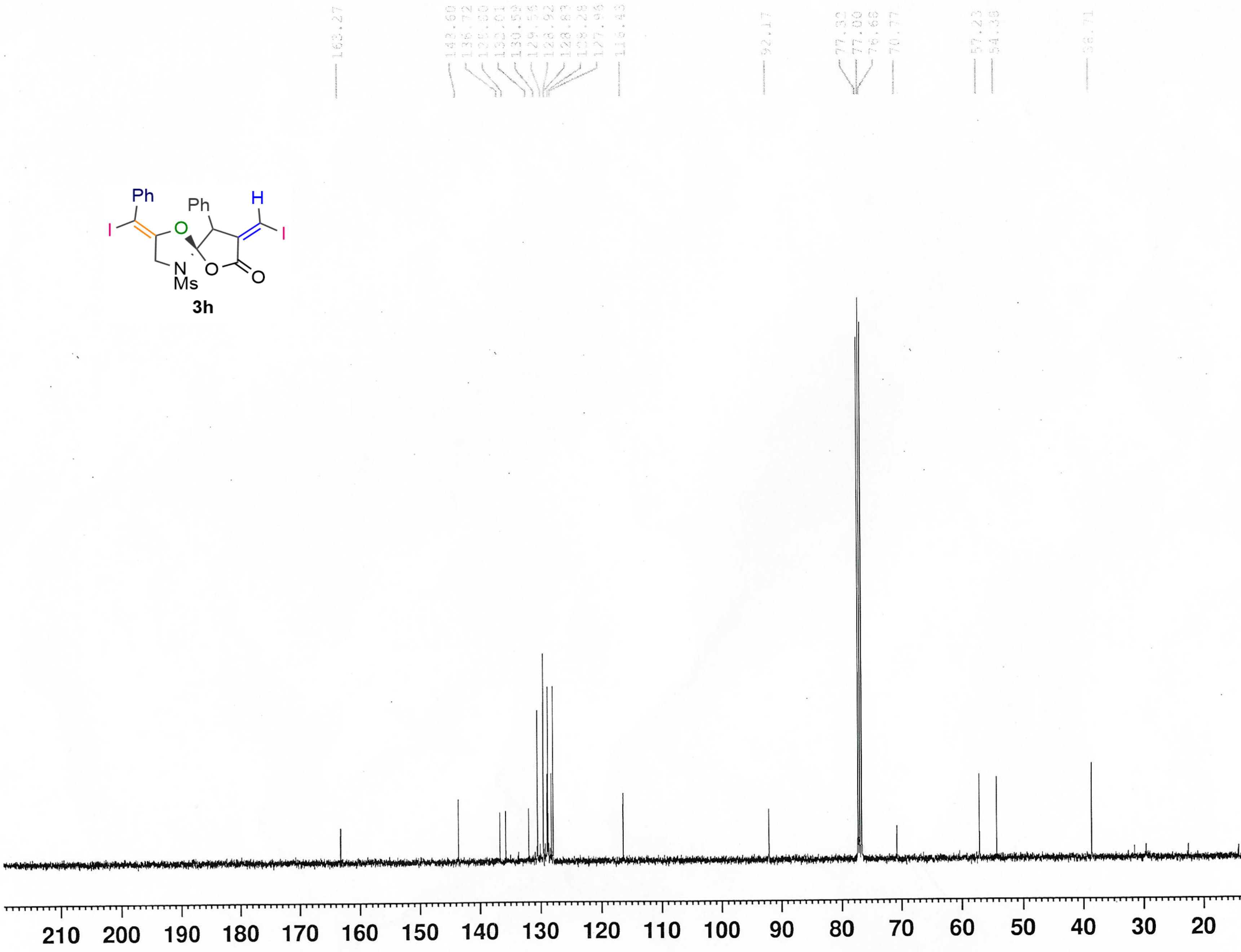


3h

Current Data Parameters
NAME 11-01-2020
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200111
Time 13.47 h
INSTRUM spect
PROBHD Z108618_0098 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 228
DW 62.400 usec
DE 16.93 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.0934706 MHz
NUC1 1H
P0 4.97 usec
P1 14.90 usec
PLW1 15.18599987 W

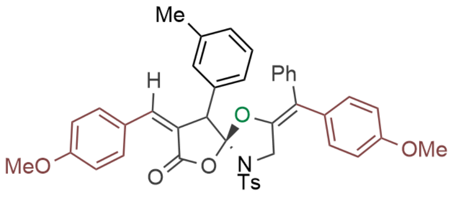
F2 - Processing parameters
SI 65536
SF 400.0910091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



