

## **A retro-Mannich mediated transformation of Morita–Baylis–Hillman ketones to saturated imidazo[1,2-*a*]pyridines**

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### **SUPPORTING INFORMATION**

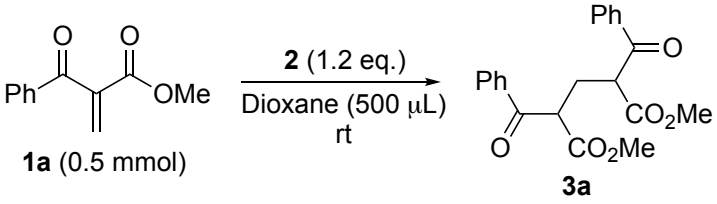
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## I. Control experiments for the degradative dimerisation of acyclic MBH Ketones

The control experiments carried out to study the mechanism of the degradative dimerisation of acyclic MBH Ketones in our previous communication<sup>1</sup> are reproduced as such below (**Table S1**) for reference.

**Table S1.** Control experiments – degradative dimerisation of acyclic MBH ketones (Note: compound numbers are reproduced from the published article in reference<sup>1</sup>)



Entry	2	H <sub>2</sub> O (µL)	Time (min)	Yield (%)
1	<sup>n</sup> PrNH <sub>2</sub> ( <b>2d</b> )	-	90	- <sup>a</sup>
2	Me <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> NMe <sub>2</sub> ( <b>2e</b> )	-	120	- <sup>b</sup>
3	Me <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> ( <b>2f</b> )	-	30	60
4	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>4</sub> NH <sub>2</sub> ( <b>2g</b> )	-	120	65
5 <sup>c</sup>	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> ( <b>2c</b> )	-	0.5	56 (33)
6 <sup>d,e</sup>	<b>2c</b> <sup>f</sup>	-	15	70
7 <sup>d,e</sup>	<b>2c</b> <sup>f,g</sup>	-	15	53
8 <sup>e</sup>	<b>2c</b> <sup>f</sup>	10	15	74
9 <sup>e</sup>	<b>2c</b> <sup>f</sup>	25	15	84

<sup>a</sup>Complex <sup>1</sup>H NMR spectrum of an isolated product. <sup>b</sup>Complex reaction mixture. <sup>c</sup>CHCl<sub>3</sub> was used as the solvent; the figure in parenthesis represents the yield of methyl 3-oxo-3-phenylpropanoate isolated from this reaction. <sup>d</sup>Reaction was carried out under inert conditions. <sup>e</sup>Anhydrous dioxane was used. <sup>f</sup>Anhydrous **2c** was used. <sup>g</sup>0.5 eq. of **2c** was used.

- The above experiments clearly revealed the requirement of both the amino groups for a successful reaction. The importance of the 2<sup>nd</sup> amino group in providing the ‘trigger’ for the transformation is corroborated by the failed attempt in its absence, as also by the decreased efficiency when its proximity is compromised.
- The reactions under moisture-free conditions and in the presence of added water were indicative of the significance of water in accelerating the transformation.
- Based on the control experiments and the above aspects, a mechanistic pathway for the reaction had been proposed in our earlier communication (*also depicted in the main text of the present manuscript*).

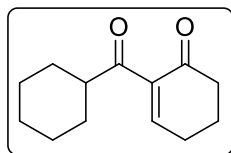
## II. Synthesis of MBH ketones:

The MBH ketones used in this work were synthesized from the corresponding MBH adducts using a literature protocol.<sup>2</sup>

The MBH ketone **4a** utilized in this work is reported in the literature.<sup>3</sup>

The data for the MBH ketone **4s** is tabulated below.

### 2-(cyclohexanecarbonyl)cyclohex-2-en-1-one (4s):

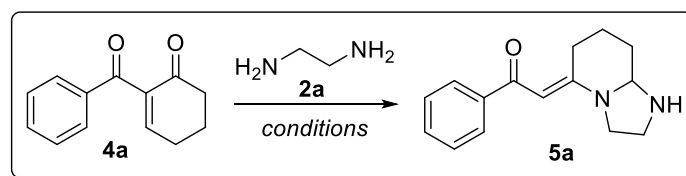


Synthesised from 1 mmol (208 mg) of the precursor MBH adduct; yield: 202 mg (98%); pale yellow oil.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz):  $\delta$  7.42 (t, 1H,  $J = 4.5$  Hz), 3.09-3.01 (m, 1H), 2.53-2.45 (m, 4H), 2.04 (p, 2H,  $J = 6.5$  Hz), 1.85-1.79 (m, 2H), 1.77-1.69 (m, 2H), 1.68-1.61 (m, 1H), 1.35-1.25 (m, 5H).  $^{13}\text{C}$   $\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 125 MHz):  $\delta$  205.3, 196.8, 154.5, 140.6, 48.9, 38.8, 28.5, 26.3, 26.0, 25.7, 22.3. HRMS (ESI-TOF):  $m/z$   $[\text{M} + \text{Na}]^+$  calculated for  $\text{C}_{13}\text{H}_{18}\text{O}_2\text{Na}$ : 229.1199; found: 229.1189.

### III. Optimisation studies on the synthesis of 5-alkylidene octahydroimidazo[1,2-*a*]pyridines from MBH Ketones

The first experiment in the study was a reaction of the MBH ketone **4a** with the diamine **2a** to yield the imidazopyridine **5a** (Table S2, Scheme). A brief optimisation study was carried out on the reaction, the details of which are collated in Table S2 below.

**Table S2.** Optimisation of the conditions for the conversion of **4a** to **5a**<sup>a</sup>



entry	<b>2a</b> , equiv	solvent [500 $\mu\text{L}$ ]	time [min]	additive [equiv]	<b>5a</b> / yield (%) <sup>b</sup>
1	1.2	dioxane	45	-	45
2	2.0	dioxane	10	-	51
3	5.0	dioxane	20	-	51
4	2.0	$\text{CH}_3\text{CN}$	10	-	65
5	2.0	$\text{CH}_3\text{CN}$	5	$\text{In}(\text{OTf})_3$ , 20 mol%	48
6	2.0	$\text{CH}_3\text{CN}$	5	$\text{Ca}(\text{OTf})_2$ (20 mol%)	43

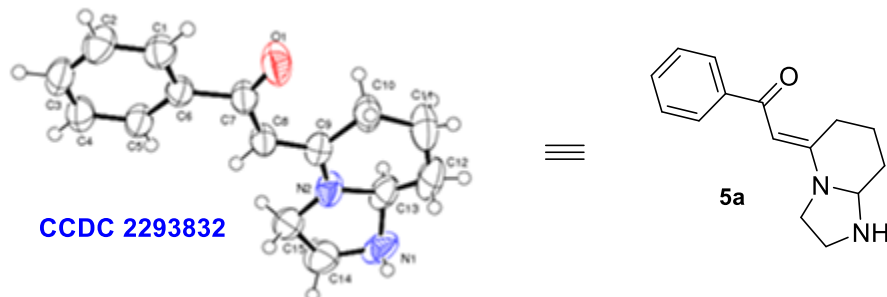
<sup>a</sup>All reactions were carried out on 0.5 mmol of **4a** at room temperature. <sup>b</sup>Refers to isolated yield after column chromatographic purification.

Our studies started with the reaction of MBH ketone **4a**, derived from cyclohex-2-en-1-one, with 1.2 equiv of ethylenediamine (**2a**) using dioxane as a solvent; to our delight, the reaction produced the product **5a**, but in modest yield (Table S2, entry 1). Increasing the equiv of ethylenediamine resulted in only marginally better yields of **5a** (entries 2 & 3). The use of  $\text{CH}_3\text{CN}$  as the solvent resulted in a more efficient reaction and afforded **5a** in 65% yield (entry 4). Further, the reaction was also carried out using Lewis acid additives in an attempt to enhance the yield; however, to our disappointment, the additives had a determinantal impact on the reaction efficiency (entries 5 & 6). Eventually, we switched to a one-pot

protocol that involved a direct conversion of MBH adducts to the corresponding heterocycles, the details of which are described in the manuscript.

#### IV. X-ray crystal structure of 5a

The colourless crystal for single crystal X-ray analysis was grown in toluene.



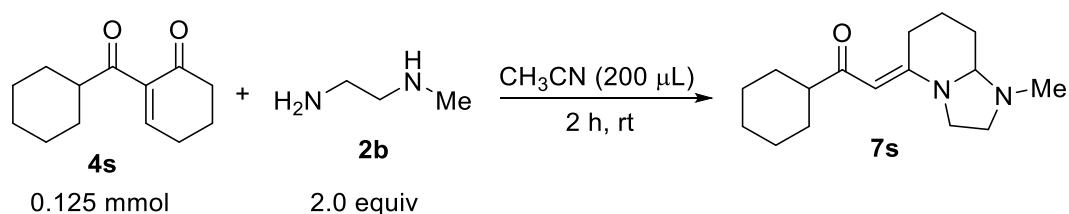
#### Crystal data and structure refinement for 5a

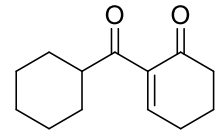
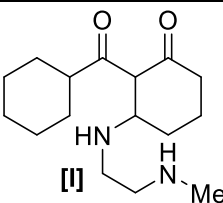
Identification code (CCDC Number)	2293832
Empirical formula	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O
Formula weight	242.31
Temperature	297(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	
a = 7.7284(5) Å	α = 77.928(2)°.
b = 7.7936(5) Å	β = 71.564(2)°.
c = 11.5229(8) Å	γ = 85.819(2)°.
Volume	643.85(7) Å <sup>3</sup>
Z	2
Density (calculated)	1.250 Mg/m <sup>3</sup>
Absorption coefficient	0.079 mm <sup>-1</sup>
F(000)	260
Crystal size	0.150 x 0.150 x 0.100 mm <sup>3</sup>
Theta range for data collection	2.778 to 24.999°.
Index ranges	-9 ≤ h ≤ 9, -9 ≤ k ≤ 9, -13 ≤ l ≤ 13
Reflections collected	27882
Independent reflections	2267 [R(int) = 0.0675]

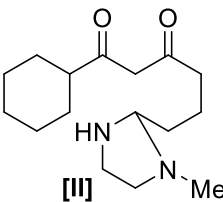
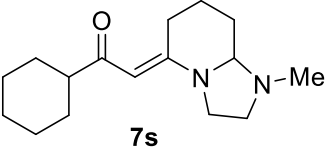
Completeness to theta = 24.999°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5029
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2267 / 72 / 197
Goodness-of-fit on F <sup>2</sup>	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1465
R indices (all data)	R1 = 0.0730, wR2 = 0.1676
Extinction coefficient	n/a
Largest diff. peak and hole	0.199 and -0.223 e.Å <sup>-3</sup>

## V. Monitoring the progress of reaction by LC-MS

A reaction of MBH ketone **4s**, derived from cyclohexane carbaldehyde, was set up with the diamine **2b** to yield the imidazopyridine **7s** under the conditions given in the Scheme below. The reaction was monitored at regular intervals by LC-HRMS (*Conditions*: Eclipse C8 column [0.1% formic acid in water/ Acetonitrile = 1:1; flow rate of 0.1 mL/min]), in an attempt to observe the intermediates **I** and **II** corresponding to the proposed mechanistic pathway (structures given in the Table below), and the eventual conversion to the saturated imidazopyridine.



Compounds	Retention time (approx.) on LC analysis (min)	m/z
 <b>4s</b>	5.4	206.1307
 [ <b>I</b> ]	-	280.2151

 <p><b>II</b></p>	-	280.2151
 <p><b>7s</b></p>	1.7	262.2045

- At the outset, the LC retention times of the starting MBH ketone **4s** (~5.4 min) and the heterocyclic product **7s** (~1.7 min) were clearly determined with the help of mass spectral correlation.
- The MBH ketone reacted quite rapidly upon the interaction with diamine **2b**; just 1 min after the addition of **2b**, nearly 50% conversion to the product **7s** could be observed using the LC-MS.
- Two minor peaks were also observed with retention times of ~3.3 min and ~4.5 min. Neither of these peaks exhibited a mass signal corresponding the expected  $m/z$  of 280 of the intermediates **I** and **II**.
- Interestingly, the above two peaks were observed with nearly similar intensity (5-7%) almost throughout the duration of the reaction, and started disappearing towards the end of the reaction. Although a mass signal of  $m/z$  263 – corresponding to the  $m/z$  of the final product itself, could be observed for both these peaks, they could not be assigned to either of the intermediates **I** or **II** unambiguously.
- Lastly, over time, the intensity of the peak at ~5.4 min corresponding to MBH Ketone **4s** gradually fades away, whereas the intensity of the peak at ~1.7 min corresponding to that of the product **7s** shows a ~92% conversion after 2 h of the reaction.

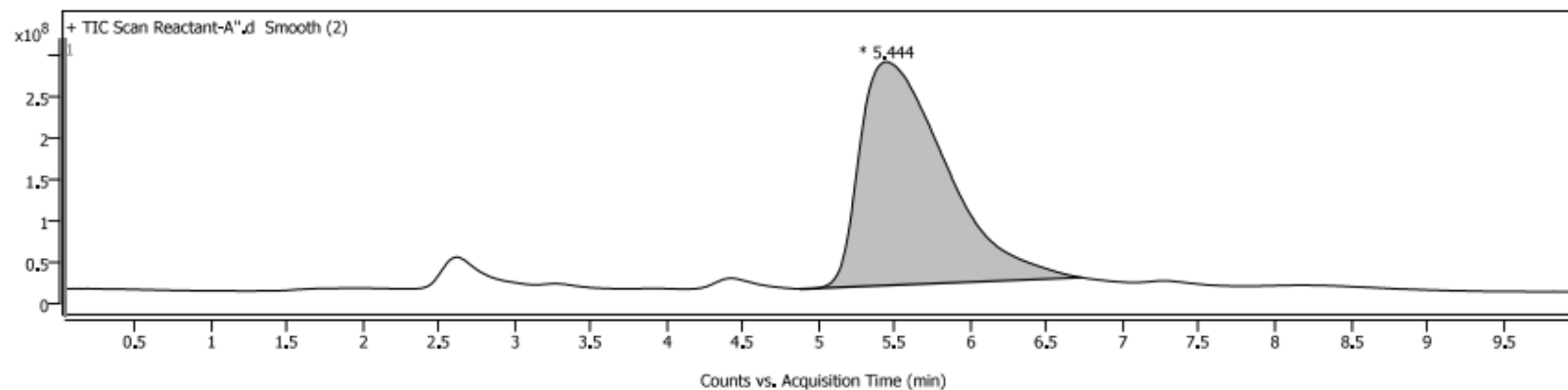
The entire study including the chromatograms along with the corresponding mass spectral analysis are reproduced below for reference. For convenience, the mass scans for the minor peaks at ~3.3 min and ~4.5 min are provided only for the “After 1 min” chromatogram.

## Chromatograms and Mass Spectral analysis

Chromatograms and MS analysis of samples of the substrate and the product:

### MBH Ketone 4s

#### Sample Chromatograms



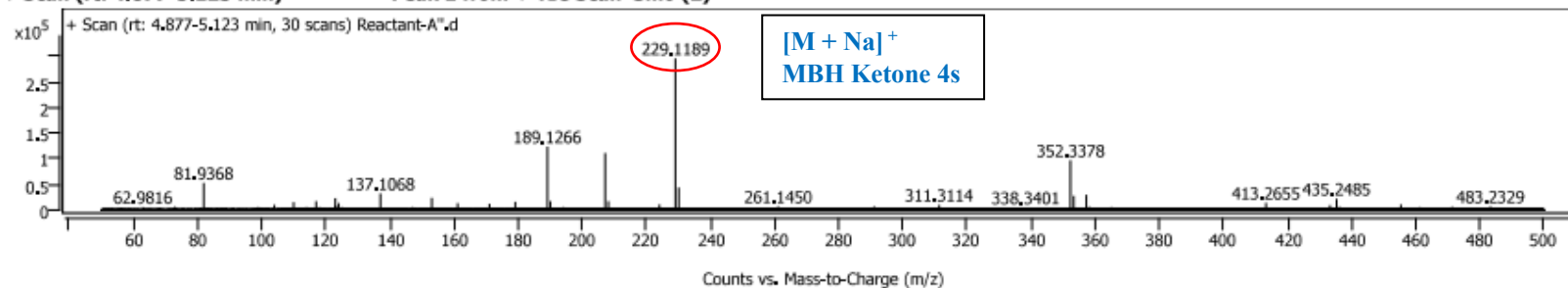
Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	4.877	5.444	6.731	269782961	10649910620	100.00	

#### Sample Spectra

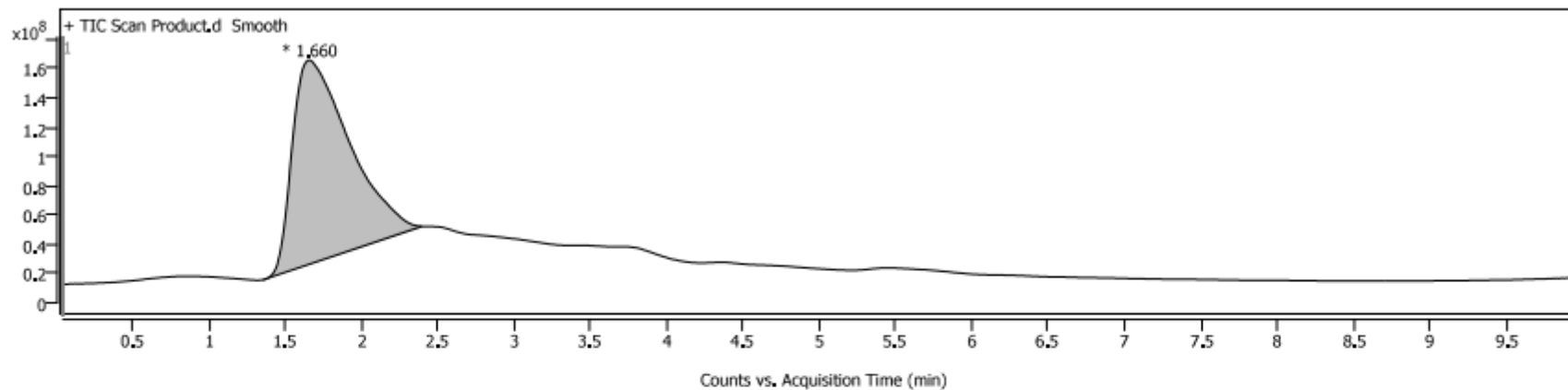
+ Scan (rt: 4.877-5.123 min)

Peak 1 from + TIC Scan Smo (2)



## Saturated Imidazopyridine 7s

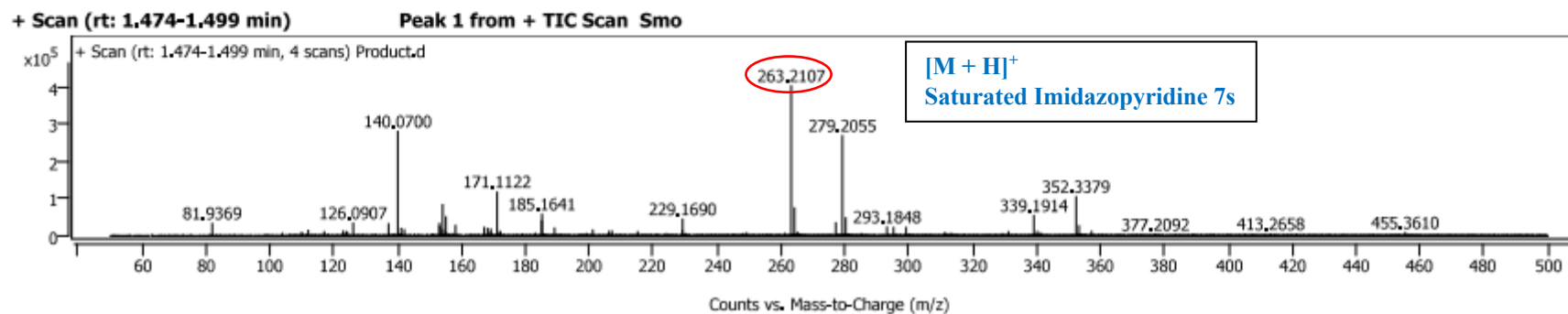
### Sample Chromatograms



Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.355	1.660	2.396	139235841	3618442909	100.00	

### Sample Spectra

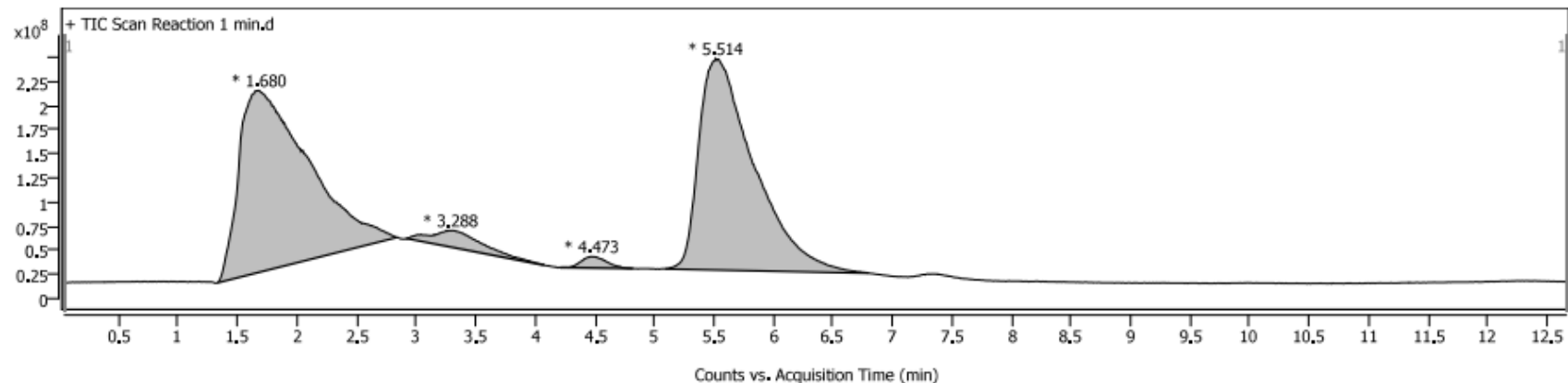




Chromatograms and MS analysis of samples of the reaction mixture:

(i) After 1 min

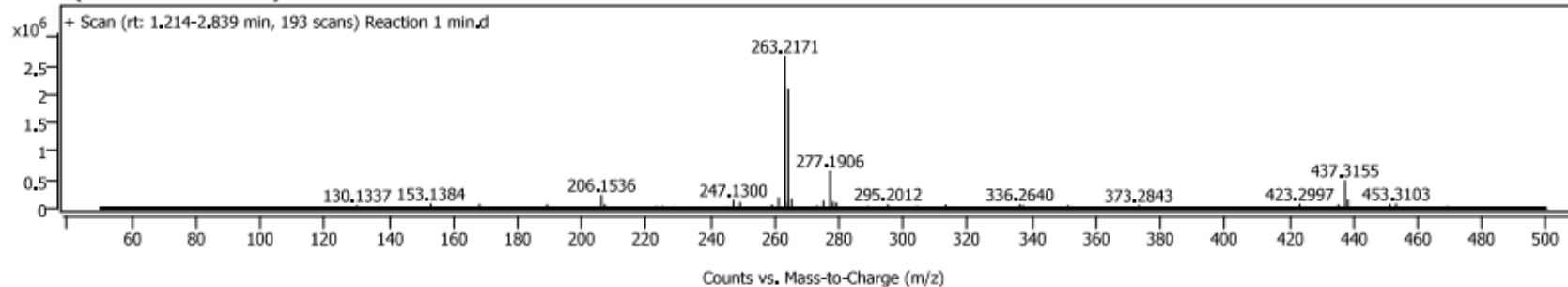
Sample Chromatograms



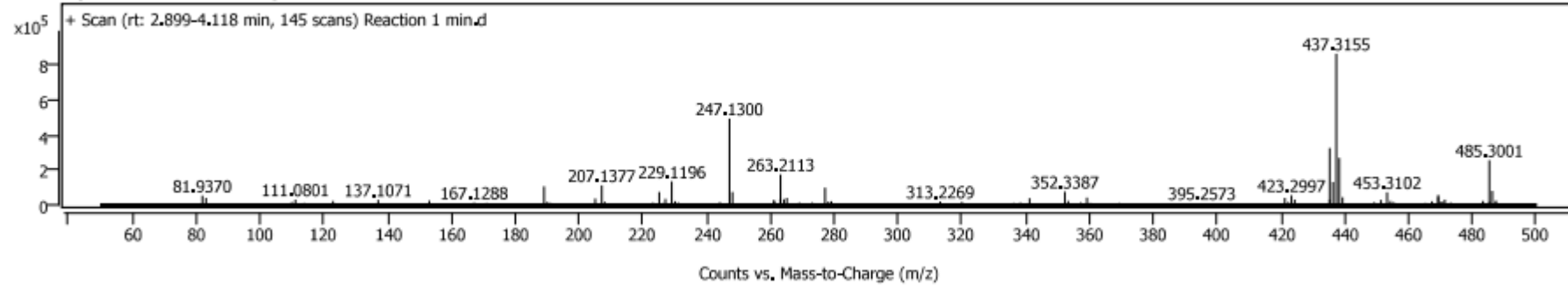
Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.333	1.680	2.839	188777512	7639900425	49.56	
2	2.916	3.288	4.075	17227543	534176510	3.47	
3	4.211	4.473	4.820	11965485	172889845	1.12	
4	5.091	5.514	6.801	219292950	7068493828	45.85	

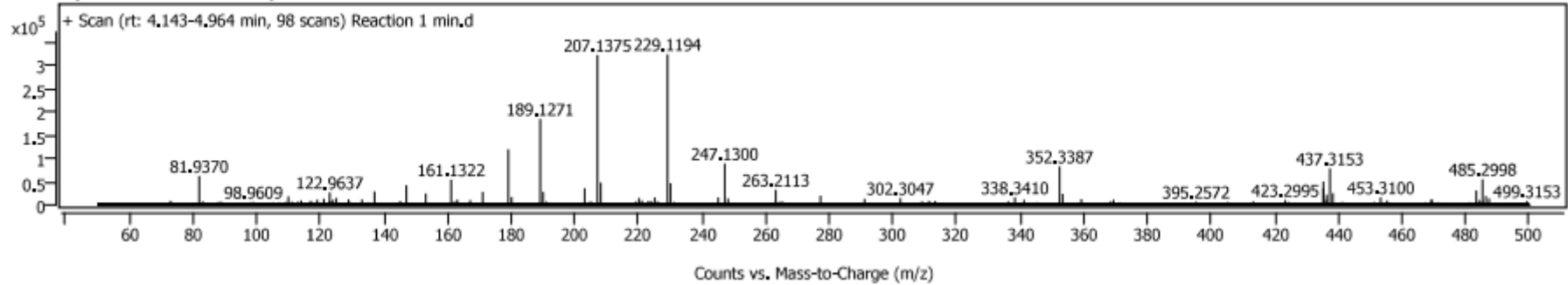
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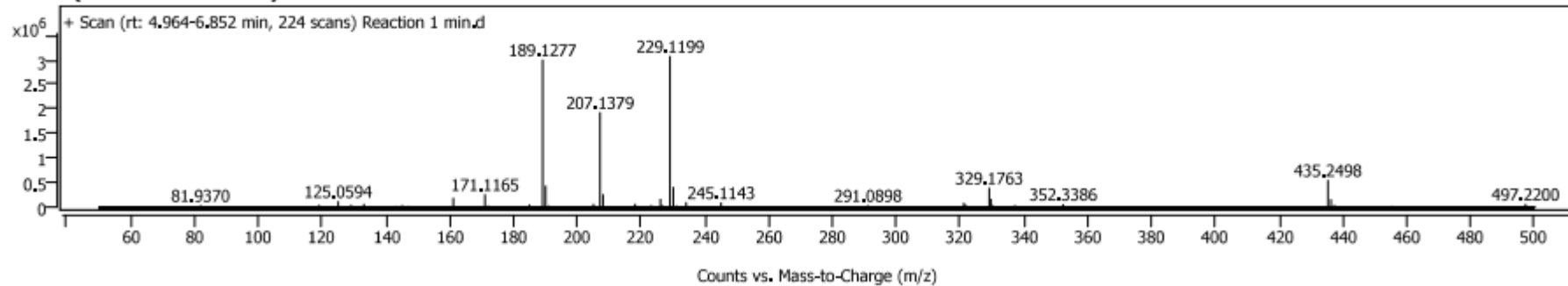
**+ Scan (rt: 2.899-4.118 min)**



**+ Scan (rt: 4.143-4.964 min)**

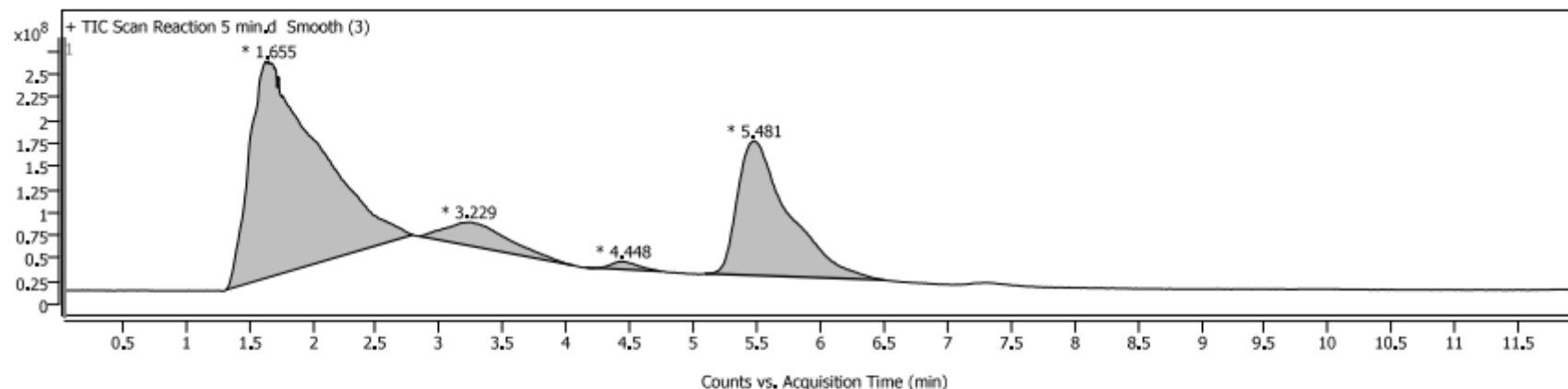


**+ Scan (rt: 4.964-6.852 min)**



(ii) After 5 min

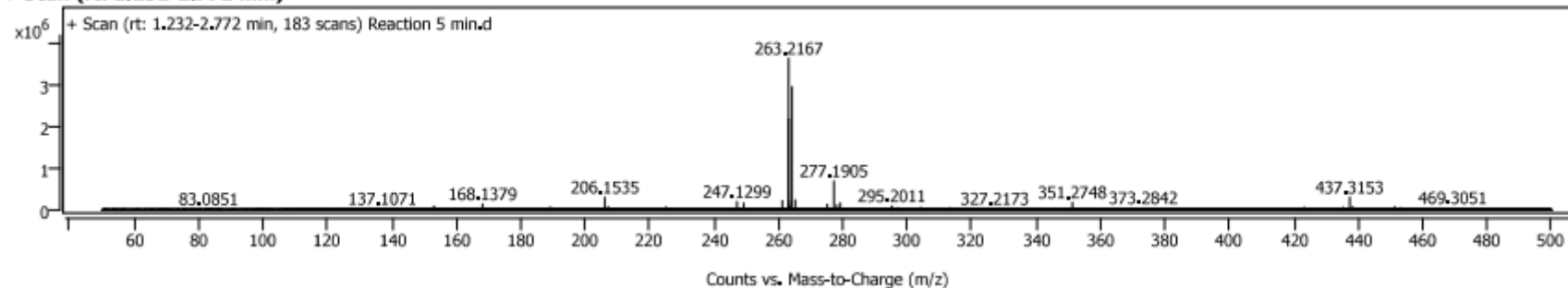
Sample Chromatograms



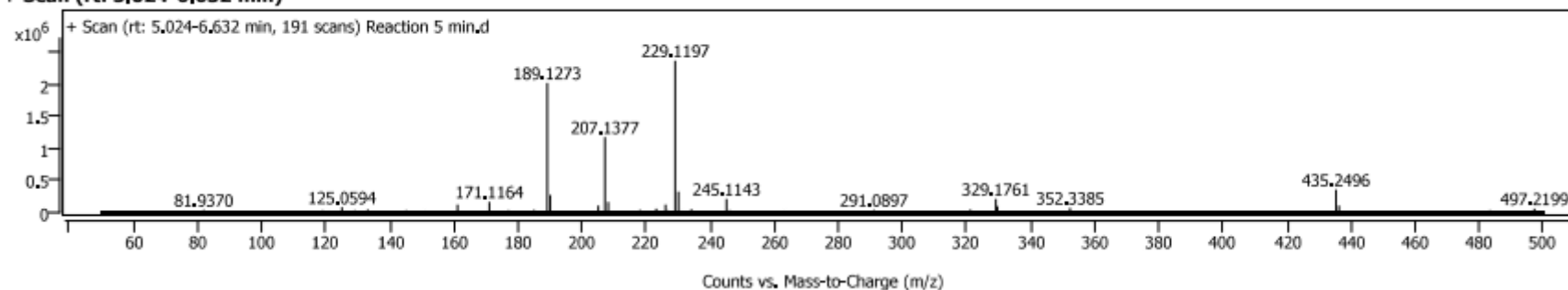
Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.316	1.655	2.789	234676644	8902971223	63.42	
2	2.840	3.229	4.059	25454591	908858886	6.47	
3	4.152	4.448	4.745	8676838	123864963	0.88	
4	5.092	5.481	6.505	146109357	4101592886	29.22	

+ Scan (rt: 1.232-2.772 min)

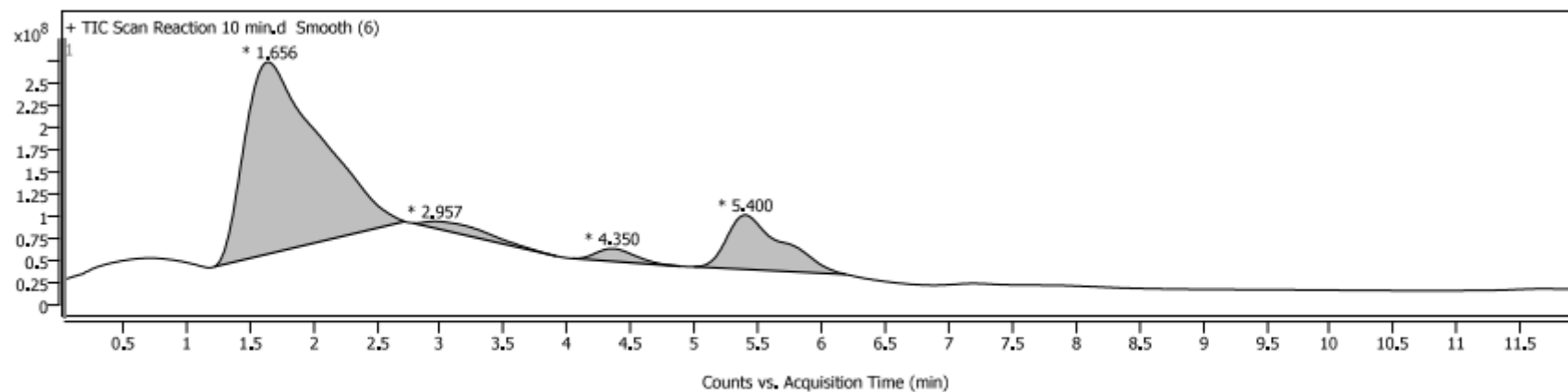


**+ Scan (rt: 5.024-6.632 min)**



**(iii) After 10 min**

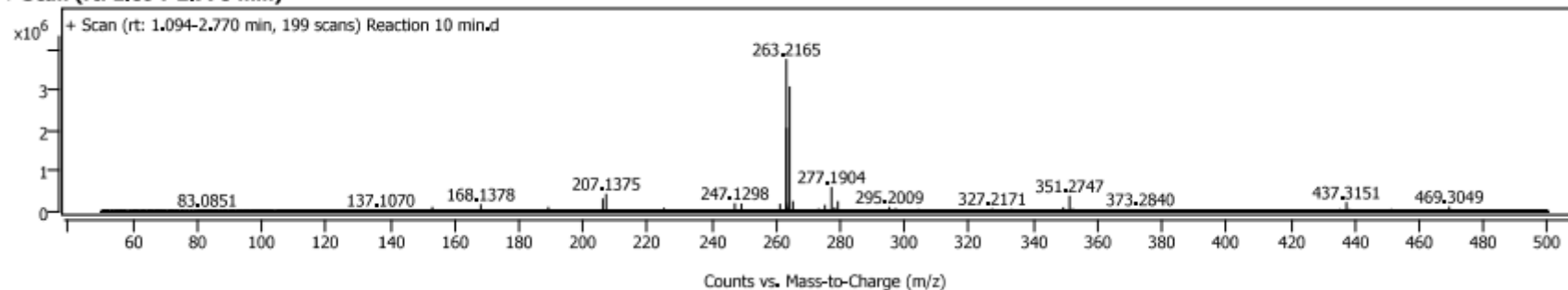
**Sample Chromatograms**



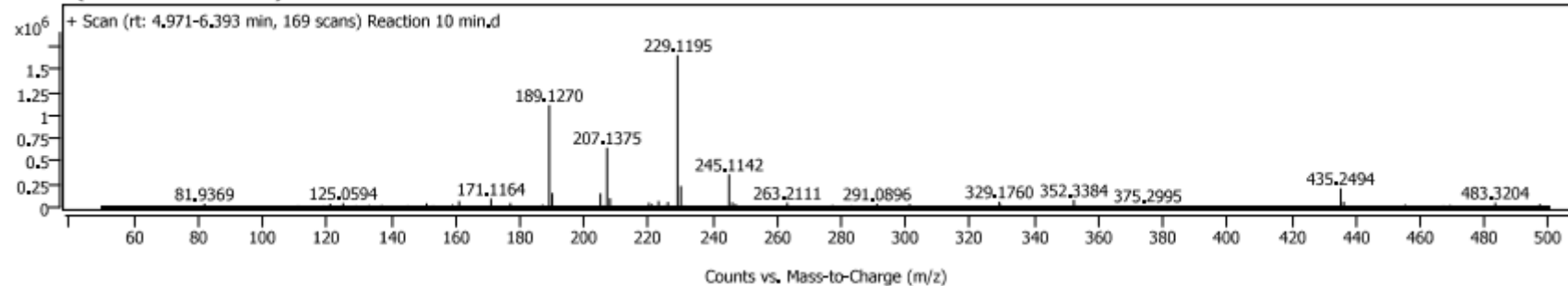
*Chromatogram Peaks*

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.221	1.656	2.720	215742118	8942086047	77.84	
2	2.787	2.957	3.913	7600439	369580376	3.22	
3	4.040	4.350	4.887	14336408	307063854	2.67	
4	4.997	5.400	6.190	61183830	1869229853	16.27	

**+ Scan (rt: 1.094-2.770 min)**

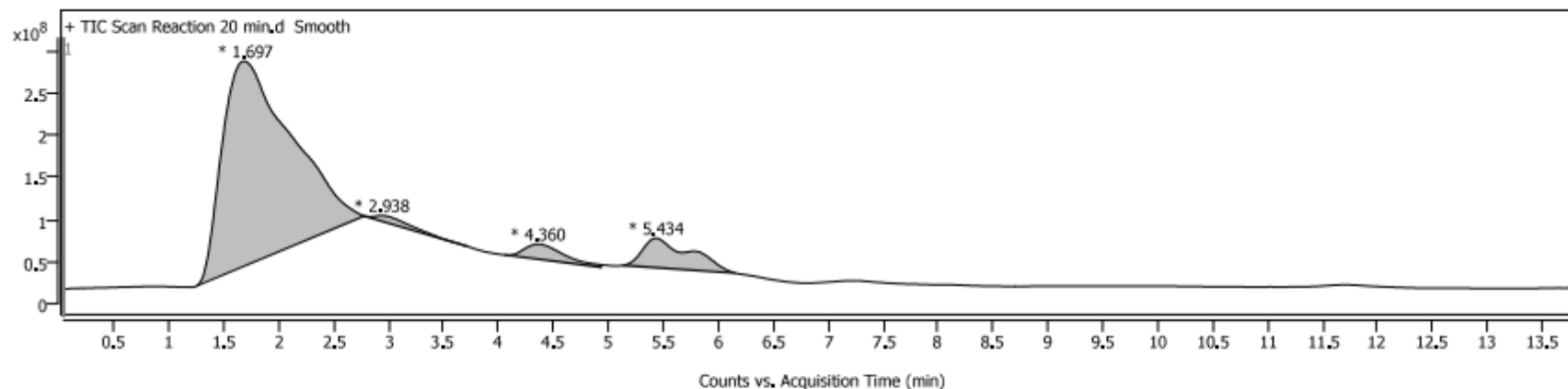


**+ Scan (rt: 4.971-6.393 min)**



(iv) After 20 min

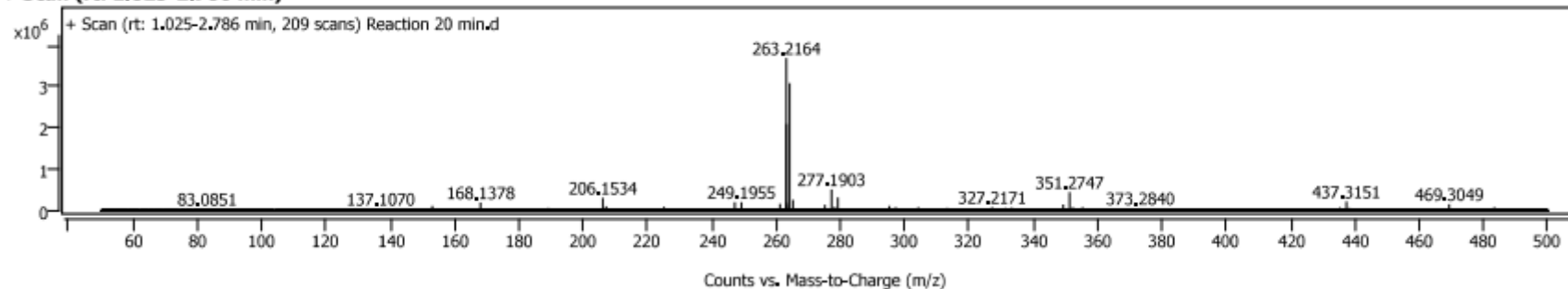
Sample Chromatograms



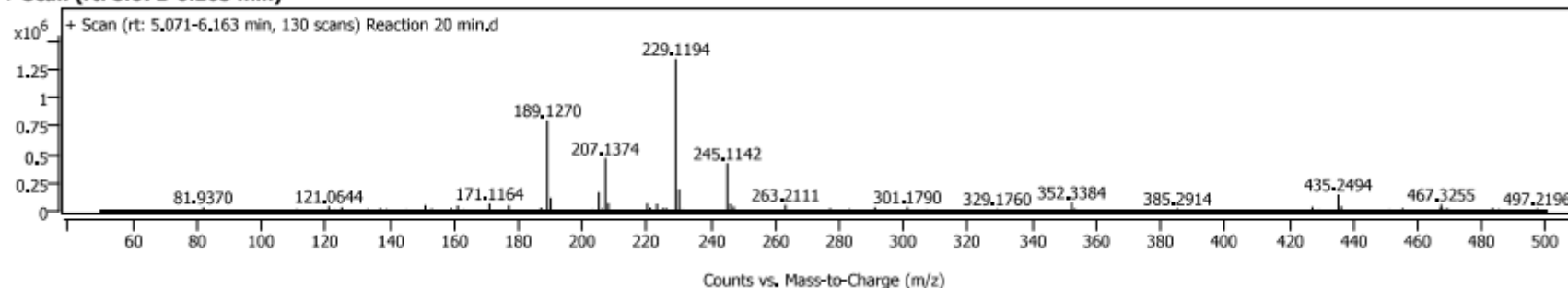
Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.254	1.697	2.777	243018211	10534631027	86.12	
2	2.777	2.938	3.725	6588104	178379431	1.46	
3	4.055	4.360	4.936	17845788	445245896	3.64	
4	5.130	5.434	6.155	34895526	1074845742	8.79	

+ Scan (rt: 1.025-2.786 min)

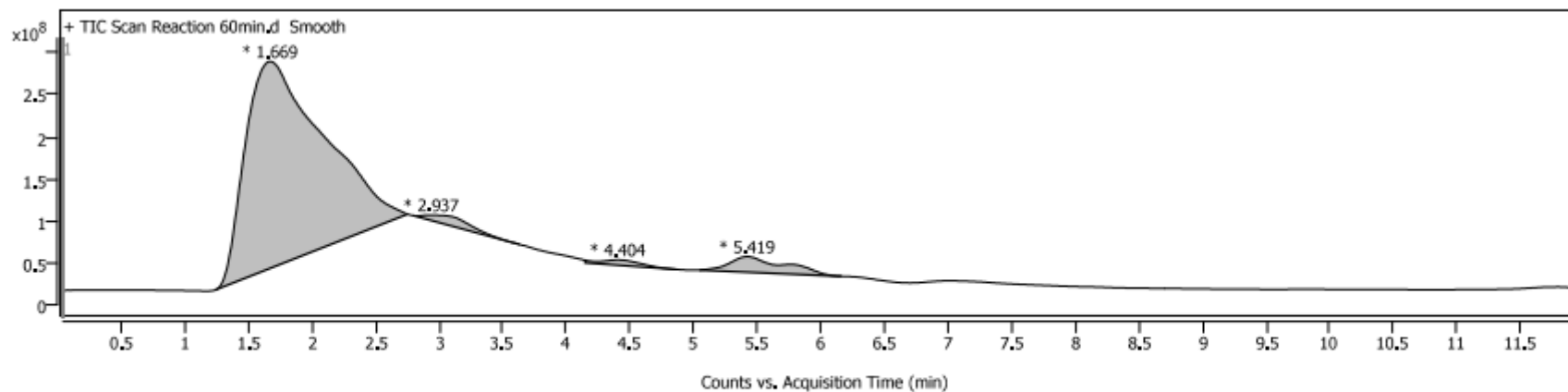


**+ Scan (rt: 5.071-6.163 min)**



**(v) After 1 h**

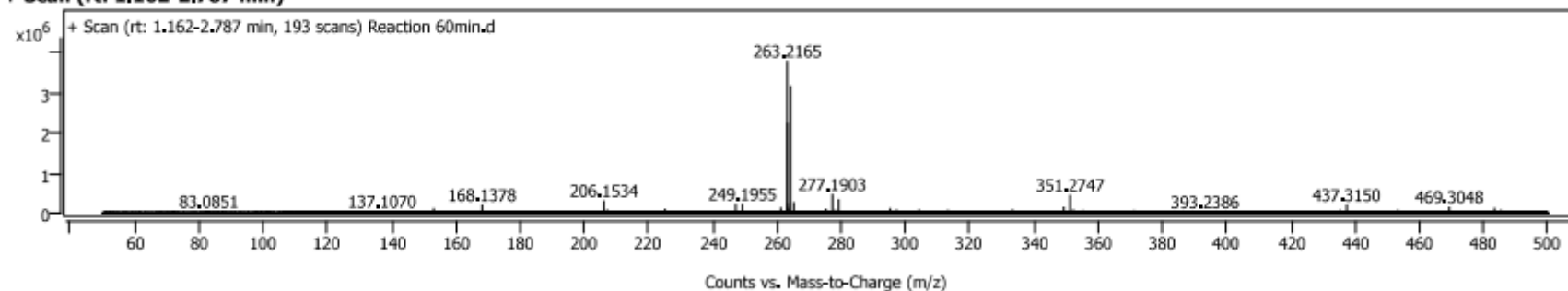
**Sample Chromatograms**



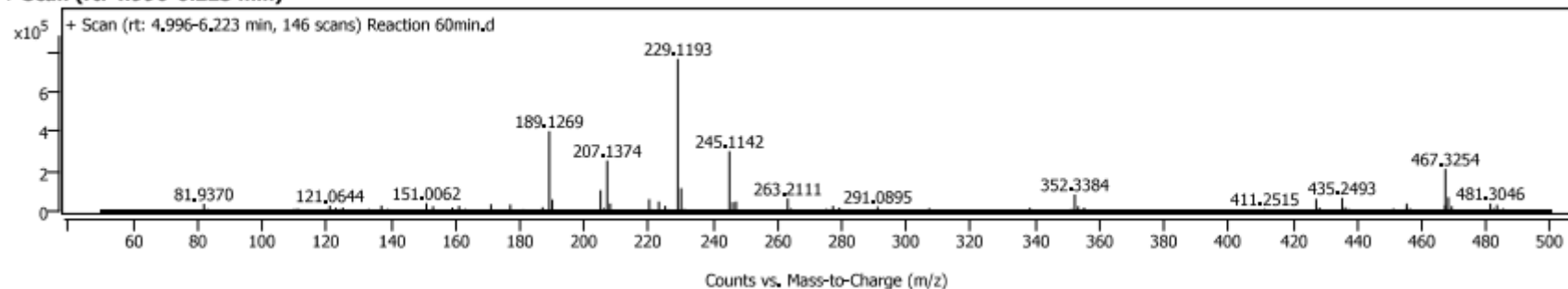
*Chromatogram Peaks*

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.238	1.669	2.753	246645655	10490002042	91.71	
2	2.795	2.937	3.633	6585160	244347876	2.14	
3	4.150	4.404	4.869	6209703	136362790	1.19	
4	5.047	5.419	6.164	18471362	567930419	4.97	

**+ Scan (rt: 1.162-2.787 min)**



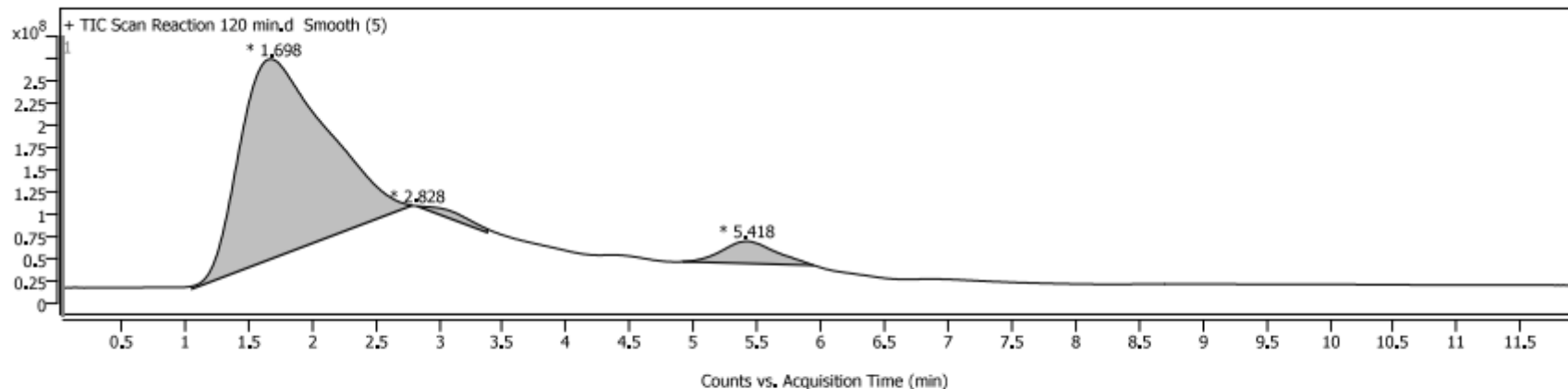
**+ Scan (rt: 4.996-6.223 min)**





(vi) After 2 h

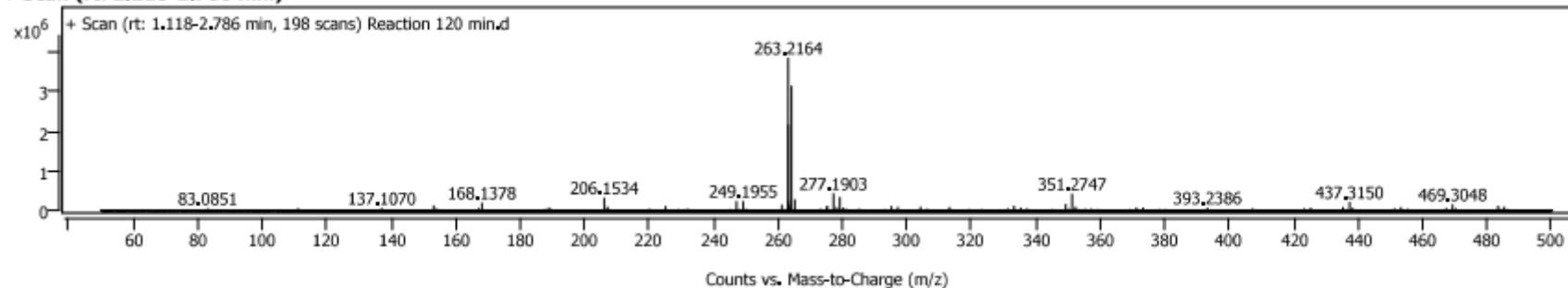
**Sample Chromatograms**



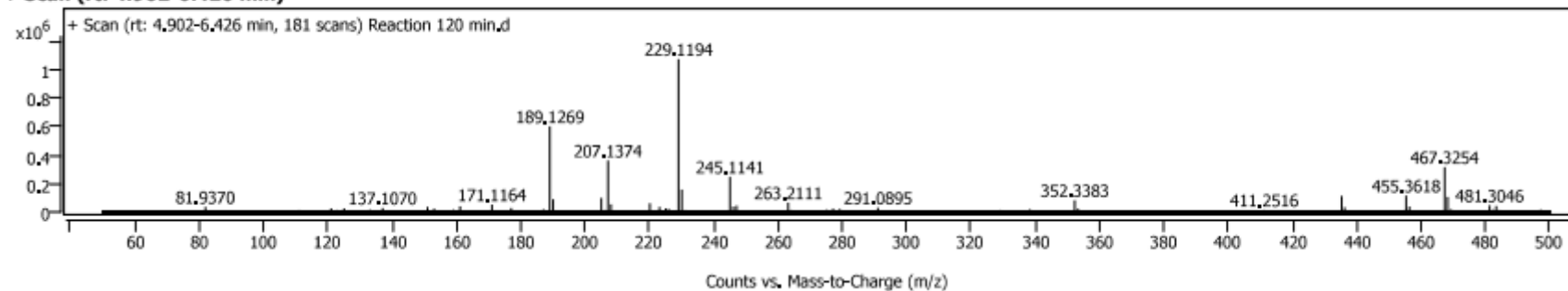
*Chromatogram Peaks*

Peak	Start	RT	End	Height	Area	Area Sum %	SNR
1	1.059	1.698	2.786	222640041	10613015719	91.95	
2	2.828	2.828	3.378	0	191512085	1.66	
3	4.910	5.418	5.943	24965537	738153308	6.39	

**+ Scan (rt: 1.118-2.786 min)**



+ Scan (rt: 4.902-6.426 min)



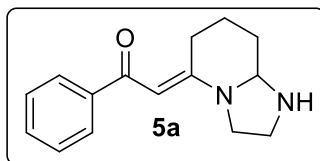
VI. References:

1. A. K. Jha, A. Kumari and S. Easwar, Diamine-mediated Degradative Dimerisation of Morita–Baylis– Hillman Ketones *Chem. Commun.*, 2020, **56**, 2949-2952.
2. A. K. Jha, R. Kumari and S. Easwar, A Hydrazine Insertion Route to N'-Alkyl Benzohydrazides by an Unexpected Carbon–Carbon Bond Cleavage, *Org. Lett.*, 2019, **21**, 8191-8195.
3. X. Tang, A.J. Blake, W. Lewis and S. Woodward, Asymmetric conjugate additions to 1,1'-diactivated cyclic enones—A comparative study, *Tetrahedron: Asymmetry*, 2009, **20**, 1881-1891.