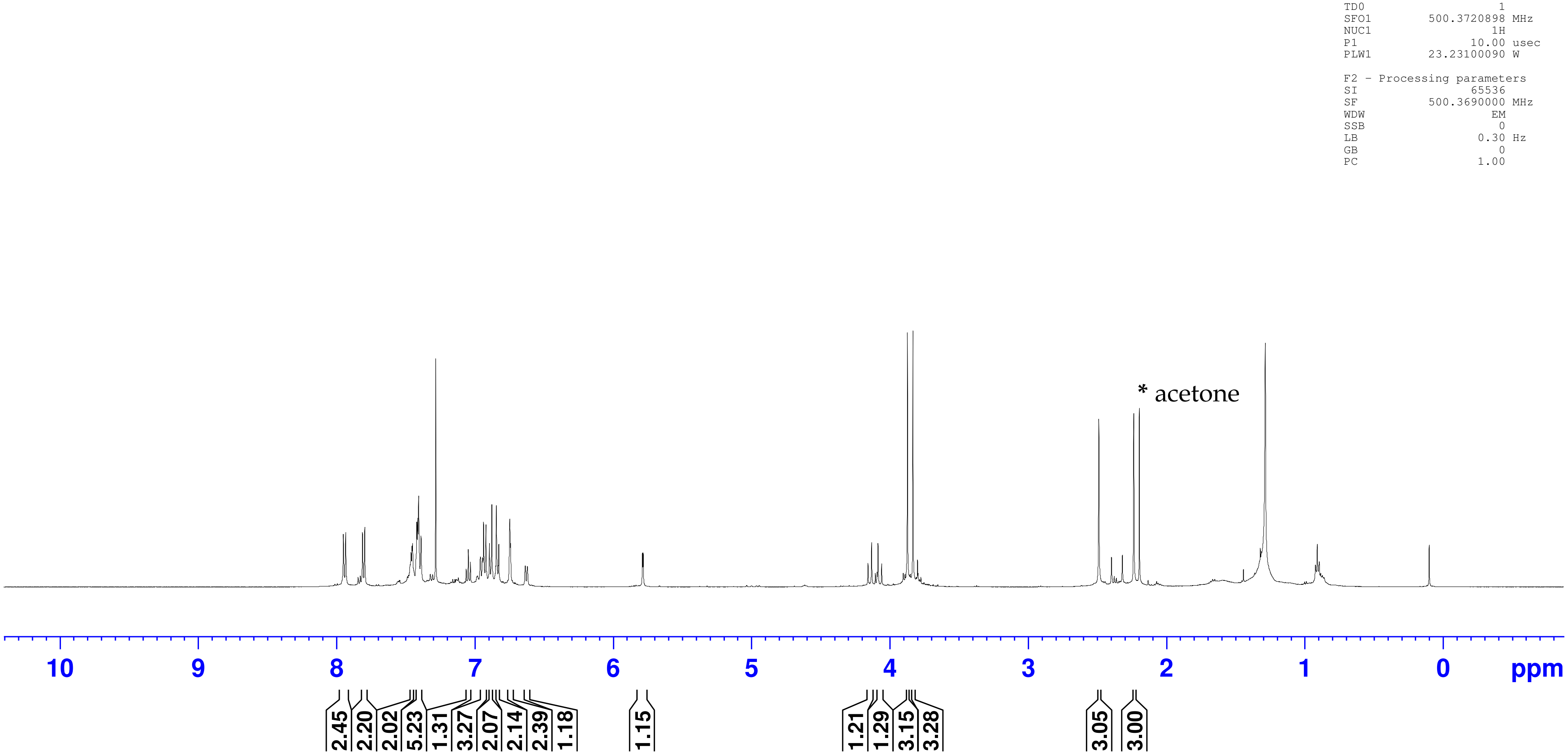
```
Current Data Parameters
NAME              11-01-2020
EXPNO                      7
PROCNO                     1

F2 - Acquisition Parameters
Date_               20200111
Time                 14.14 h
INSTRUM                spect
PROBHD   Z108618_0098 (
PULPROG              zgpg30
TD                    65536
SOLVENT                CDCl3
NS                      460
DS                        4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                1.3631488 sec
RG                      203
DW                   20.800 usec
DE                     6.50 usec
TE                    297.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1
SFO1            100.6130223 MHz
NUC1                    13C
P0                     3.33 usec
P1                    10.00 usec
PLW1            49.43999863 W
SFO2            400.0926004 MHz
NUC2                     1H
CPDPRG[2            waltz65
PCPD2                 90.00 usec
PLW2            15.18599987 W
PLW12            0.41622999 W
PLW13            0.20936000 W

F2 - Processing parameters
SI                    32768
SF              100.6029658 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



5

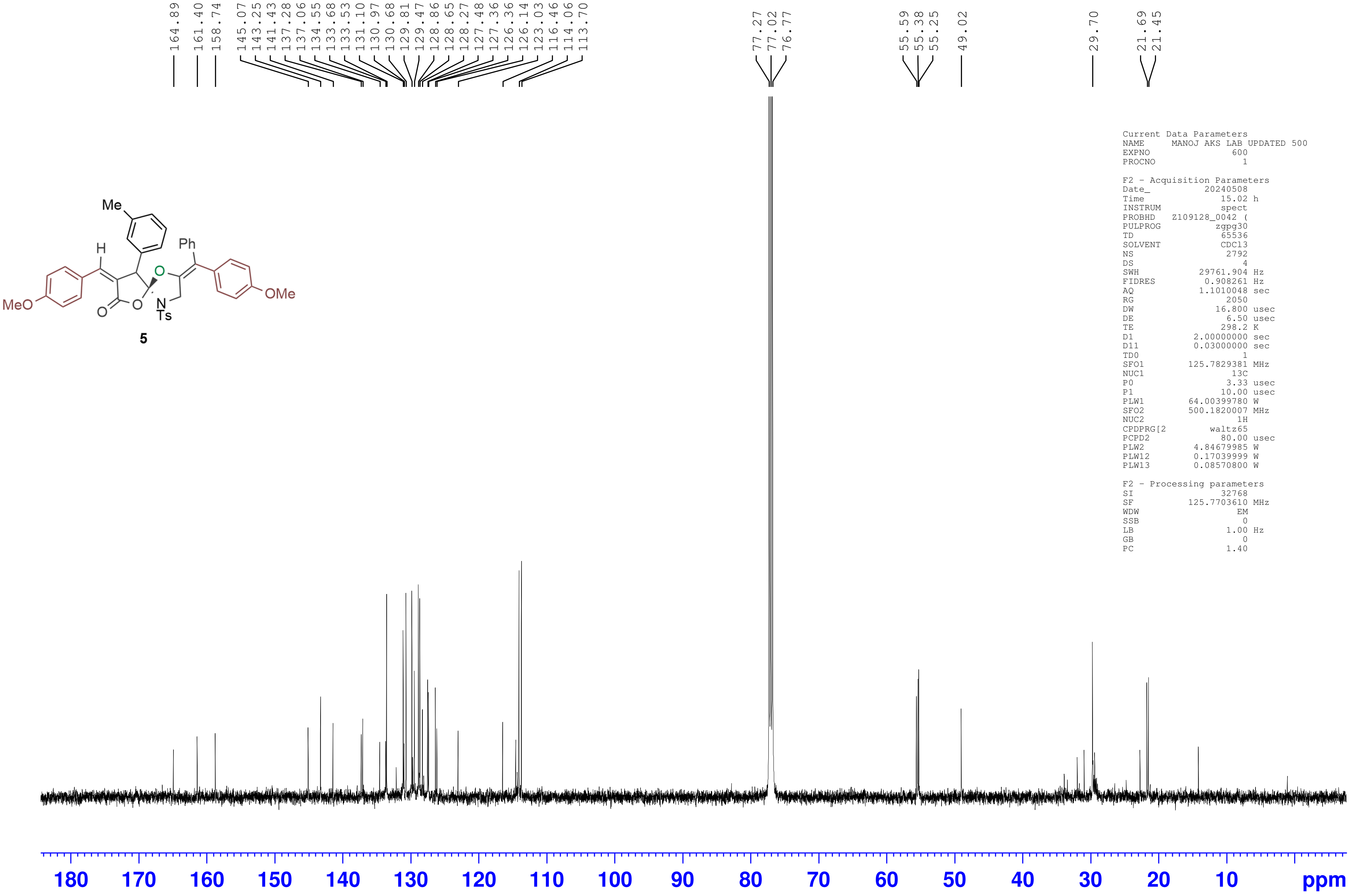