# <sup>1</sup>H and <sup>13</sup>C NMR spectra of the synthesised products

ES-SS-324R re, <sup>1</sup>H, CDCl<sub>3</sub>, 11-07-2022

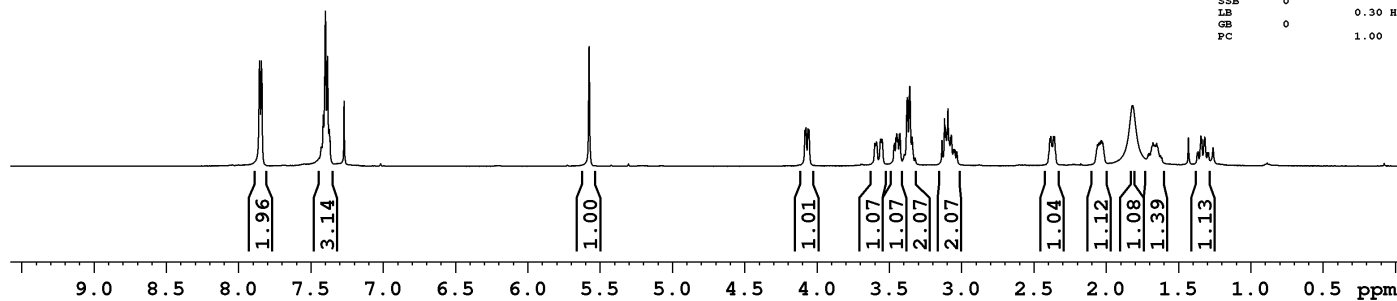
7.856  
7.854  
7.841  
7.838  
7.428  
7.424  
7.413  
7.398  
7.383  
7.374  
7.371  
7.366  
7.269  
5.575  
4.081  
4.074  
4.060  
4.053  
3.597  
3.586  
3.559  
3.548  
3.466  
3.461  
3.452  
3.447  
3.443  
3.437  
3.428  
3.423  
3.373  
3.356  
3.340  
3.134  
3.116  
3.109  
3.099  
3.092  
3.075  
3.069  
2.387  
2.381  
2.363  
2.356  
2.058  
2.050  
2.044  
2.036  
2.030  
2.023  
1.816  
1.674  
1.663  
1.648  
1.337  
1.322  
1.316



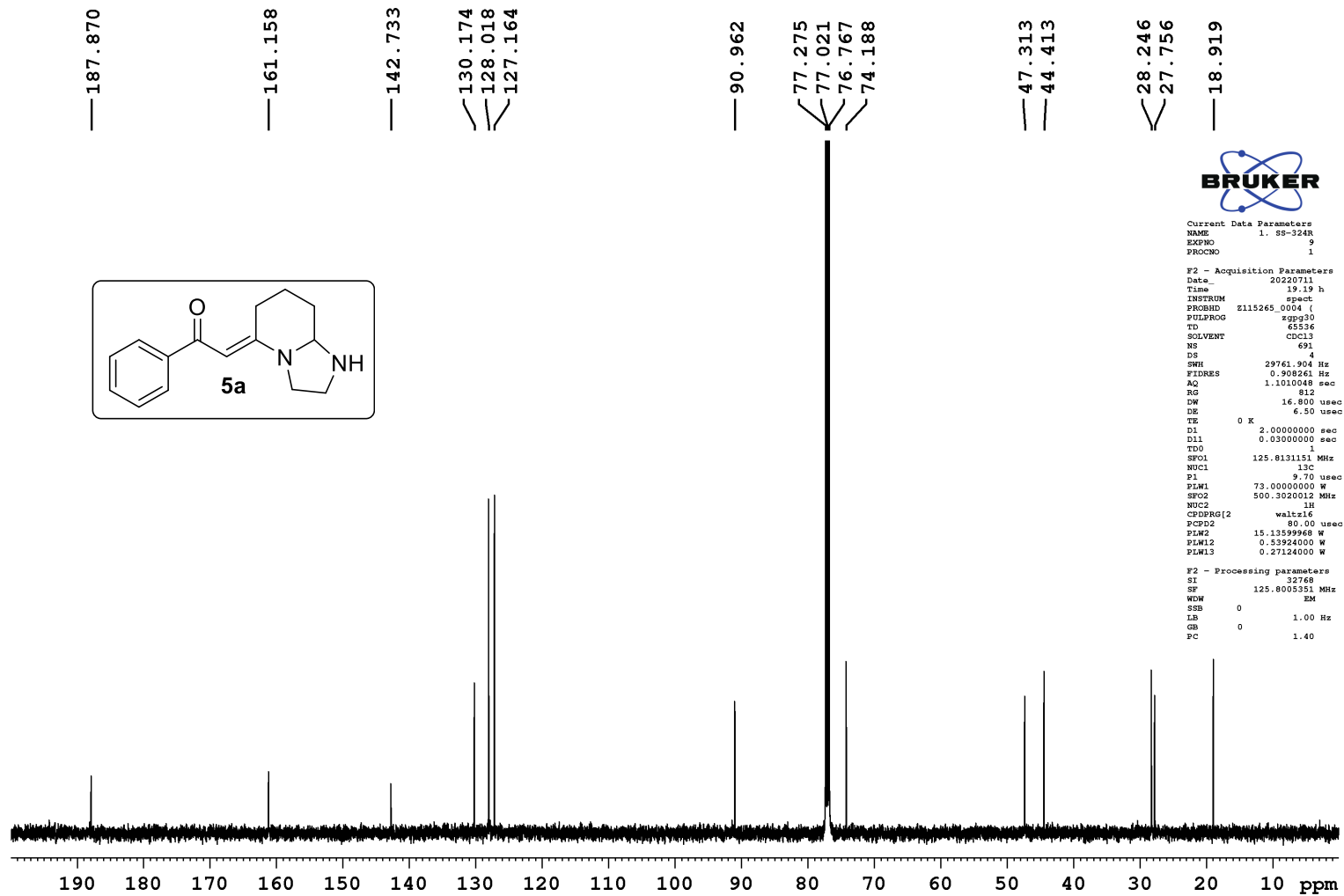
Current Data Parameters  
 NAME 1. SS-324R  
 EXPNO 8  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220711  
 Time 18.40 h  
 INSTRUM spect  
 PROBHD Z115265.0004 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.2767999 sec  
 RG 203  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.0000000 sec  
 TD0 1  
 SFO1 500.3030896 MHz  
 NUC1 <sup>1</sup>H  
 P1 15.10 usec  
 PLW1 15.13599968 W

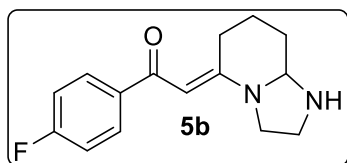
F2 - Processing parameters  
 SI 65536  
 SF 500.3000101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



ES-SS-324R re, 13C, CDCl3, 11-07-2022



ES-SS-282, 1H, CDC13, 22-06-2022



7.869  
7.858  
7.853  
7.841

7.066  
7.049  
7.032

5.520  
4.089  
4.082  
4.068  
4.062  
3.576  
3.567  
3.538  
3.528  
3.477  
3.473  
3.463  
3.458  
3.454  
3.449  
3.439  
3.434  
3.375  
3.358  
3.341  
3.145  
3.128  
3.121  
3.110  
3.104  
3.096  
3.086  
3.073  
3.058  
2.394  
2.387  
2.369  
2.362  
2.023  
1.702  
1.697  
1.675  
1.661  
1.648  
1.625  
1.621  
1.371  
1.364  
1.345

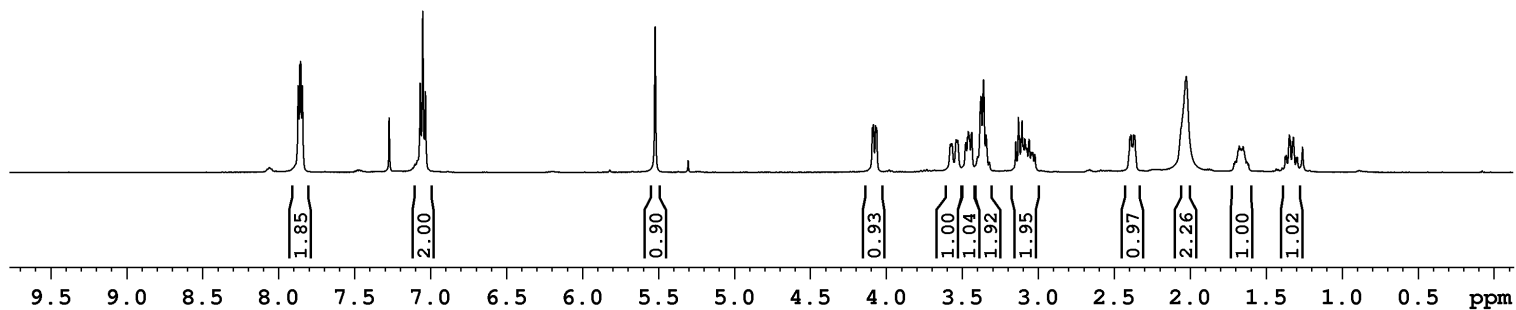


```

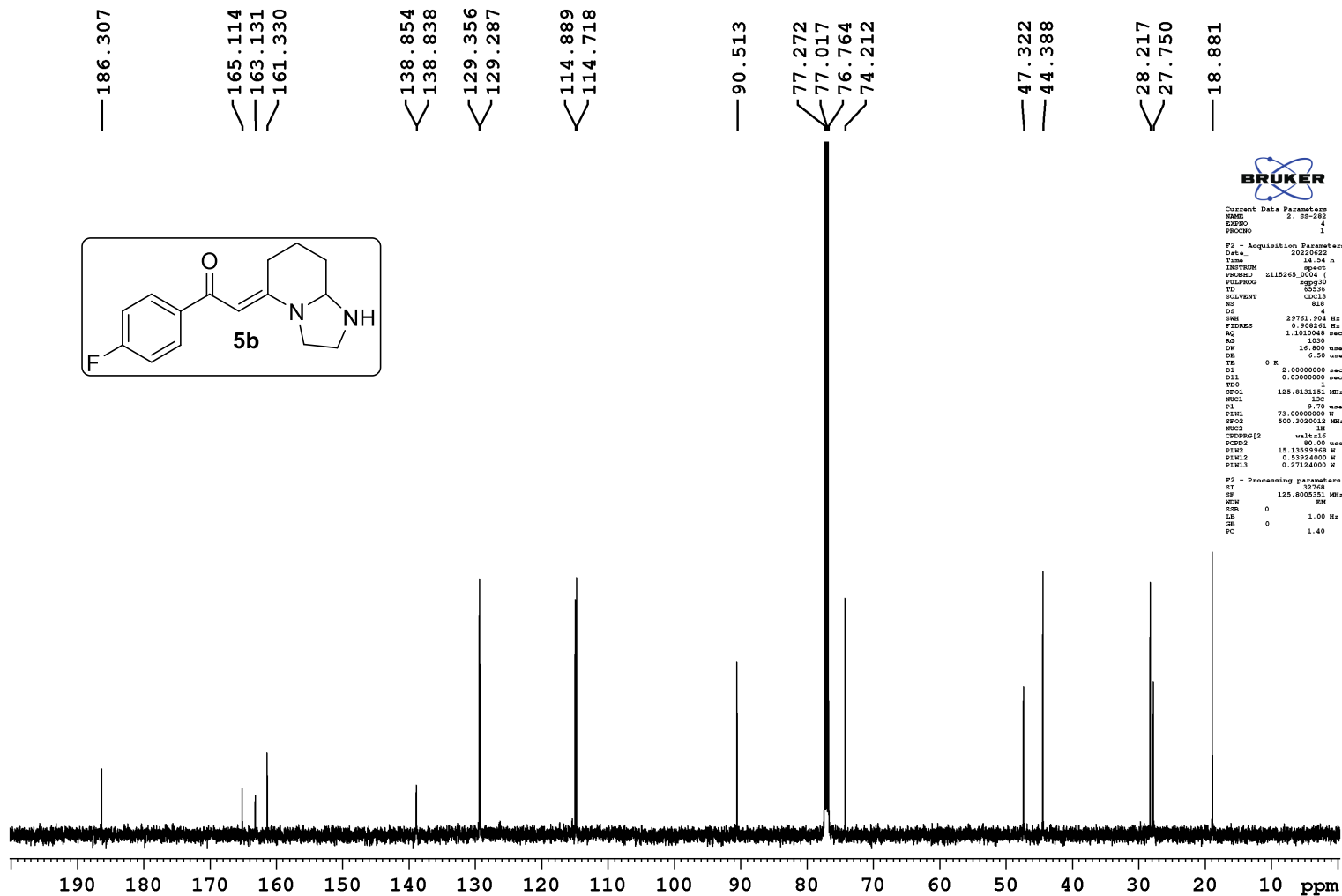
Current Data Parameters
NAME      2_ SS-282
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20220622
Time     14.08 h
INSTRUM  spect
PROBHD   z115265_0004 (
PULPROG  zgpg
TD        65536
SOLVENT  cdcl3
NS        16
DS        2
SFO      10000.000 Hz
FIDRES   0.305176 Hz
AQ        3.2767399 sec
RG        181
WDW       50.000 usec
DE        6.50 usec
TE        0 K
D1        1.0000000 sec
TBO
SFO1     500.3030624 MHz
NUC1      1H
P1        15.10 usec
PL1      15.13599968 W

F2 - Processing parameters
SI        65536
SF        500.3000023 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```



ES-SS-282, 13C, CDC13, 22-06-2022



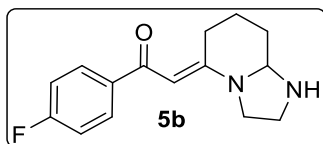
Current Data Parameters  
NAME 2: ES-282  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220622  
Time 14:54 h  
INSTRUM spect  
PROBHD E11245.0004 (4  
PULPROG zgpg30  
TU 8536  
SOLVENT CDCl3  
NS 818  
DS 4  
SWH 29761.904 Hz  
F2CHES 0.208061 Hz  
AQ 1.1010048 sec  
RG 1020  
DN 16.890 usec  
DE 6.50 usec  
TE 0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD 1  
YD0 125.813151 MHz  
NUC1 13C  
P1 9.70 usec  
PL1 73.0000000 W  
SFO2 900.350915 MHz  
NUC2 1H  
CROSSP2 waltz16  
PCPD2 80.00 usec  
PLA2 15.1358958 W  
PLM12 0.5352400 W  
PLM13 0.2714000 W

F2 - Processing parameters  
SI 32768  
SF 125.800551 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-282\_19F\_CDCl3\_26-12-2023

— -110.862

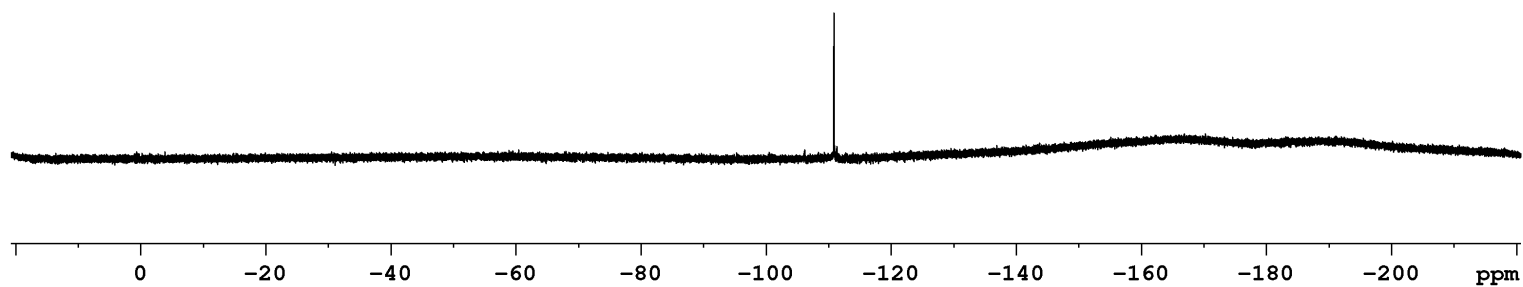


```
Current Data Parameters
NAME      19f spectra
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20211216
Time     16:14 h
INSTRUM  spect
PROBHD   E115245.0084
PULPROG  zgpg30p2
TD       131072
SOLVENT  CDCl3
NS       16
DS       4
SFR      115626.367 Hz
FIDRES   1.722950 Hz
AQ       0.5747161 sec
RG       724
DF       4.400 usec
DE       6.50 usec
TE       0 K

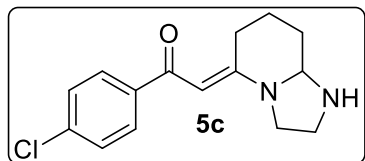
D1       1.0000000 sec
D11      0.0000000 sec
D12      0.0002000 sec
TD0      0.0002000 sec
SFO1     470.6582195 MHz
NUC1     19F
P1       15.00 usec
P1A1    27.0000000 W
SFO2     500.2520010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    60.00 usec
PLM2     15.23529963 W
PLM12    0.53324000 W

F2 - Processing parameters
SI       32768
SF       470.7652000 MHz
WDW      0
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```



ES-SS-277, 1H, CDC13, 06-06-2022

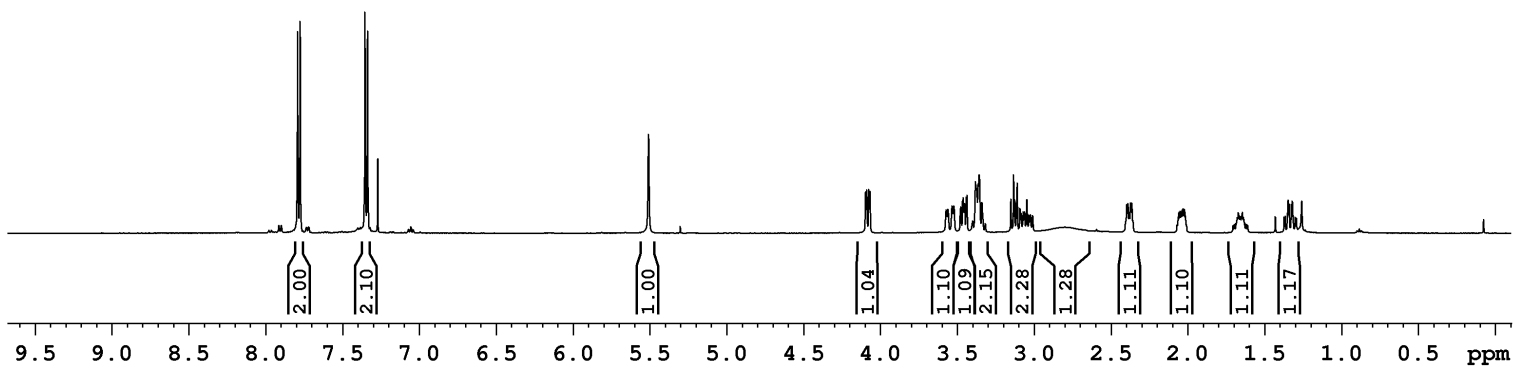
7.791  
7.773  
7.352  
7.335  
7.269  
5.507  
4.094  
4.087  
4.073  
4.066  
3.570  
3.559  
3.531  
3.520  
3.478  
3.474  
3.463  
3.459  
3.454  
3.449  
3.439  
3.434  
3.397  
3.380  
3.355  
3.337  
3.149  
3.132  
3.125  
3.114  
3.107  
3.090  
3.083  
3.069  
3.060  
3.045  
3.031  
3.022  
3.008  
2.395  
2.388  
2.370  
2.363  
2.055  
2.047  
2.041  
2.033  
2.027  
2.019  
1.676  
1.674  
1.669  
1.666  
1.658  
1.655  
1.647  
1.643  
1.636  
1.631  
1.627  
1.371  
1.364  
1.350  
1.345  
1.338  
1.324  
1.318  
1.313  
1.299  
1.292



Current Data Parameters  
NAME 3. SS-277 R  
EXPNO 1  
PROCNO 1

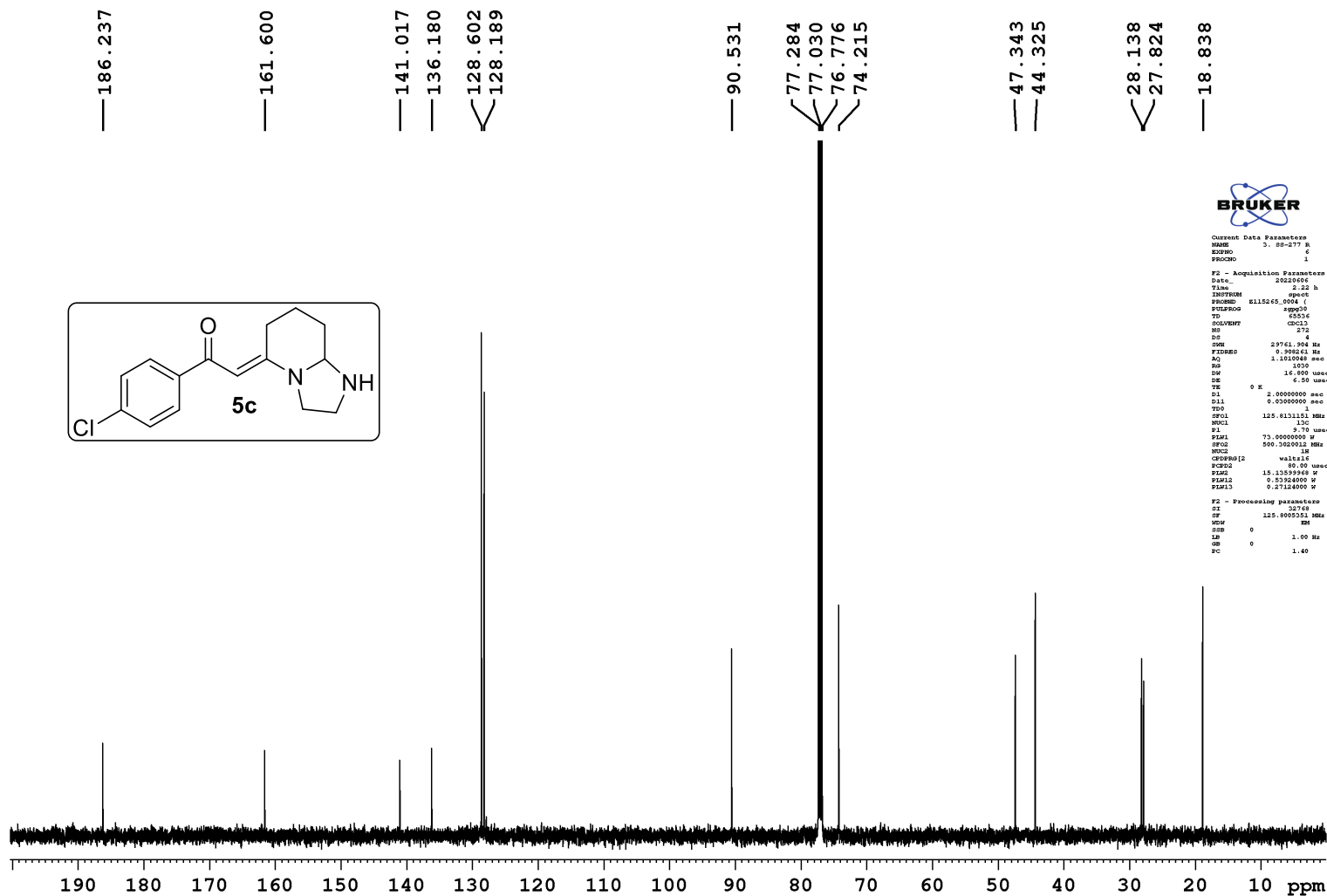
F2 - Acquisition Parameters  
Date\_ 20220606  
Time 2.04 h  
INSTRUM spect  
PROBHD z115265.0004 (C  
PULPROG zgpg  
TD 65536  
SOLVENT cdcl3  
NS 16  
DS 2  
SFO 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2757399 sec  
RG 181  
WDW 50.000 usec  
DE 6.50 usec  
TE 300 K  
D1 1.0000000 sec  
TBO 1  
SFO1 500.3030624 MHz  
NUC1 1H  
P1 15.10 usec  
P1M1 15.13599268 W

F2 - Processing parameters  
SI 65536  
SF 500.3000294 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





ES-SS-277, 13C, CDC13, 06-06-2022



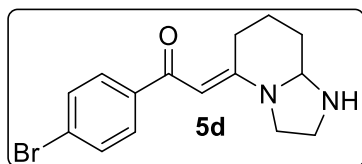
Current Data Parameters  
NAME 5\_08-277.k  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220606  
Time 2.22 h  
INSTRUM spect  
PROBHD E115245.0004 (4  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 272  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.990261 Hz  
AQ 1.1010048 sec  
RG 1050  
DF 16.800 usec  
DE 6.50 usec  
TE 0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD 0  
SFO1 125.811151 MHz  
NUC1 13C  
P1 9.70 usec  
PL1 0.0000000 W  
SFO2 500.1320012 MHz  
NUC2 1H  
CDEPRG2 waltz16  
PCPD2 80.00 usec  
PL22 15.1535568 W  
PL12 0.25324000 W  
PL13 0.27154000 W

F2 - Processing parameters  
SI 32768  
SF 125.805512 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-290, 1H, CDC13, 13-06-2022

7.725  
7.708  
7.517  
7.500  
7.269  
5.506  
4.097  
4.090  
4.076  
4.069  
3.574  
3.564  
3.536  
3.526  
3.486  
3.481  
3.471  
3.466  
3.461  
3.457  
3.446  
3.442  
3.386  
3.377  
3.368  
3.361  
3.343  
3.153  
3.135  
3.128  
3.118  
3.111  
3.093  
3.076  
3.067  
3.052  
3.038  
3.029  
3.015  
2.401  
2.394  
2.376  
2.369  
2.062  
2.055  
2.048  
2.041  
2.034  
2.027  
1.691  
1.683  
1.676  
1.672  
1.664  
1.661  
1.653  
1.649  
1.644  
1.633  
1.626  
1.621  
1.614  
1.373  
1.366  
1.348  
1.341  
1.327  
1.320  
1.301  
1.295

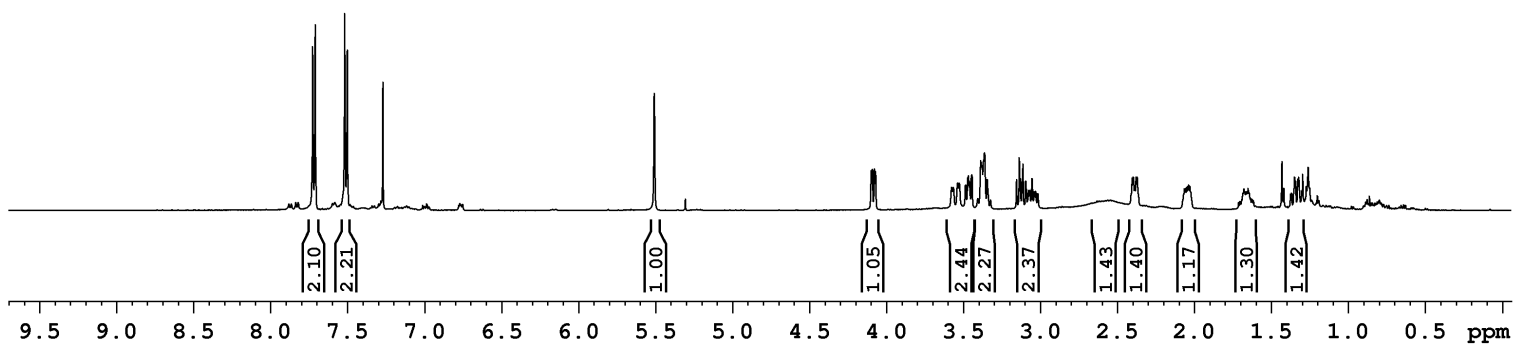


```

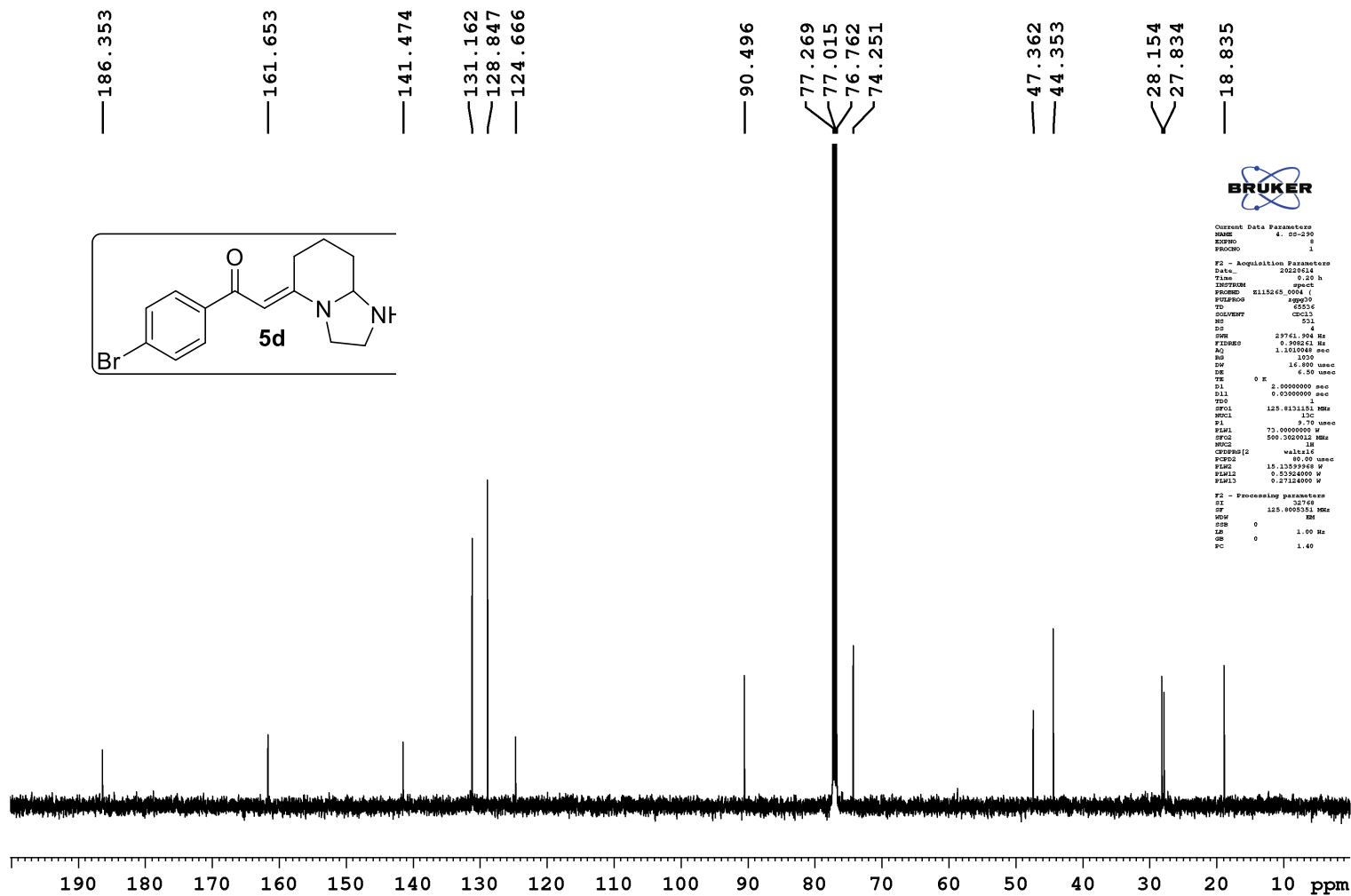
Current Data Parameters
NAME      4_SS-290
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20220613
Time      23.49 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SFO      10000.000 Hz
FIDRES    0.305176 Hz
AQ        3.2757959 sec
RG        181
DM        50.000 usec
DE        6.50 usec
TE        0 K
D1        1.00000000 sec
TDO       1
SFO2     500.300856 MHz
NUC1      1H
P1        15.10 usec
PL1       15.13599968 W

F2 - Processing parameters
SI        65536
SF        500.300856 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```



ES-SS-290, 13C, CDC13, 13-06-2022



```
Current Data Parameters
NAME      4_05-290
EXPNO    1
PROCNO   1

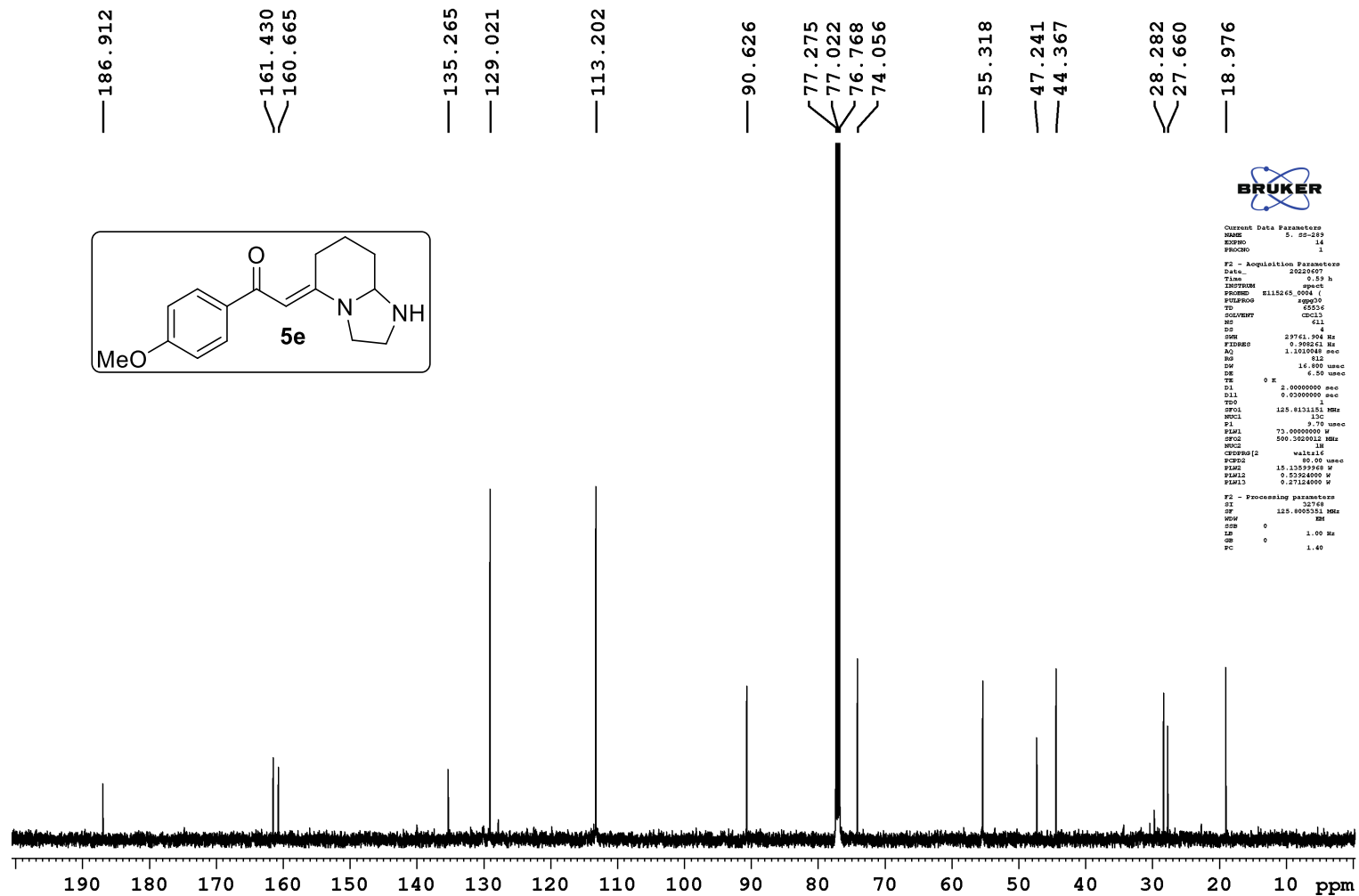
F2 - Acquisition Parameters
Date_    20220114
Time     0.20 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  cdcl3
NS        2
DS        4
SFO      29761.994 MHz
FIDRES   0.398261 MHz
AQ        1.101048 sec
RG        4028
DM        14.800 usec
DE        6.50 usec
TE        300.2 K
D1        2.0000000 sec
d11       0.0200000 sec
TD0       1
SFO1     125.815151 MHz
NUC1      13C
PC1       150 usec
P1        1.70 usec
P1M1     73.0000000 MHz
SFO2     500.1362912 MHz
NUC2      1H
PC2       18 usec
P2M1     18.1359948 MHz
P2M2     80.00 usec
P2M3     18.1359948 MHz
P2M4     0.53264000 MHz
P2M5     0.27124000 MHz

F2 - Processing parameters
SI        32768
SF        125.8055151 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

ES-SS-289 r, 1H, CDC13, 06-06-2022

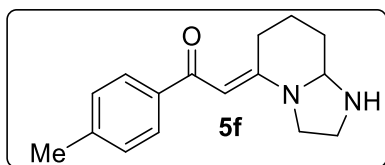


ES-SS-289, 13C, CDC13, 06-06-2022



```
Current Data Parameters
NAME      5_SS-289
EXPNO    14
PROCNO   1
F2 - Acquisition Parameters
Date_    20220601
Time     0.55 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD       65536
SOLVENT  cdcl3
NS       614
DS       4
SFO     29761.994 MHz
FIDRES   0.398261 Hz
AQ       1.302048 sec
RG       812
DM       16.800 usec
DE       6.50 usec
TE       300 K
D1       2.0000000 sec
d11      0.2000000 sec
TD0      1
SFO1     125.813151 MHz
NUC1     13C
NUC2     13C
PC1      1.70 usec
P1M1     70.0000000 W
SFO2     500.302012 MHz
PC2      18
P1M2     18.1359948 W
SFO3     411.141 MHz
PC3      80.00 usec
P1M3     0.53924000 W
SFO4     0.27124000 W
P1M4     0.27124000 W
F2 - Processing parameters
SI       32768
SF       125.805511 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

ES-SS-276R, 1H, CDC13, 09-07-2022

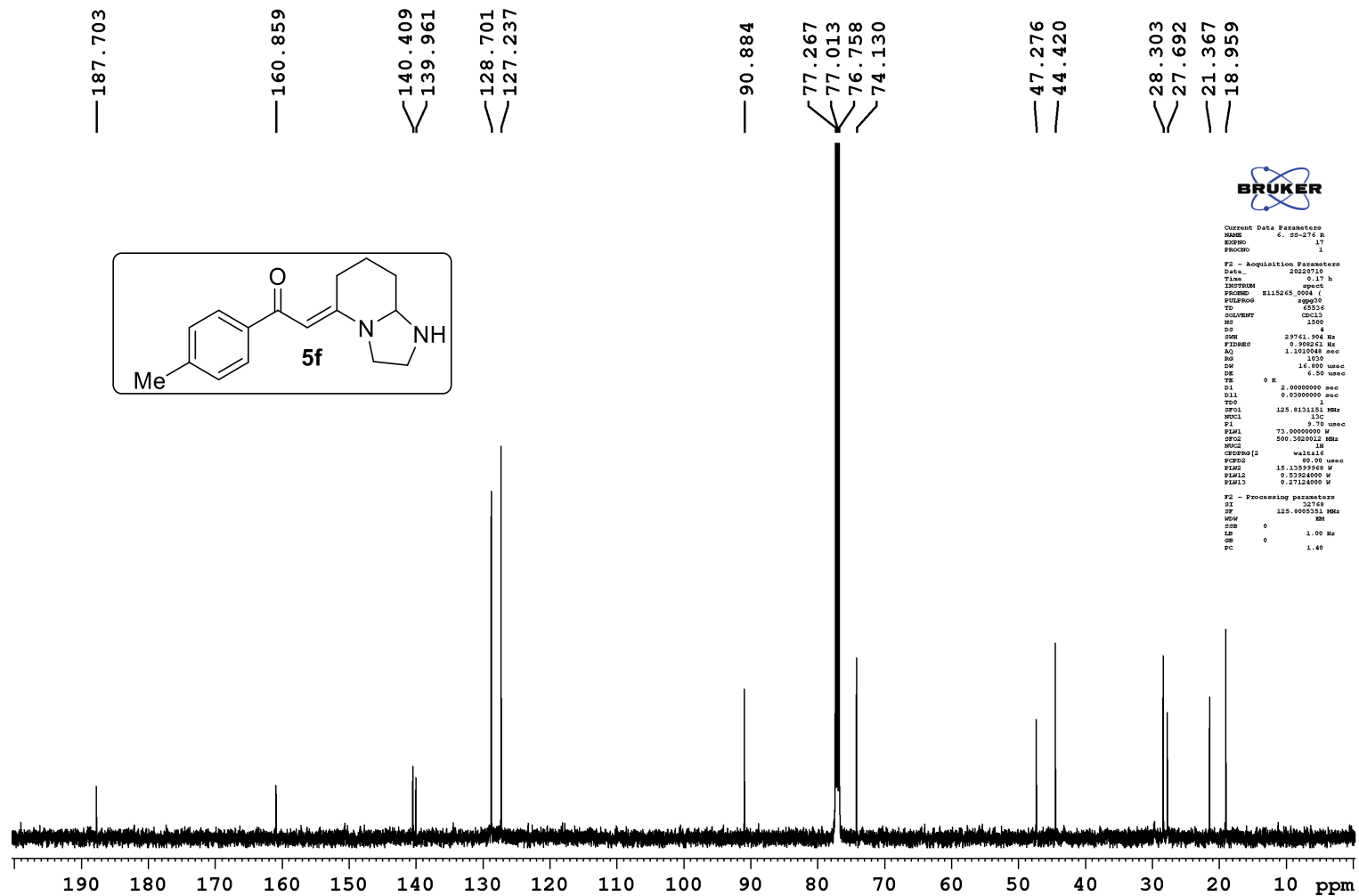


Current Data Parameters  
NAME 6\_SS-276 R  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220705  
Time 22.54 h  
INSTRUM spect  
PROBHD 115265\_0004 (4  
PULPROG zgpg  
TD 65536  
SOLVENT cdcl3  
NS 16  
DS 2  
SFO 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2757959 sec  
RG 256  
DM 50.000 umm  
DE 6.50 umm  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.300856 MHz  
NUC1 1H  
P1 15.10 umm  
PLM1 15.13599968 M

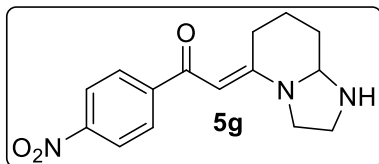
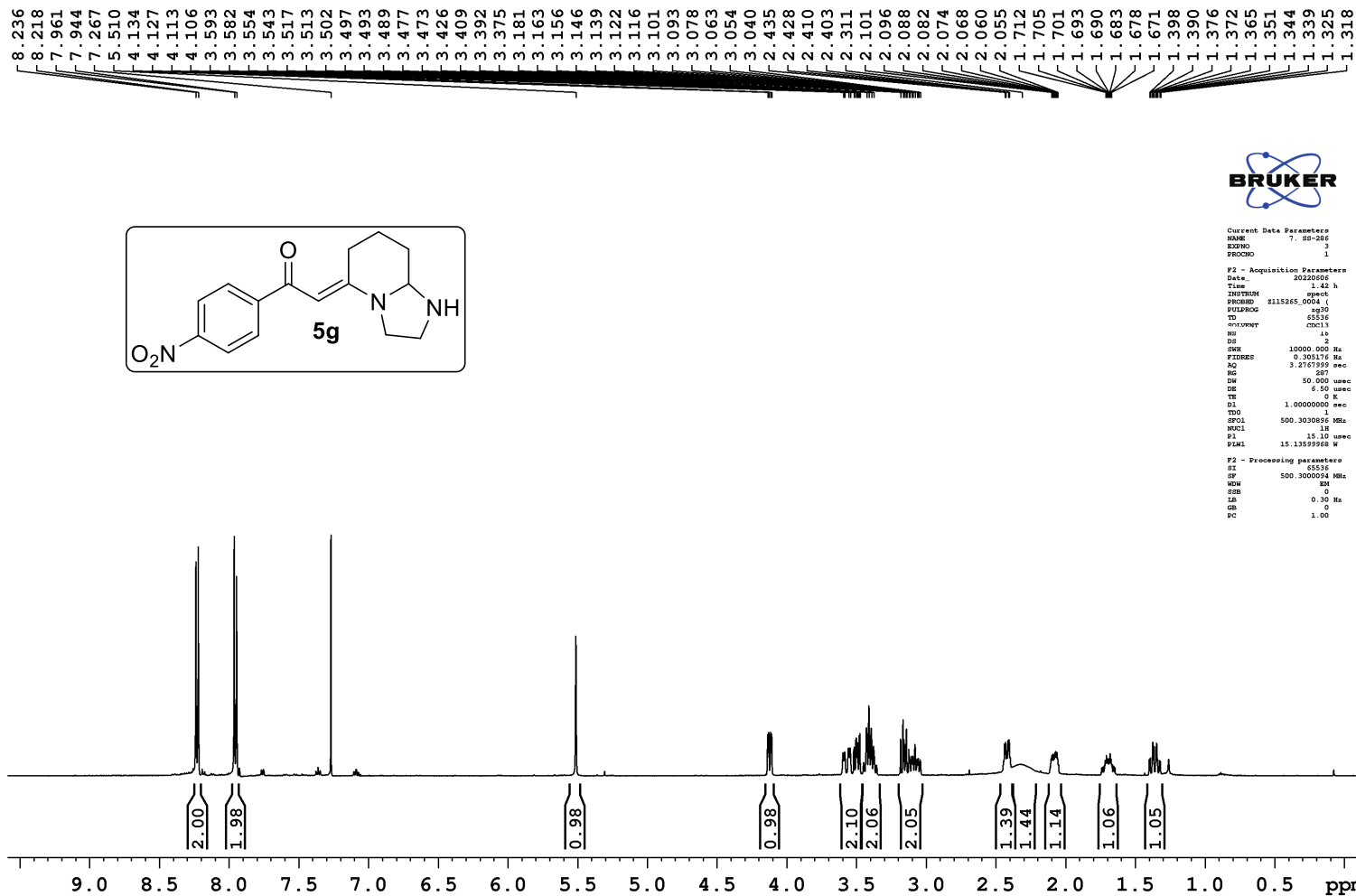
F2 - Processing parameters  
SI 65536  
SF 500.3000104 MHz  
WDW EM  
SFB 0  
GB 0  
PC 1.00

ES-SS-276R, 13C, CDC13, 09-07-2022



Current Data Parameters  
NAME: 6\_02-276 R  
EXPNO: 17  
PROCNO: 1  
F2 - Acquisition Parameters  
Date\_: 20220710  
Time: 0.17 h  
INSTRUM: spect  
PROBHD: BBO51  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: cdcl3  
NS: 4  
DS: 4  
SWH: 23761.904 Hz  
FIDRES: 0.398261 Hz  
AQ: 1.101068 sec  
RG: 4028  
DM: 16.800 usec  
DE: 6.50 usec  
TE: 300 K  
D1: 2.0000000 sec  
D11: 0.0200000 sec  
TD0: 1  
SFO1: 125.813151 MHz  
NUC1: 13C  
P1: 3.70 usec  
PL1: 75.0000000 W  
SFO2: 500.302012 MHz  
NUC2: 1H  
CROSSP2: 90.00 usec  
PCP2: 18.1335948 W  
PL2: 0.53264000 W  
PL13: 0.27124000 W  
F2 - Processing parameters  
SI: 32768  
SF: 125.805511 MHz  
WDW: EM  
SSB: 0  
LB: 1.00 Hz  
GB: 0  
PC: 1.40

ES-SS-286, 1H, CDC13, 06-06-2022



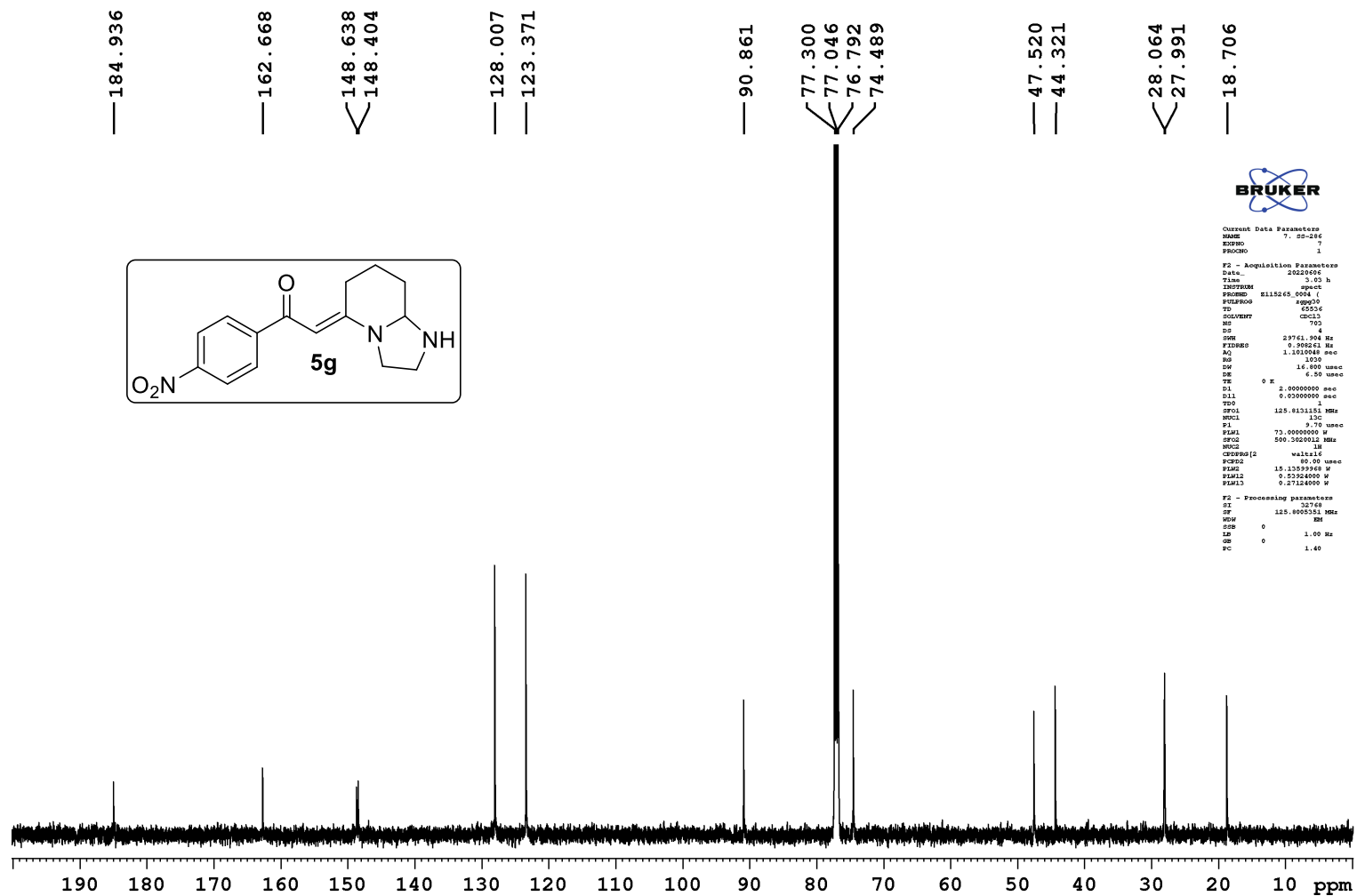
Current Data Parameters  
 NAME 7\_SS-286  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220606  
 Time 1.42 h  
 INSTRUM spect  
 PROBRD s115265\_0004 (   
 PULPROG zgpg30  
 TD 65536  
 SFO 500.136299  
 AQ 1.42  
 DE 2  
 DSX 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.2757999 sec  
 RG 287  
 DM 50.000 umax  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 500.3030856 MHz  
 NUC1 1H  
 P1 15.10 usec  
 PLW1 15.13599968 W

F2 - Processing parameters  
 SI 65536  
 SF 500.3000054 MHz  
 DSX 0  
 MSH 0.30 Hz  
 GB 0  
 PC 1.00



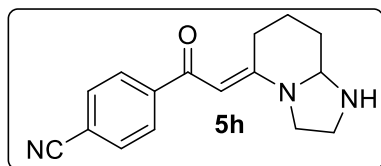
ES-SS-286, 13C, CDC13, 06-06-2022



Current Data Parameters  
NAME 7\_05-286  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220604  
Time 09:07  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 703  
DS 4  
SFO 29761.994 Hz  
FIDRES 0.098261 Hz  
AQ 1.101068 sec  
RG 4028  
DM 16.800 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
D11 0.2000000 sec  
TD0 1  
SFO1 125.813151 MHz  
NUC1 13C  
PC1 1.70 usec  
P1 132  
P1P1 73.0000000 W  
SFO2 500.302012 MHz  
NUC2 1H  
PCP2 18  
SFO2 500.302012 MHz  
P2P2 80.00 usec  
P2P2 18.1359948 W  
P1P12 0.53924000 W  
P1P13 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.805511 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-280, 1H, CDC13, 07-06-2022

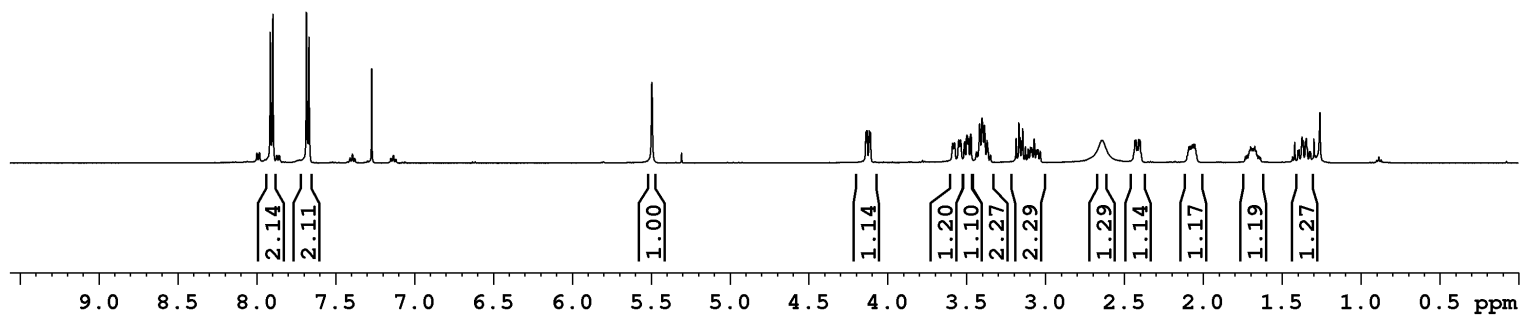
7.912  
7.895  
7.683  
7.666  
7.269  
5.493  
4.136  
4.129  
4.115  
4.108  
3.586  
3.575  
3.547  
3.536  
3.513  
3.509  
3.498  
3.494  
3.489  
3.485  
3.474  
3.470  
3.415  
3.400  
3.385  
3.368  
3.184  
3.167  
3.160  
3.149  
3.142  
3.125  
3.093  
3.084  
3.069  
3.639  
2.431  
2.424  
2.406  
2.399  
2.088  
2.080  
2.073  
2.065  
2.060  
2.052  
1.697  
1.693  
1.686  
1.682  
1.676  
1.670  
1.376  
1.371  
1.365  
1.350  
1.344  
1.339



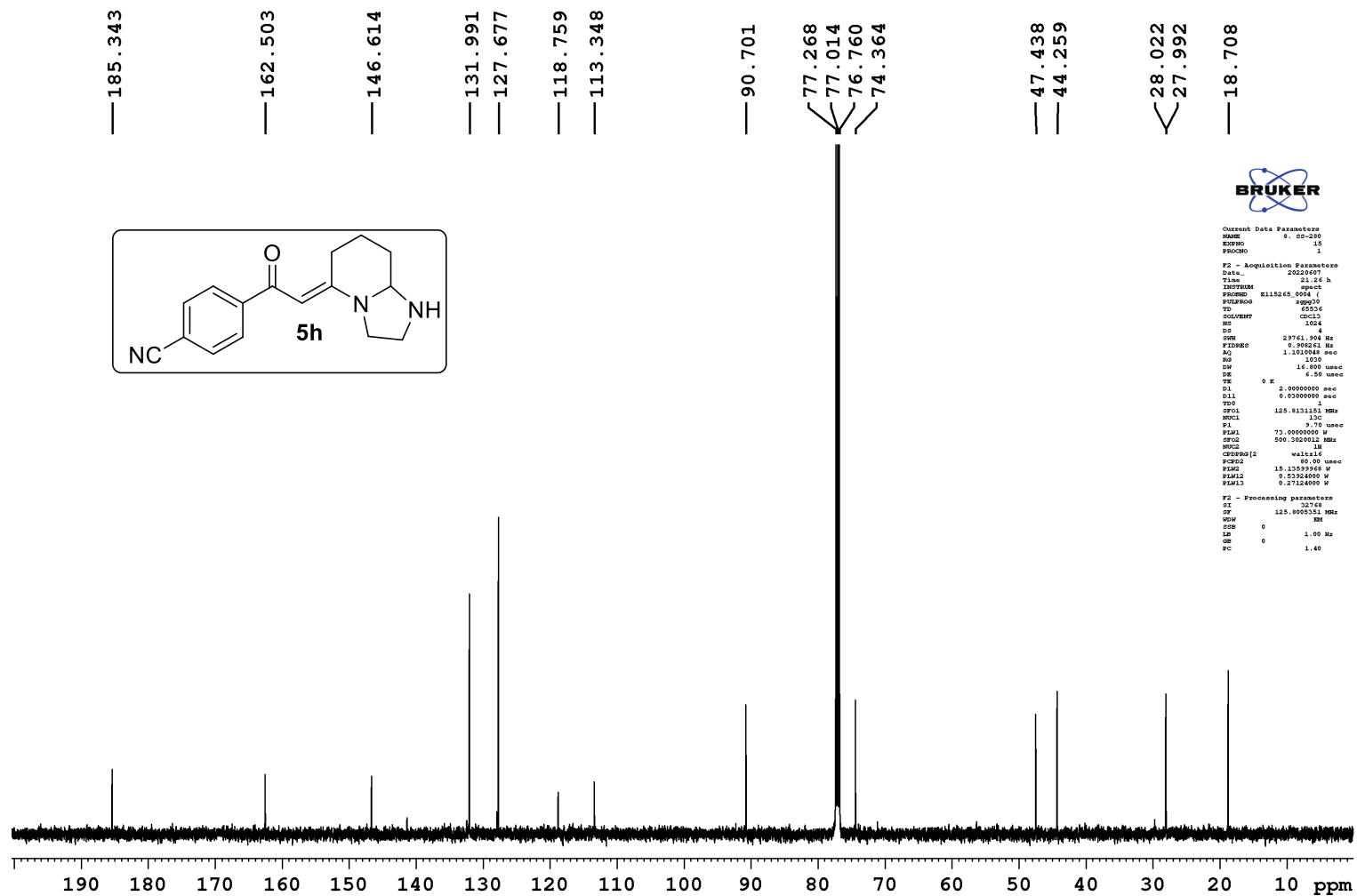
Current Data Parameters  
NAME 8. SS-280  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220607  
Time 20.29 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 287  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLN1 15.1359996 W

F2 - Processing parameters  
SI 65536  
SF 500.300093 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



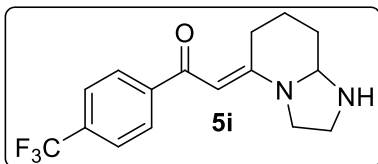
ES-SS-280, 13C, CDC13, 07-06-2022