```
Current Data Parameters
NAME     Aradhana Ascend 500
EXPNO                  288
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240507
Time                 16.14 h
INSTRUM              spect
PROBHD   Z119470_0291 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES            0.305176 Hz
AQ               3.2767999 sec
RG                   87.13
DW                  50.000 usec
DE                    6.50 usec
TE                   300.9 K
D1              1.00000000 sec
TD0                      1
SFO1           500.3720898 MHz
NUC1                    1H
P1                   10.00 usec
PLW1           23.23100090 W

F2 - Processing parameters
SI                   65536
SF             500.3690000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

5



```
Current Data Parameters
NAME     MANOJ AKS LAB UPDATED 500
EXPNO                 600
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240508
Time                15.02 h
INSTRUM              spect
PROBHD   Z109128_0042 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2792
DS                      4
SWH             29761.904 Hz
FIDRES           0.908261 Hz
AQ              1.1010048 sec
RG                   2050
DW                 16.800 usec
DE                   6.50 usec
TE                  298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          125.7829381 MHz
NUC1                  13C
P0                   3.33 usec
P1                  10.00 usec
PLW1          64.00399780 W
SFO2          500.1820007 MHz
NUC2                   1H
CPDPRG[2           waltz65
PCPD2               80.00 usec
PLW2           4.84679985 W
PLW12          0.17039999 W
PLW13          0.08570800 W

F2 - Processing parameters
SI                  32768
SF            125.7703610 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```