```
Current Data Parameters
NAME      8_05-280
EXPNO    15
PROCNO   1
F2 - Acquisition Parameters
Date_    20220607
Time     21.24 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  cdcl3
NS        4
DS        4
SFO      29761.994 MHz
FIDRES   0.988261 Hz
AQ        1.101068 sec
RG         4028
DF         14.808 usec
DE         6.50 usec
TE        0 K
D1         2.0000000 sec
d11        0.2000000 sec
TD0        1
SFO1      125.8131011 MHz
NUC1       13C
P1         1.70 usec
PC1        150
P1P1      73.0000000 W
SFO2      500.1325012 MHz
NUC2       1H
CPDPRG2  waltz16
PCPD2     80.00 usec
P1P2      18.1335948 W
P1P12     0.53264000 W
P1P13     0.27124000 W
F2 - Processing parameters
SI         32768
SF         125.8055151 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-310R3\_1H\_CDCl3\_10-09-2023

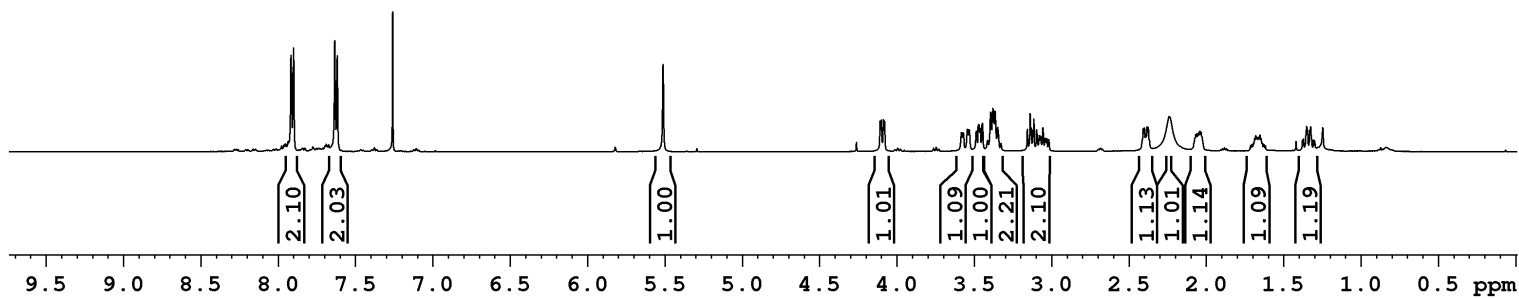
7.916  
7.900  
7.634  
7.618  
7.260  
5.511  
4.108  
4.100  
4.087  
4.079  
3.582  
3.571  
3.543  
3.532  
3.489  
3.484  
3.469  
3.460  
3.449  
3.445  
3.394  
3.378  
3.365  
3.348  
3.156  
3.138  
3.132  
3.114  
3.096  
3.079  
3.070  
3.055  
3.040  
2.407  
2.400  
2.391  
2.382  
2.375  
2.238  
2.208  
2.060  
2.053  
2.046  
2.040  
2.032  
2.027  
1.679  
1.675  
1.668  
1.664  
1.657  
1.652  
1.646  
1.356  
1.351  
1.345  
1.331  
1.324



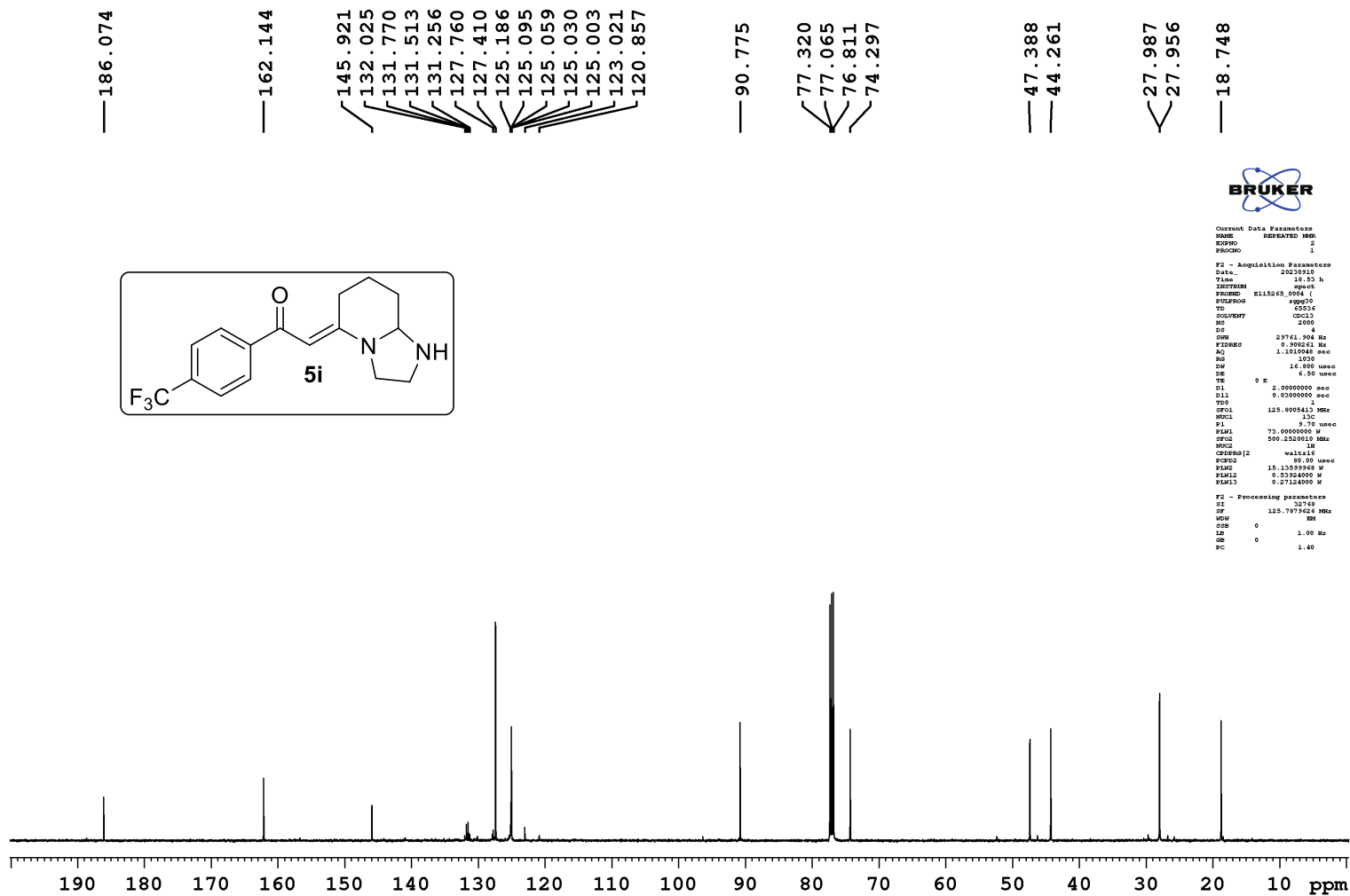
Current Data Parameters  
NAME REPEATED NMR  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230910  
Time 16.57 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 228  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLN1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500148 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



ES-SS-310R3\_13C\_CDC13\_10-09-2023



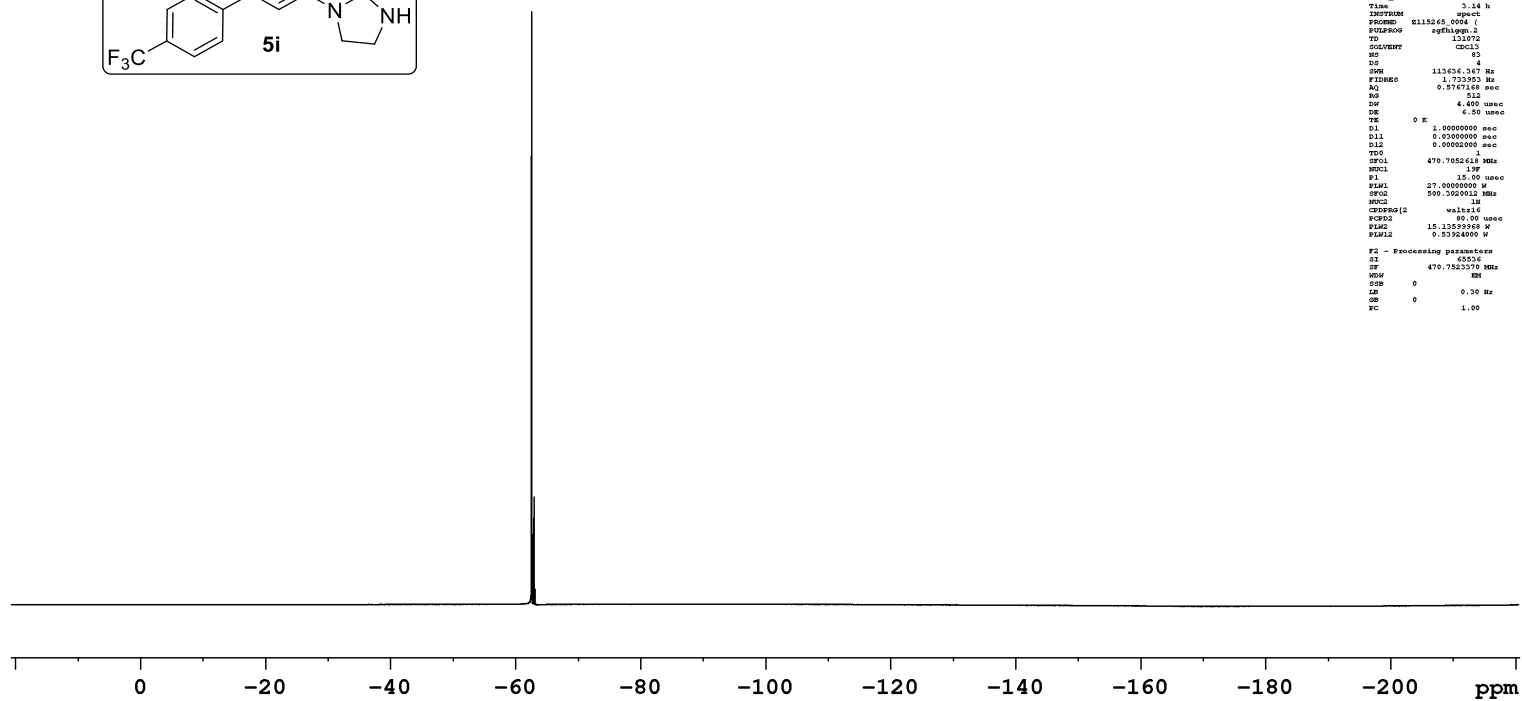
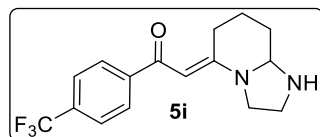
```
Current Data Parameters
NAME          REPEATED 160
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20230910
Time          16.55 h
INSTRUM       spect
PROBHD        5mmBBO
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            2000
DS            4
SFO          29761.994 MHz
FIDRES        0.986261 MHz
AQ            1.101068 sec
RG            3078
DF            14.908 usec
DE            6.50 usec
TE            300 K
D1            2.0000000 sec
d11           0.0200000 sec
TD0           1
SFO1          125.905411 MHz
NUC1          13C
PC1           150
P1           3.70 usec
P1M1          73.0000000 MHz
SFO2          500.1302610 MHz
NUC2          1H
PCPDW2        18
PCPDW22       441414
PCPDW23       80.00 usec
P1M2          16.1335948 MHz
P1M12         0.53264000 MHz
P1M13         0.27124000 MHz

F2 - Processing parameters
SI            32768
SF            125.7679624 MHz
WDW           EM
SSB           0
LB            1.00 MHz
GB            0
PC            1.40
```

ES-SS-310r\_19F; CDC13; 11-07-2022

— -62.647



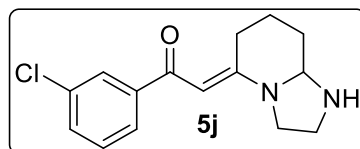
```
Current Data Parameters
NAME      9: ES-310r
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20220711
Time      7:14 h
INSTRUM   spect
PROBHD    E115265.0064
PULPROG   zgpg30
TD        131072
SOLVENT   CDCl3
NS        4
DS        4
SWH        113436.367 Hz
FIDRES    1.732393 Hz
AQ         0.5747168 sec
RG         512
DQ         4.400 usec
DE         6.50 usec
TE         300 K

D1         1.0000000 sec
D11        0.0200000 sec
D12        0.0002000 sec
TD0
SF01       470.752518 MHz
NUC1       19F
P1         15.00 usec
PL11       27.0000000 W
SF02       500.325012 MHz
NUC2
CPDPRG2   waltz16
PCPD2     80.00 usec
PLM2       15.1352999 W
PLM12     0.53524000 W

F2 - Processing parameters
SI         32768
SF         470.752518 MHz
DF         80
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

ES-SS-300R, 1H, CDC13, 15-06-2022



7.799  
7.724  
7.709  
7.380  
7.365  
7.328  
7.313  
7.297  
7.269

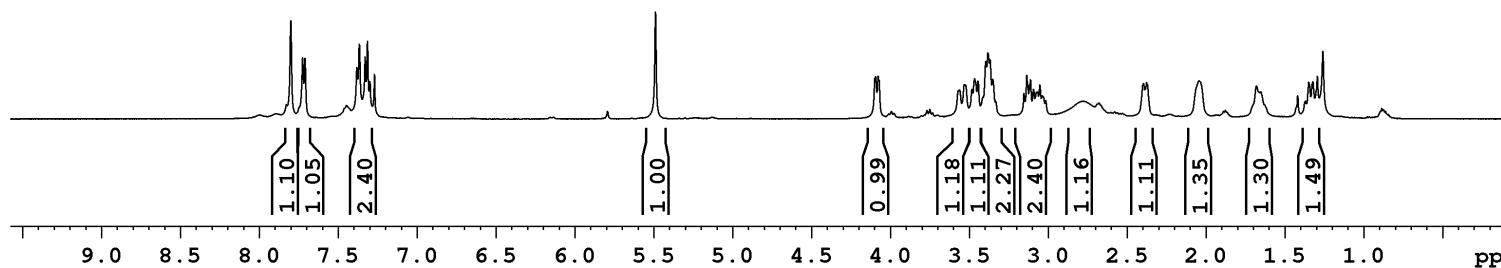
5.487  
4.096  
4.091  
4.076  
3.568  
3.559  
3.530  
3.521  
3.480  
3.464  
3.444  
3.394  
3.380  
3.367  
3.349  
3.151  
3.134  
3.110  
3.092  
3.073  
3.066  
3.051  
3.036  
3.028  
3.014  
2.775  
2.393  
2.375  
2.041  
2.034  
1.677  
1.650  
1.372  
1.366  
1.346



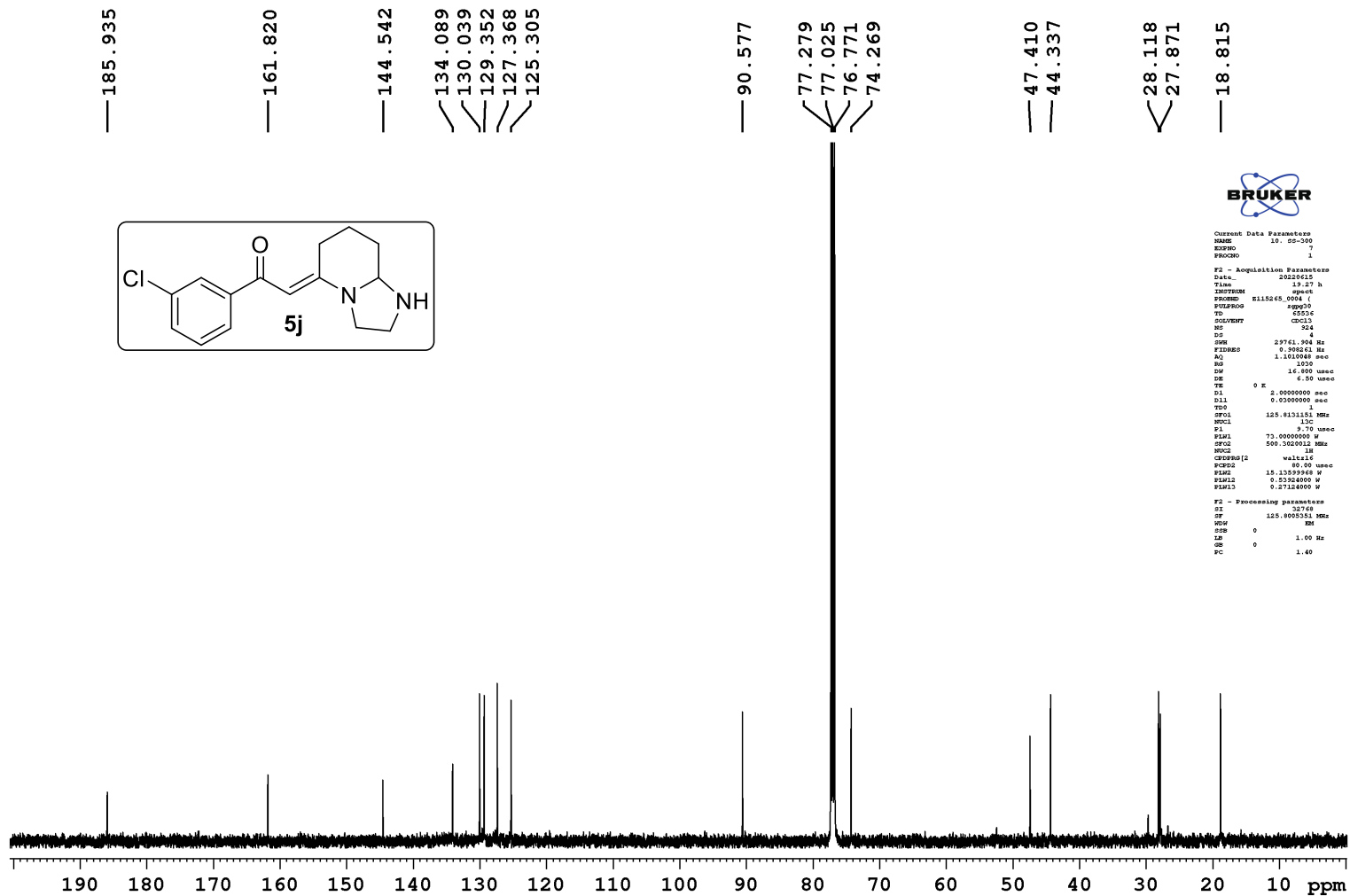
```
Current Data Parameters
NAME      10. SS-300
EXPNO     8
PROCNO    1

F2 - Acquisition Parameters
Date_     20220615
Time      19.32 h
INSTRUM   spect
PROBHD    Z115265.0004 (
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ         3.2747999 sec
RG         181
DW         50.000 usec
DE         6.50 usec
TE         0 K
D1         1.00000000 sec
TDO        1
SFO1       500.3030896 MHz
NUC1       1H
P1         15.10 usec
PLM1       15.13599968 W

F2 - Processing parameters
SI         65536
SF         500.300106 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



ES-SS-300, 13C, CDC13, 15-06-2022

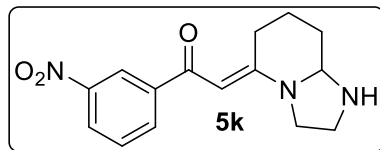


```
Current Data Parameters
NAME      10_05-200
EXPNO     1
PROCNO    1
F2 - Acquisition Parameters
Date_     20220615
Time      15.27 h
INSTRUM   spect
PROBHD    BBO51
PULPROG   zgpg30
TD        65536
SOLVENT   cdcl3
NS        204
DS        4
SFO      29761.994 MHz
FIDRES    0.988261 Hz
AQ        1.102068 sec
RG        4028
DM        14.800 usec
DE        6.50 usec
TE        0 K
D1        2.0000000 sec
d11       0.2000000 sec
TD0       1
SFO1      125.8151511 MHz
NUC1       13C
PC1        150 usec
P1         1.70 usec
P1M1      70.00000000 W
SFO2      500.1320212 MHz
NUC2       1H
PC2M2     18
PC2M2(2)  18
P2M2      80.00 usec
P2M2      18.1359948 W
P1M12     0.53264000 W
P1M13     0.27124000 W
F2 - Processing parameters
SI        32768
SF        125.8055151 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```



ES-SS-298R3\_1H\_CDCl3\_07-09-2023

8.631  
8.258  
8.244  
8.242  
8.198  
8.183  
7.579  
7.563  
7.547  
7.269  
5.536  
4.126  
4.120  
4.105  
4.099  
3.589  
3.579  
3.551  
3.541  
3.515  
3.500  
3.496  
3.492  
3.476  
3.445  
3.425  
3.406  
3.388  
3.175  
3.158  
3.152  
3.140  
3.134  
3.113  
3.097  
3.089  
3.073  
3.058  
3.050  
3.027  
2.420  
2.420  
2.412  
2.402  
2.395  
2.089  
2.083  
2.075  
2.068  
2.062  
2.055  
1.826  
1.701  
1.697  
1.686  
1.674  
1.368  
1.342

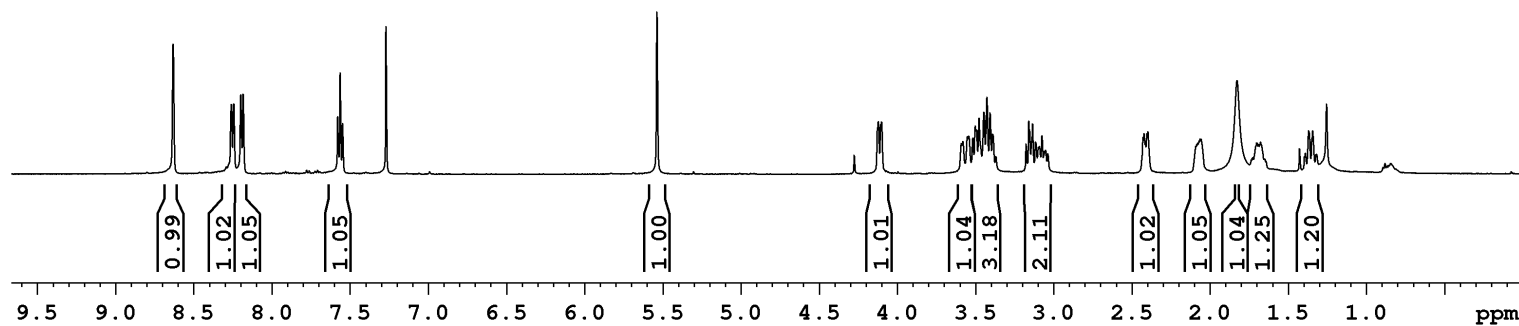


```

Current Data Parameters
NAME      REPEATED.nmr
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20230908
Time      0.59 h
INSTRUM   spect
PROBRD    Z115245.004 /
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         0
SWH        10000.000 Hz
FIDRES     0.305176 Hz
AQ          3.276799 sec
RG          228
DW          50.000 usec
DE          6.50 usec
TE          0 K
D1          1.00000000 sec
TDO         1
SFO1       500.2530890 MHz
NUC1        1H
P1          15.10 usec
PLN1        15.13599968 W

F2 - Processing parameters
SI          65536
SF          500.2500091 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
    
```



ES-SS-298R3\_13C\_CDC13\_07-09-2023

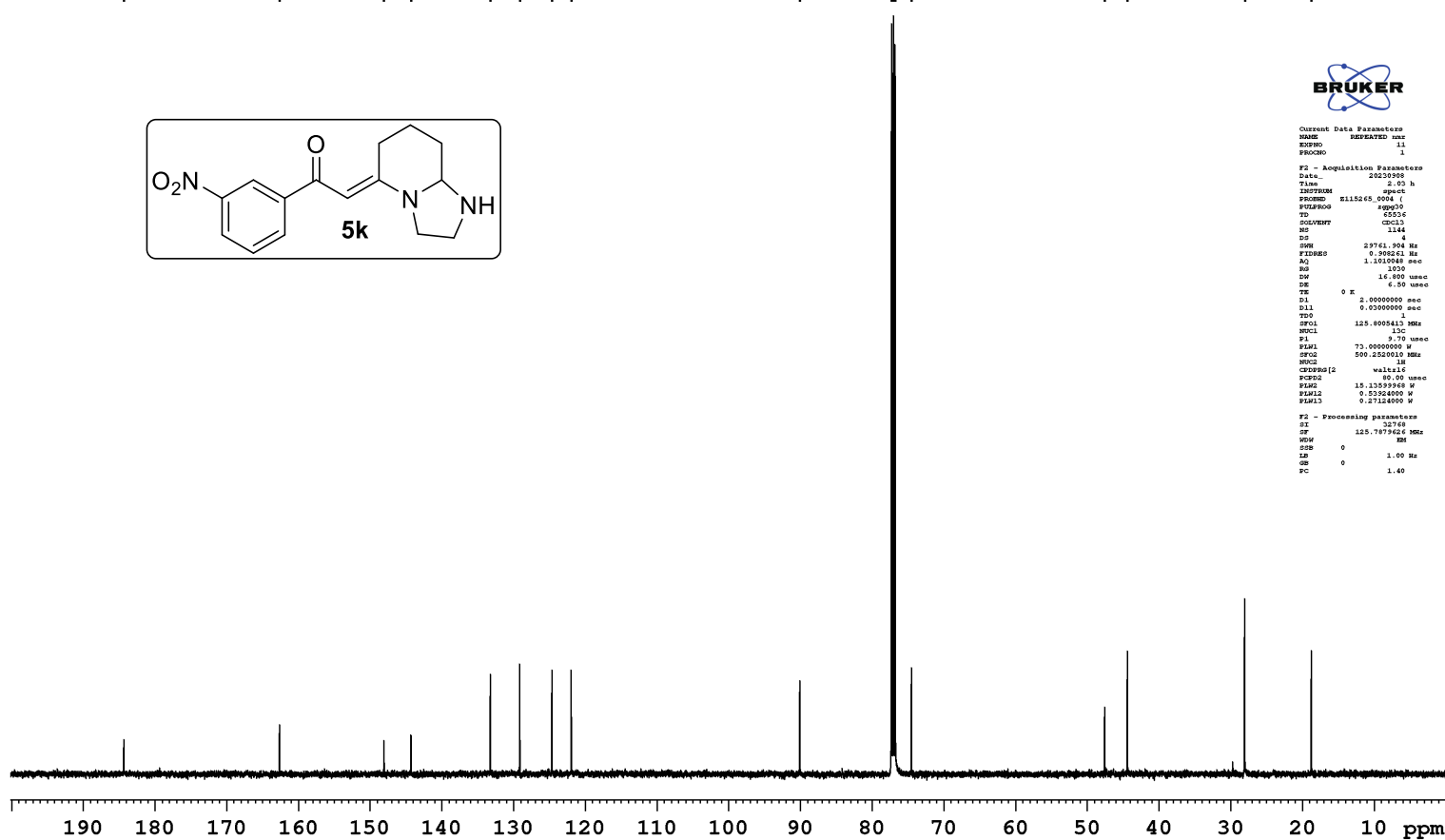
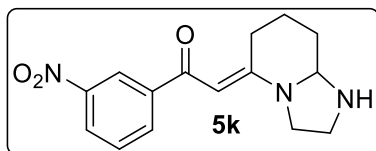
— 184.318  
— 162.628  
— 148.065  
— 144.291  
— 133.223  
— 129.124  
— 124.627  
— 121.944

— 90.081  
77.280  
77.026  
76.773  
74.505

— 47.558  
— 44.376

— 28.028

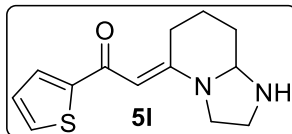
— 18.736



Current Data Parameters  
NAME REPEATED Hz  
EXPRM 11  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20230908  
Time 21.05 h  
INSTRUM spect  
PROBHD 5mm  
PULPROG zgpg30  
TD 65536  
SOLVENT cdc13  
NS 1144  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.398261 MHz  
AQ 1.1010048 sec  
RG 4028  
DM 14.900 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
D11 0.2000000 sec  
TD0 1  
SFO1 125.9054113 MHz  
NUC1 13C  
PC1 150 usec  
P1 1.50 usec  
PL1 0.0000000 W  
SFO2 500.1320101 MHz  
NUC2 1H  
CROSSP2  
PCP2 80.00 usec  
P2 18.1335948 W  
PL2 0.53264000 W  
PL13 0.27124000 W  
F2 - Processing parameters  
F1 29761.994 MHz  
SFO 125.9054113 MHz  
NUC 13C  
SFO 500.1320101 MHz  
PC 1.40

ES-SS-2-100R\_1H\_CDC13\_17-09-2023

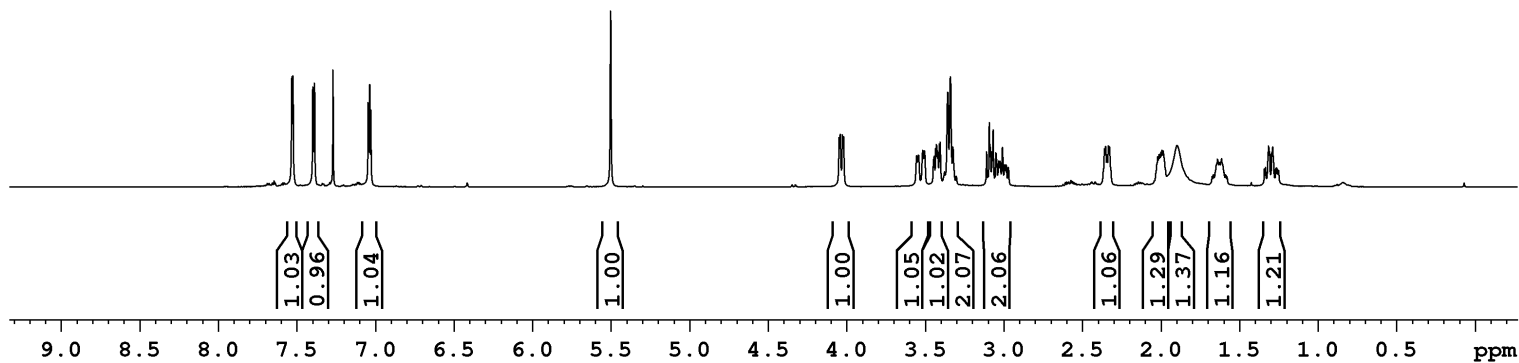
7.531  
7.525  
7.524  
7.398  
7.396  
7.388  
7.387  
7.269  
7.045  
7.038  
7.036  
7.028  
5.502  
4.047  
4.040  
4.026  
4.019  
3.553  
3.542  
3.515  
3.504  
3.447  
3.442  
3.433  
3.427  
3.423  
3.418  
3.409  
3.404  
3.355  
3.338  
3.323  
3.108  
3.091  
3.084  
3.073  
3.067  
3.049  
3.022  
3.008  
2.357  
2.351  
2.333  
2.326  
2.019  
2.011  
2.005  
1.997  
1.991  
1.984  
1.895  
1.639  
1.635  
1.612  
1.314  
1.307  
1.293  
1.287



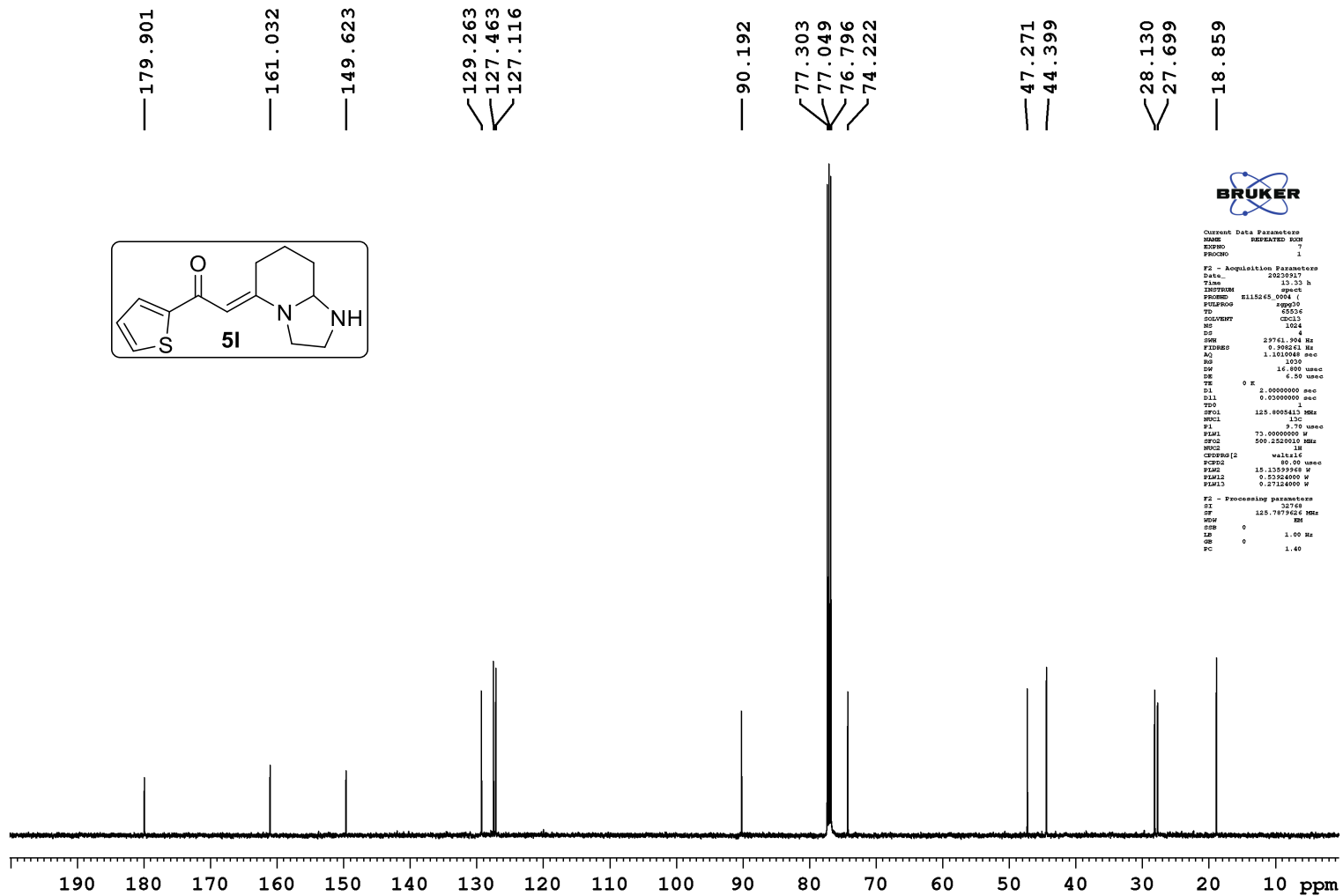
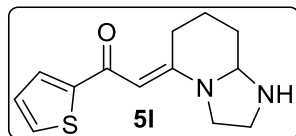
Current Data Parameters  
NAME REPEATED RUN  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230917  
Time 12.36 h  
INSTRUM spect  
PROCNO 2115245\_004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 161  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500093 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

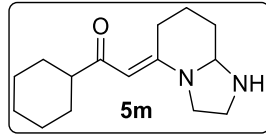


ES-SS-2-100\_13C\_CDC13\_17-09-2023

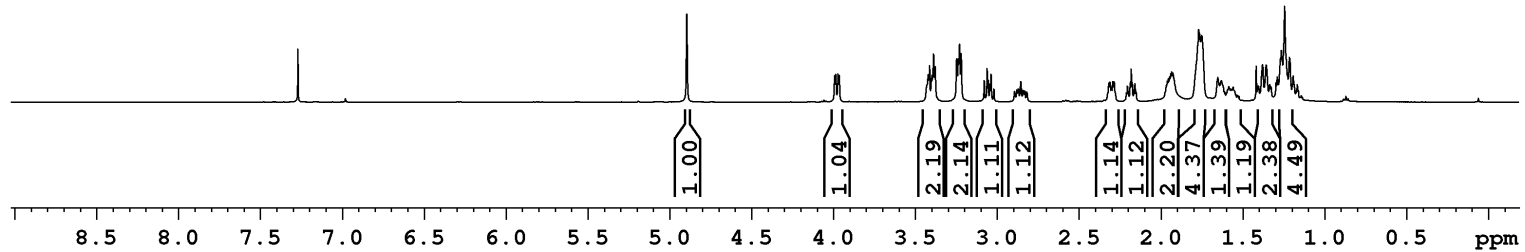


Current Data Parameters  
NAME REPEATED RUN  
EXPNO 7  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20230917  
Time 13:25 h  
INSTRUM spect  
PROBHD 515265.004 (1  
PULPROG zgpg30  
TD 65534  
SOLVENT cdc13  
NS 404  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.988261 Hz  
AQ 1.102048 sec  
RG 4028  
DM 14.800 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
D11 0.2000000 sec  
TD0 1  
SFO1 125.805413 MHz  
NUC1 13C  
P1 150 usec  
PL1 0  
PL12 70.0000000 W  
SFO2 500.132010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
PL2 18.1335948 W  
PL13 0.53264000 W  
PL14 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.767942 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-2-114\_1H\_CDC13\_20-11-2023



7.269



4.894  
3.991  
3.983  
3.970  
3.962  
3.420  
3.411  
3.396  
3.386  
3.377  
3.245  
3.235  
3.228  
3.218  
3.077  
3.059  
3.052  
3.042  
3.035  
3.017  
2.891  
2.877  
2.868  
2.854  
2.839  
2.830  
2.816  
2.309  
2.291  
2.203  
2.179  
2.173  
2.156  
1.931  
1.924  
1.767  
1.748  
1.650  
1.629  
1.592  
1.556  
1.533  
1.401  
1.376  
1.354  
1.332



Current Data Parameters  
NAME 20 nov 2023  
EXPNO 1  
PROCNO 1

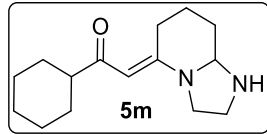
F2 - Acquisition Parameters  
Date\_ 20231120  
Time 19.46 h  
INSTRUM spect  
PROBHD Z115265.004 ( 1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2747999 sec  
RG 101  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500091 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-2-114\_13C\_CDC13\_20-11-2023

— 200.681

— 159.531

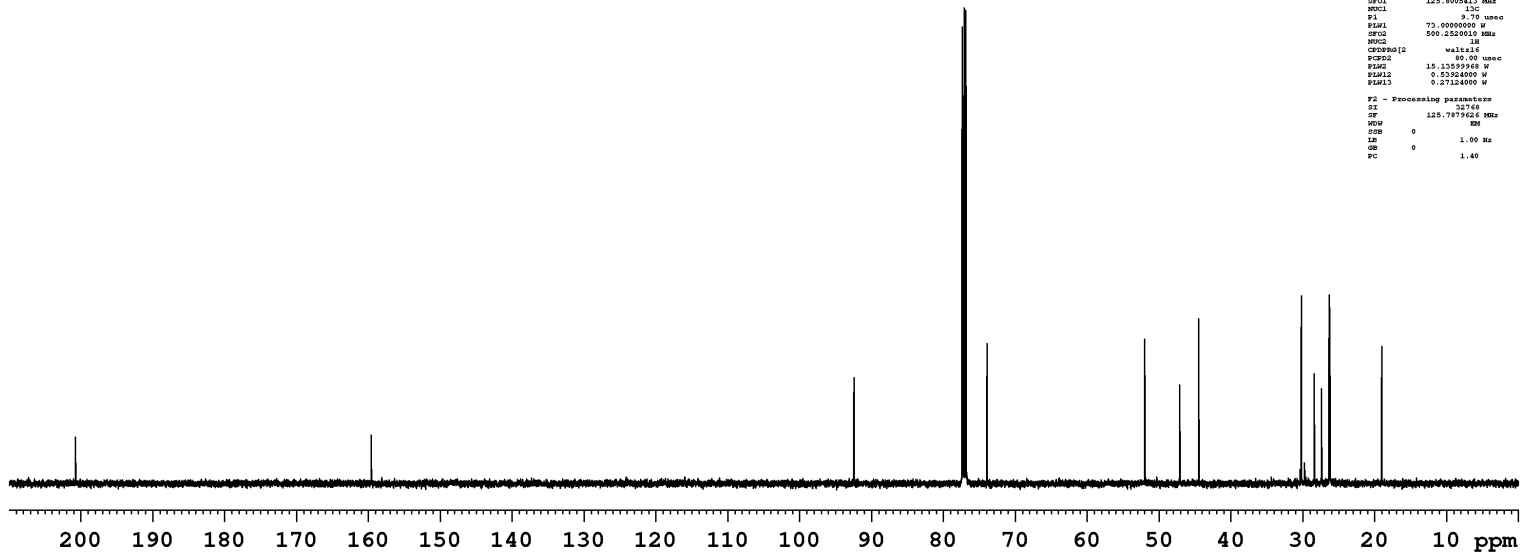


— 92.384

77.305  
77.050  
76.797  
73.851

— 51.914  
— 47.040  
— 44.398

30.143  
30.123  
28.327  
27.323  
26.266  
26.152  
18.948

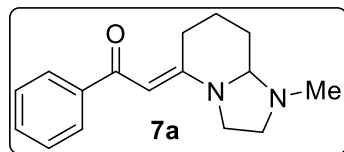


```
Current Data Parameters
NAME      20 nov 2023
EXPNO    2
PROCNO    1

F2 - Acquisition Parameters
Date_     20211120
Time      15:59 h
INSTRUM   spect
PROBHD    E115245.0054 (
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        207
DS        4
SWH        29761.904 Hz
FIDRES    0.398241 Hz
AQ         1.102068 sec
RG         2050
DM         164.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
d11        0.2000000 sec
TDO        125.8005413 MHz
SFO1       125.8005413 MHz
NUC1       13C
P1         8.75 usec
PLM1       73.0000000 W
SFO2       500.1325010 MHz
NUC2       1H
CFO2WD2    14111.6
PCPD2      80.00 usec
PLM2       15.13259950 W
PLM12      0.53324000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7673614 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-2-77, 1H, CDCl3, 13-05-2022



7.842  
7.828  
7.377  
7.363  
7.269

5.544

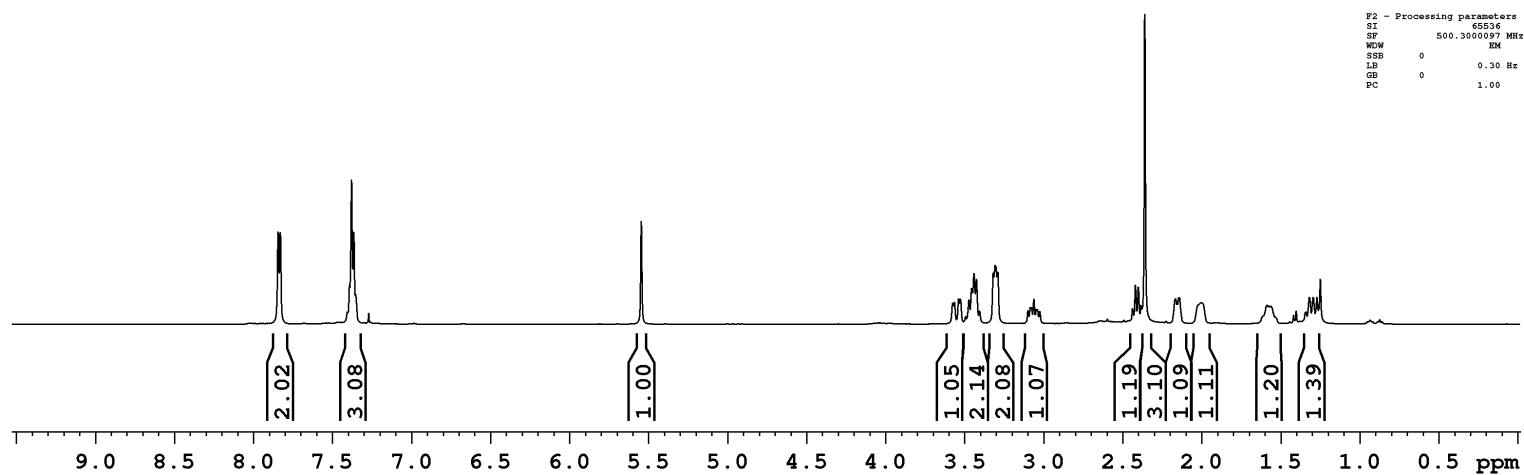
3.573  
3.563  
3.535  
3.524  
3.470  
3.438  
3.403  
3.317  
3.304  
3.288  
3.097  
3.060  
3.022  
2.435  
2.417  
2.399  
2.380  
2.358  
2.162  
2.138  
1.997  
1.582  
1.571  
1.559  
1.338  
1.292  
1.269



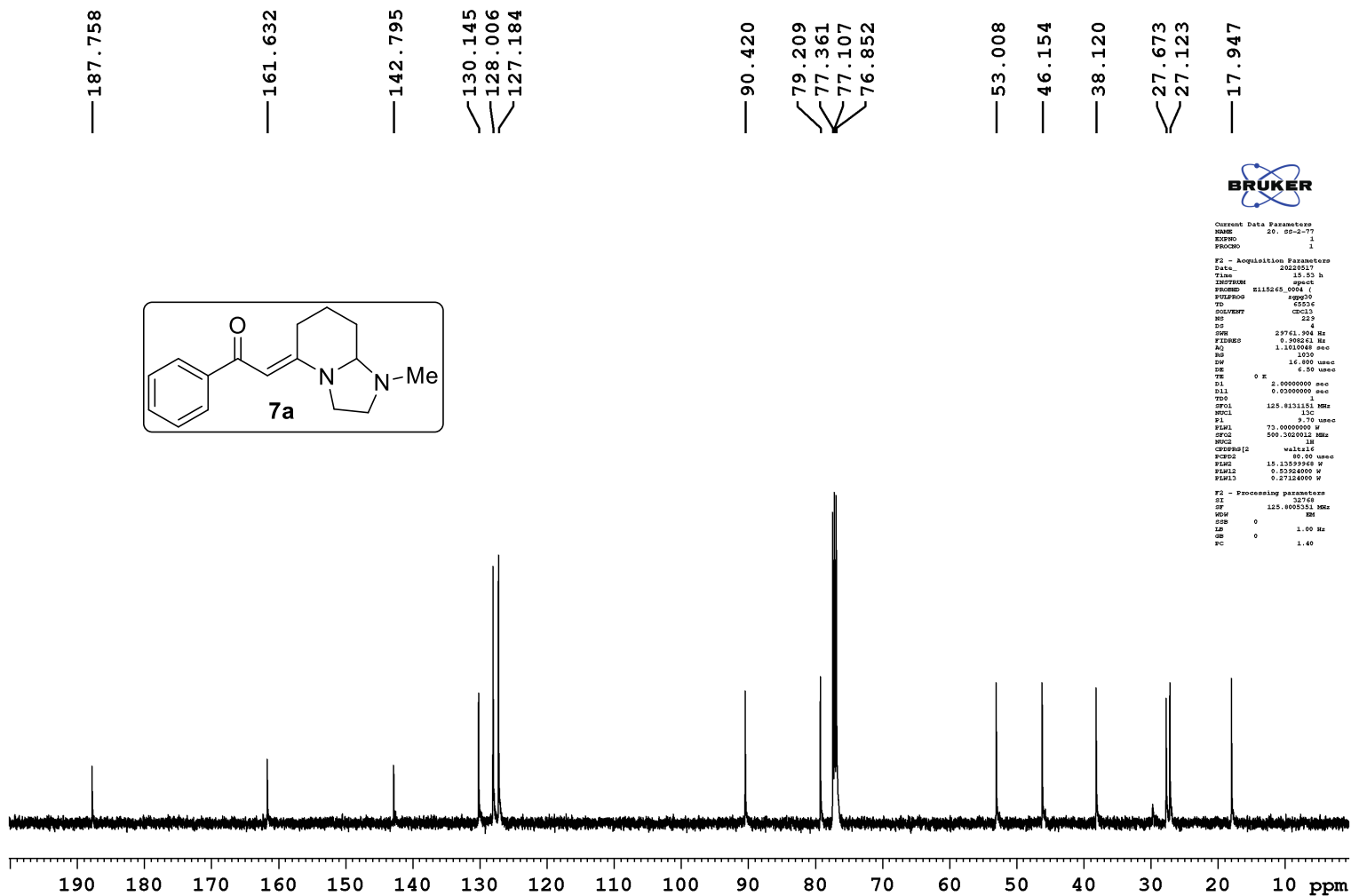
Current Data Parameters  
NAME 13-SS-2-77  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220513  
Time 15.46 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 71.8  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.0000000 sec  
TD0 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.300097 MHz  
NOM RM  
SSB 0  
LP 0.30 Hz  
GB 0  
PC 1.00



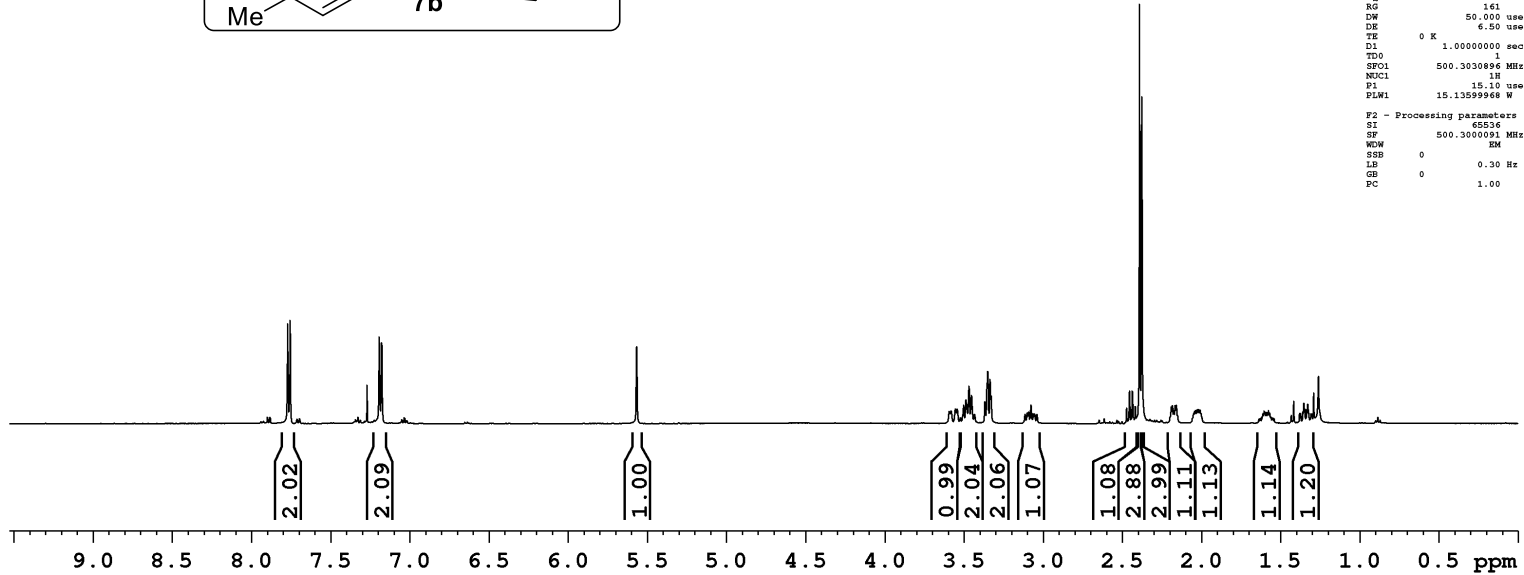
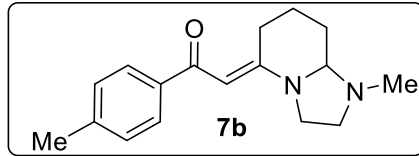
ES-SS-2-77, 13C, CDC13, 17-05-2022





ES-SS-PBP-26, 1H, CDC13, 13-05-2022

7.771  
7.754  
7.192  
7.176  
5.566  
3.591  
3.580  
3.553  
3.542  
3.501  
3.486  
3.481  
3.467  
3.451  
3.367  
3.365  
3.353  
3.349  
3.334  
3.327  
3.099  
3.090  
3.075  
3.061  
2.471  
2.390  
2.375  
2.189  
2.182  
2.165  
2.157  
2.048  
2.043  
2.035  
2.029  
2.021  
2.015  
2.008  
2.002  
1.610  
1.602  
1.598  
1.591  
1.587  
1.580  
1.575  
1.568  
1.379  
1.372  
1.358  
1.352  
1.347  
1.333  
1.327  
1.321  
1.307  
1.259

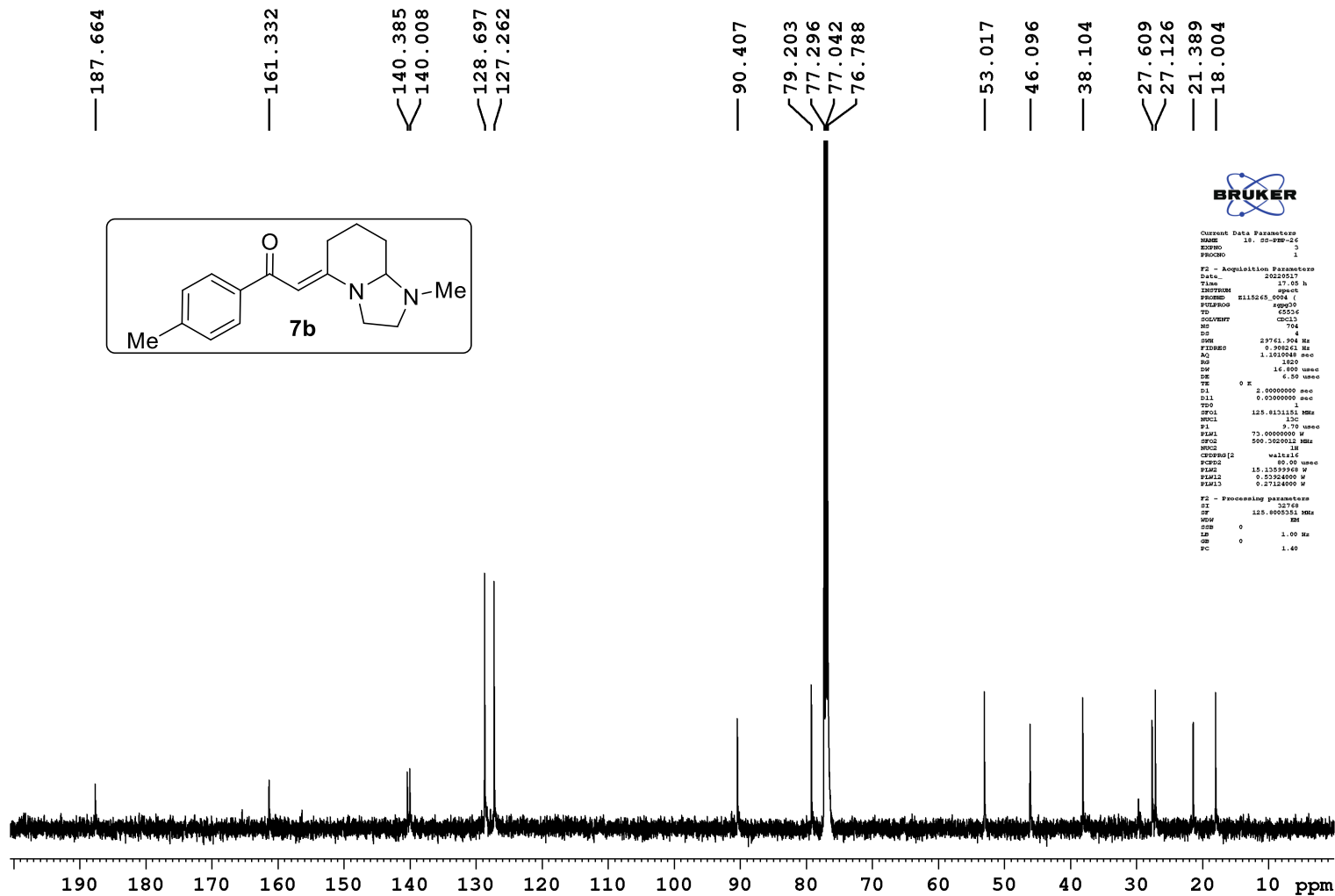


Current Data Parameters  
NAME 18\_SS-PBP-26  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220513  
Time 15:37 h  
INSTRUM spect  
PROBRD Z115245.004 f  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 161  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLN1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.300091 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-PBP-26; 13C, CDC13, 17-05-2022

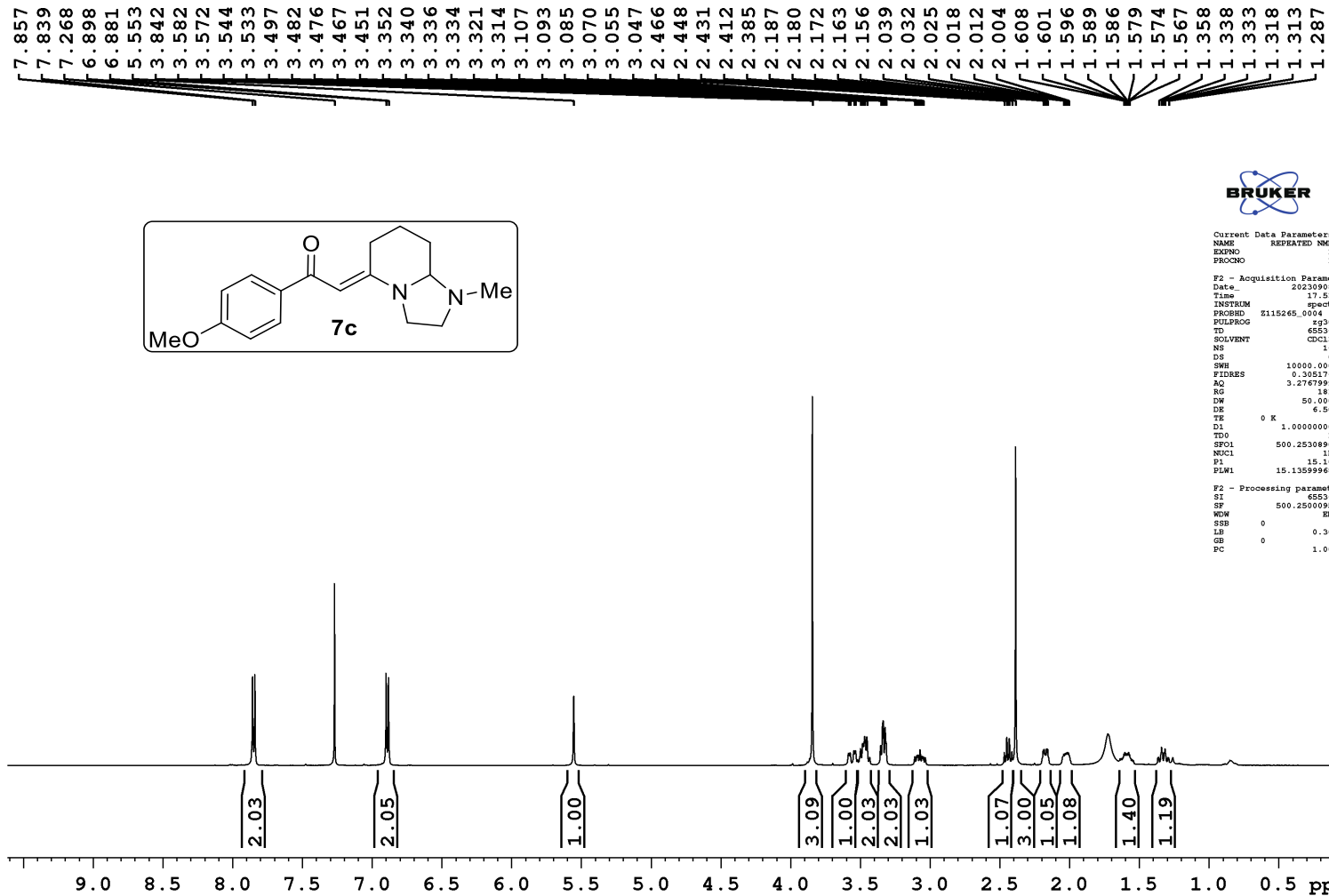


```
Current Data Parameters
NAME      18_SS-PBP-26
EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_    20220517
Time     11:05 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  cdcl3
NS        704
DS        4
SFO      29761.994 MHz
FIDRES   0.398261 MHz
AQ        1.101068 sec
RG        320
DM        14.800 usec
DE        6.50 usec
TE        300.2 K
D1        2.0000000 sec
d11       0.2000000 sec
TD0       1
SFO1      125.8151515 MHz
NUC1       13C
PC1        150 usec
P1         3.70 usec
P1P1      70.0000000 W
SFO2      500.302012 MHz
NUC2       1H
PC2P2[2]  18 usec
P2P2[2]   80.00 usec
P1P2      18.1359948 W
P1P12     0.53924000 W
P1P13     0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.8055151 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-2-82R\_1H\_CDC13\_08-09-2023



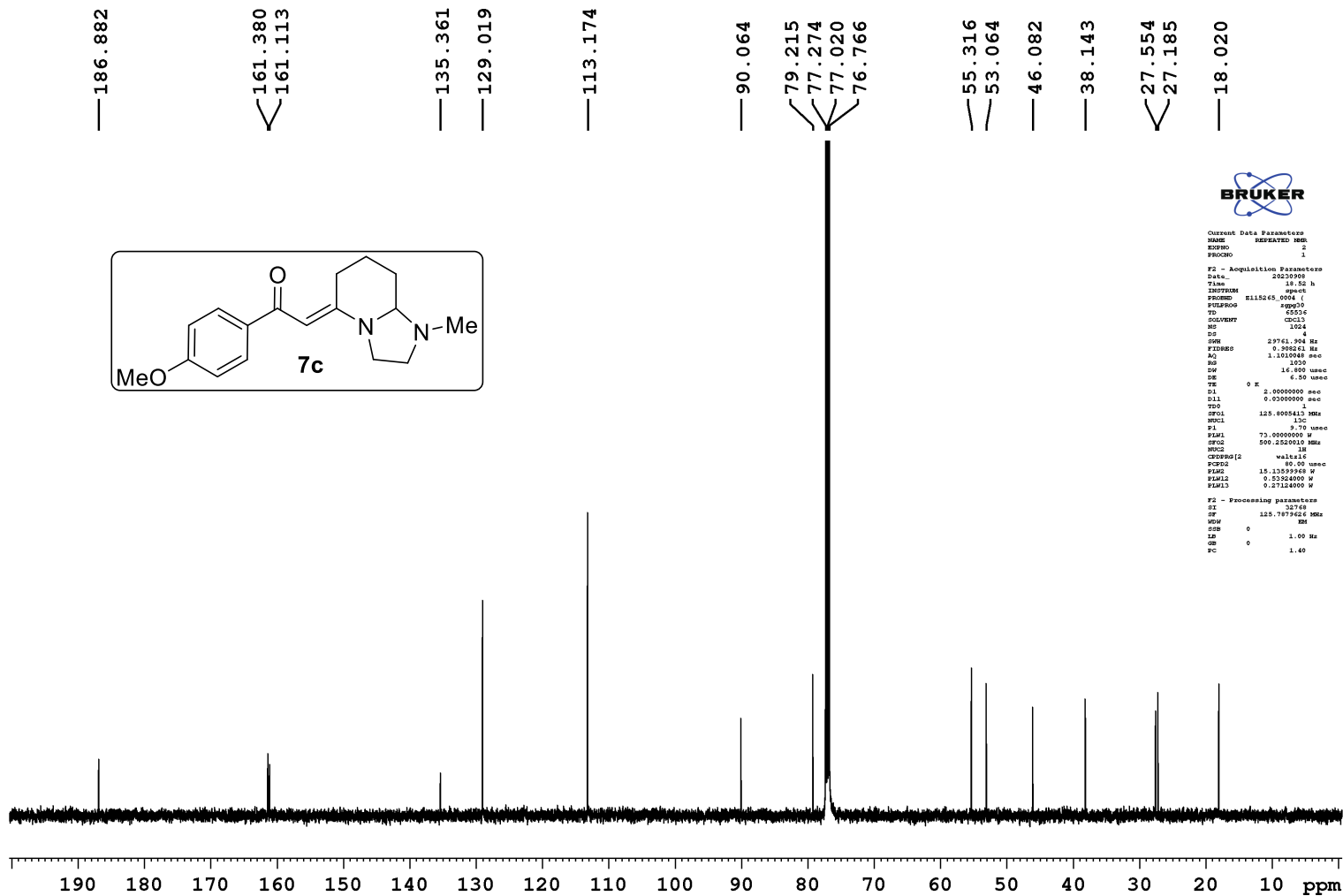
```

Current Data Parameters
NAME      REPEATED NMR
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20230908
Time     17.53 h
INSTRUM  spect
PROBHD   Z115265.0004 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        0
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ        3.2747999 sec
RG        181
DW        50.000 usec
DE        6.50 usec
TE        0 K
D1        1.00000000 sec
TDO       1
SFO1     500.2530090 MHz
NUC1      1H
P1        15.10 usec
PLW1     15.13599968 W

F2 - Processing parameters
SI        65536
SF        500.2500095 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

ES-SS-2-82R\_13C\_CDC13\_08-09-2023

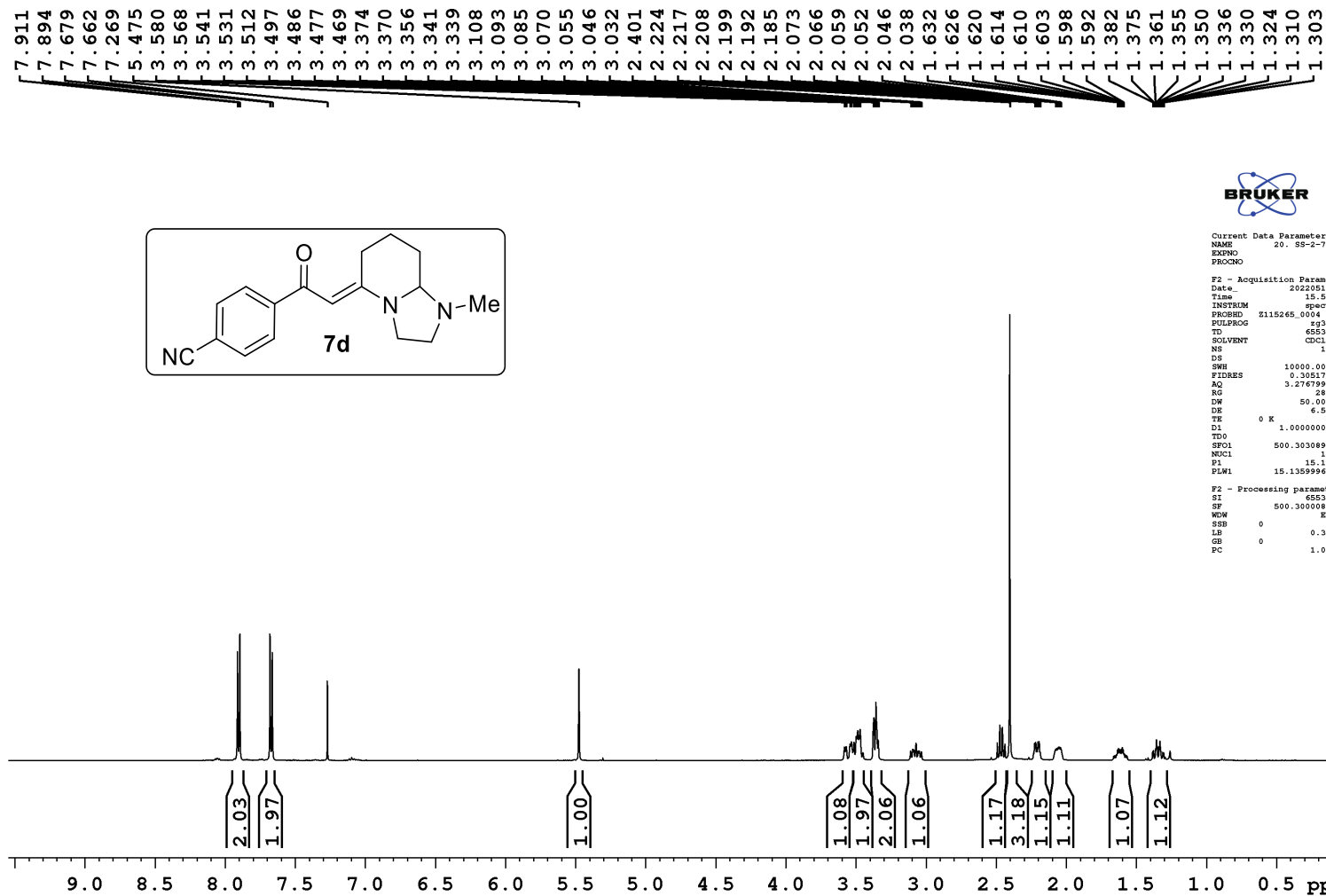


```
Current Data Parameters
NAME      REVEATED.MS
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20230908
Time     15:52 h
INSTRUM  spect
PROBHD   E15245.0064
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       29761.904 Hz
FIDRES   0.998261 Hz
AQ        1.1037048 sec
RG         1020
DQ        16.800 usec
DE         6.50 usec
TE        0 K
D1         2.0000000 sec
d11       0.0000000 sec
TDS       125.4004413 MHz
SFO1      125.4004413 MHz
NUC1       13C
P1         150 usec
PL1       70.0000000 W
SFO2      500.1325010 MHz
NUC2       1H
CPDPRG2  waltz16
PCPD2     80.00 usec
PL2      15.1325000 W
PL12     0.5324000 W
PL13     0.2712400 W

F2 - Processing parameters
SI         32768
SF         125.7679244 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-2-78, 1H, CDC13, 13-05-2022

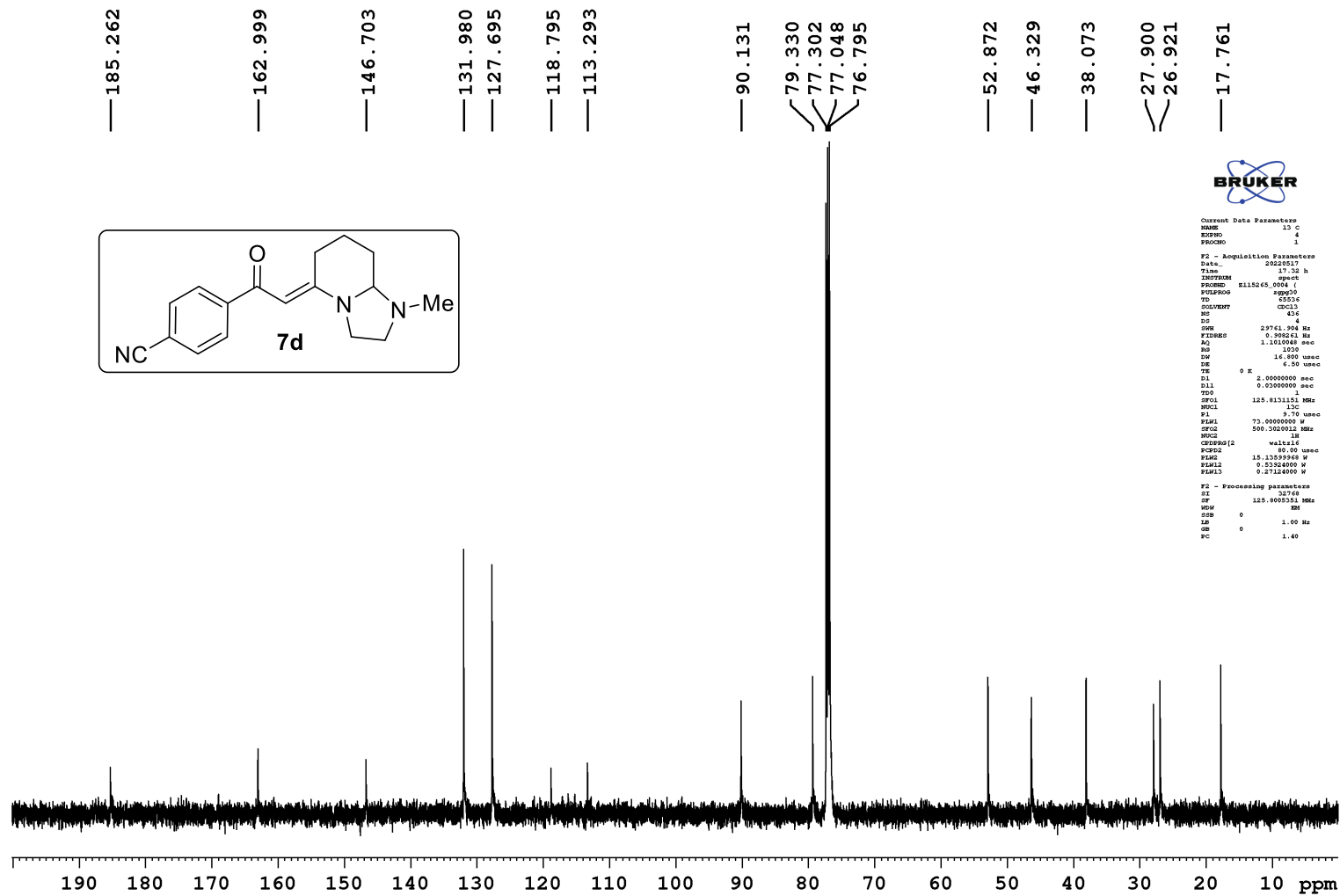


Current Data Parameters  
NAME 20. SS-2-78  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220513  
Time 15.55 h  
INSTRUM spect  
PROBRD Z115245.004 f  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 287  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

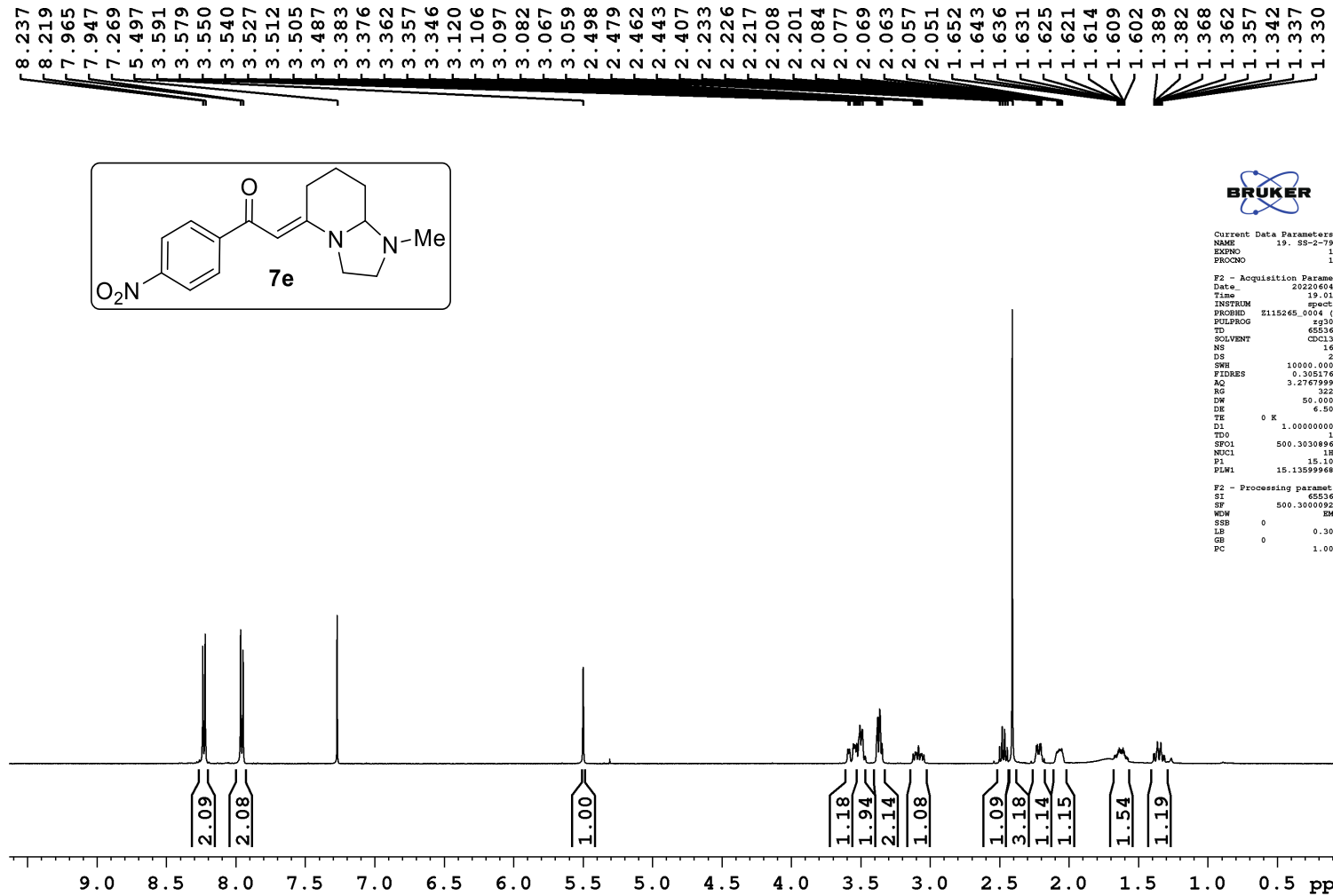
F2 - Processing parameters  
SI 65536  
SF 500.3000089 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-78; 13C, CDC13, 17-05-2022



Current Data Parameters  
NAME 13 C  
EXPNO 4  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220517  
Time 17:32 h  
INSTRUM spect  
PROBHD 5mmBBO  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 4  
DS 4  
SFO 29761.994 Hz  
FIDRES 0.988261 Hz  
AQ 1.102048 sec  
RG 4028  
DM 14.808 usec  
DE 6.50 usec  
TE O K  
D1 2.0000000 sec  
D11 0.0200000 sec  
TD0 1  
SFO1 125.813151 MHz  
NUC1 13C  
P1 1.70 usec  
PL11 70.0000000 W  
SFO2 500.302012 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
PL12 18.1339948 W  
PL13 0.53264000 W  
PL14 0.27124000 W  
F2 - Processing parameters  
F1 125.805521 MHz  
SF 500.302012 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-2-79, 1H, CDC13, 04-06-2022

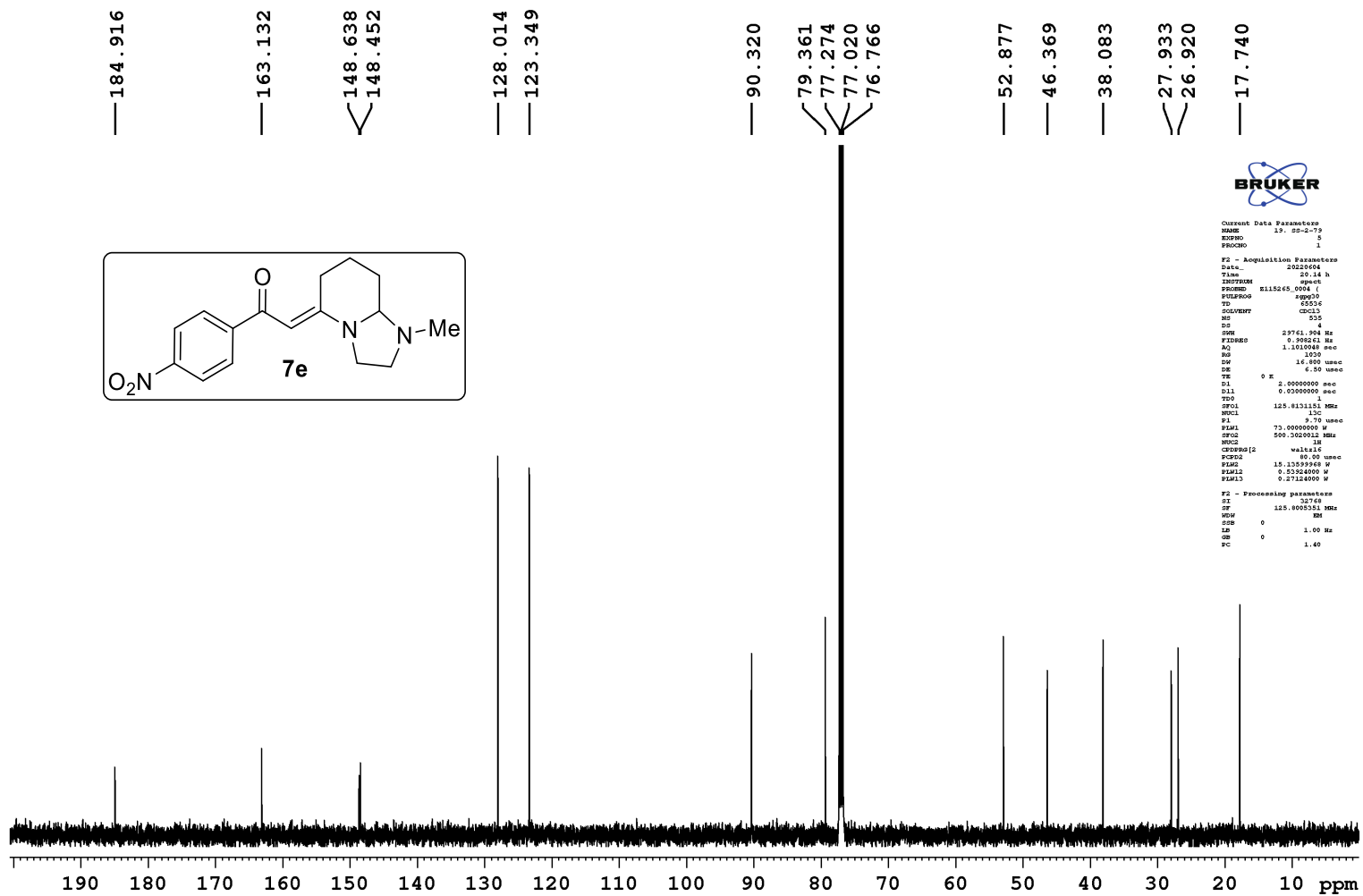


Current Data Parameters  
NAME 19-SS-2-79  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220604  
Time 19.01 h  
INSTRUM spect  
PROBHD Z115265.004 ( eg30  
PULPROG gms36  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.274799 sec  
RG 322  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.0000000 sec  
TDO 1  
SFO1 500.300092 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.300092 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

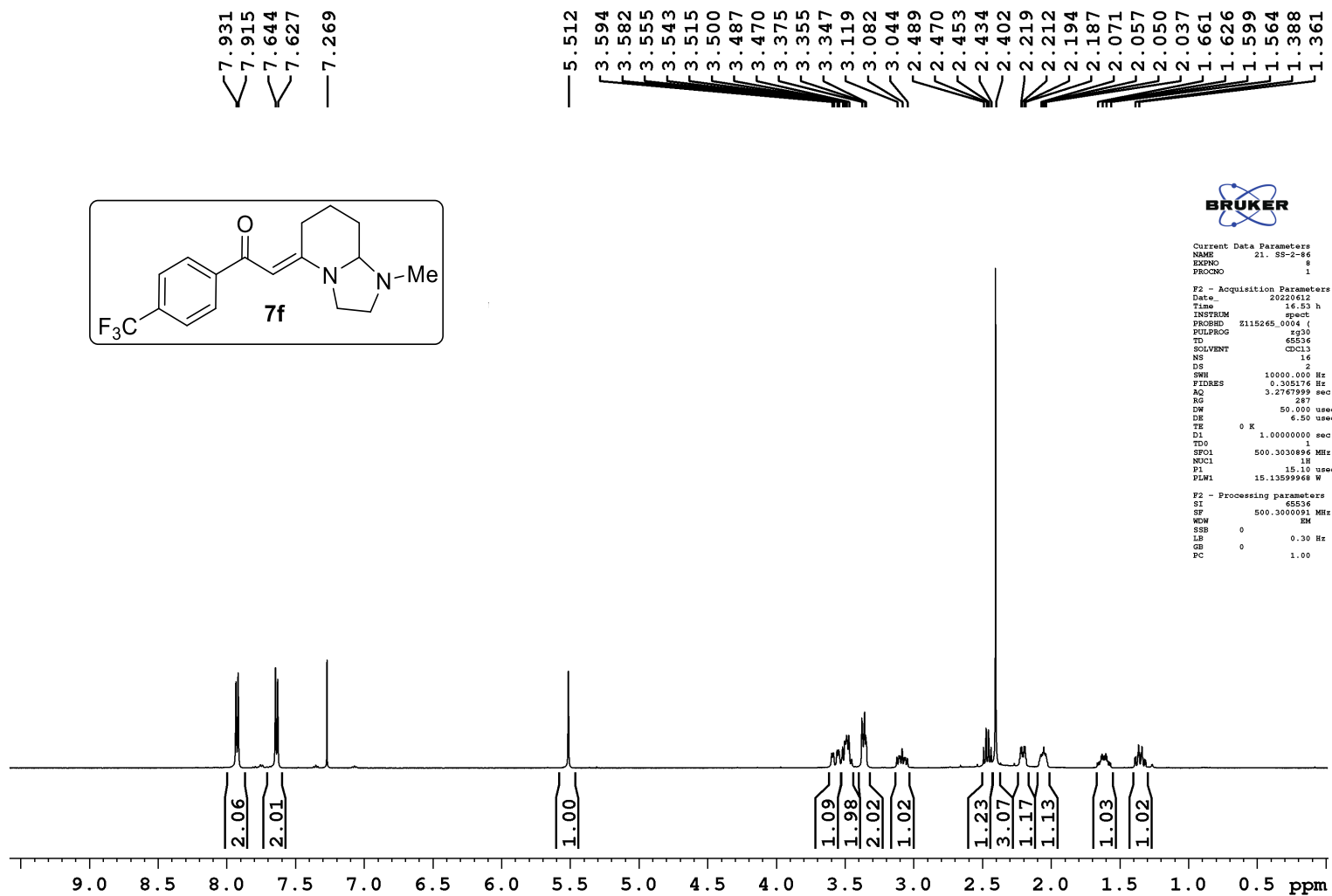
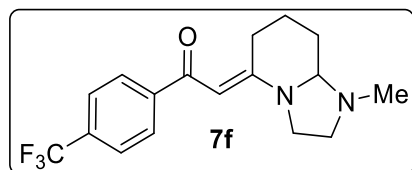
ES-SS-2-79, 13C, CDCl3, 04-06-2022



Current Data Parameters  
NAME 19\_SS-2-79  
EXPNO 5  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220604  
Time 20:14 h  
INSTRUM spect  
PROBHD 5115265.0004 (1  
PULPROG zgpg30  
TD 65534  
SOLVENT cdcl3  
NS 512  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.098261 MHz  
AQ 1.101068 sec  
RG 4028  
DM 14.800 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
S11 0.2000000 sec  
TD0 1  
SFO1 125.815151 MHz  
NUC1 13C  
PC1 150 usec  
P1 1.70 usec  
PL11 70.0000000 W  
SFO2 500.302012 MHz  
NUC2 1H  
PCP2 18  
PL2 15.1359948 W  
P112 0.53244000 W  
P113 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.805511 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



ES-SS-2-86, 1H, CDC13, 12-06-2022

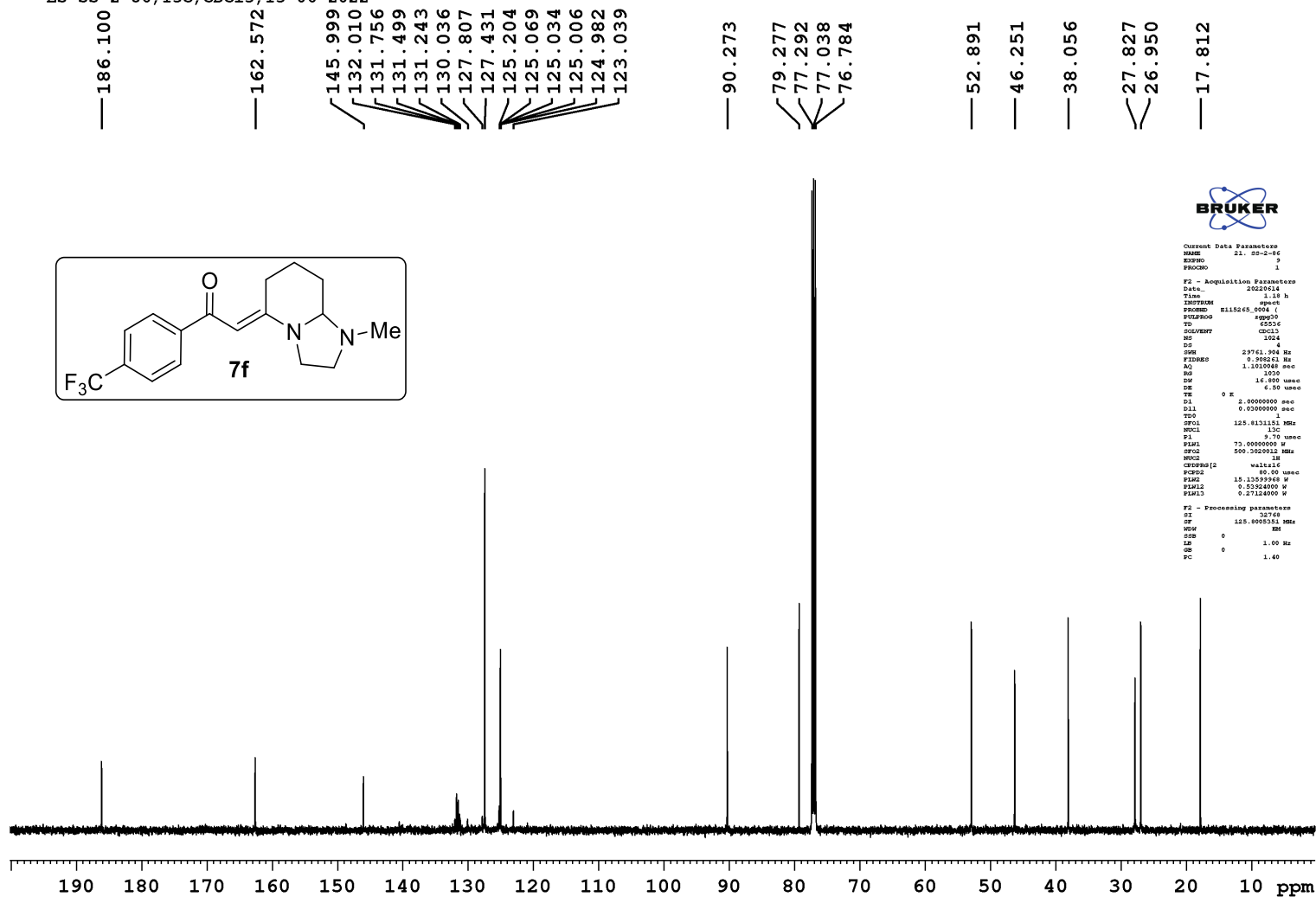


Current Data Parameters  
NAME 21. SS-2-86  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220612  
Time 16.53 h  
INSTRUM spect  
PROCNO Z115265\_0004 ( )  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.275799 sec  
RG 287  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.3000091 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-2-86, 13C, CDC13, 13-06-2022



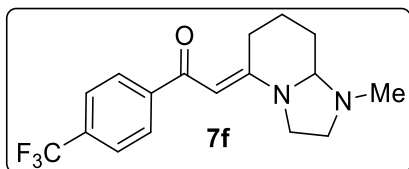
Current Data Parameters  
NAME 21. SS-2-86  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220614  
Time 11:18 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 4  
DS 4  
SFO 29761.994 Hz  
FIDRES 0.398261 Hz  
AQ 1.101008 sec  
RG 4028  
DM 14.800 usec  
DE 6.50 usec  
TE 300 K

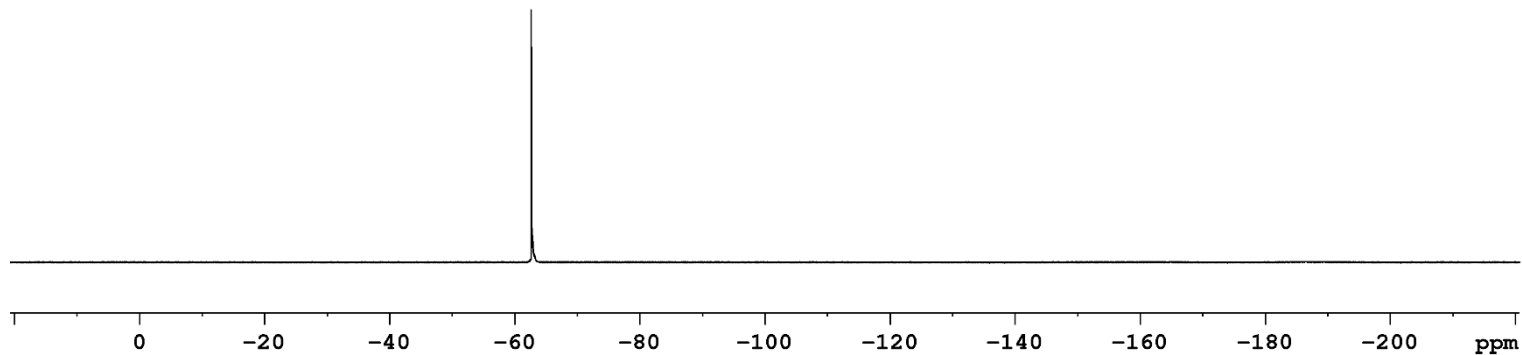
D1 2.0000000 sec  
S21 0.0200000 sec  
TD0 1  
SFO1 125.815151 MHz  
NUC1 13C  
P1 3.70 usec  
PL11 70.0000000 W  
SFO2 500.302012 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
PL12 18.1359948 W  
PL13 0.53264000 W  
PL14 0.27124000 W

F2 - Processing parameters  
SI 32768  
SF 125.805521 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-2-86\_19F\_CDC13\_26-12-2023



---62.590



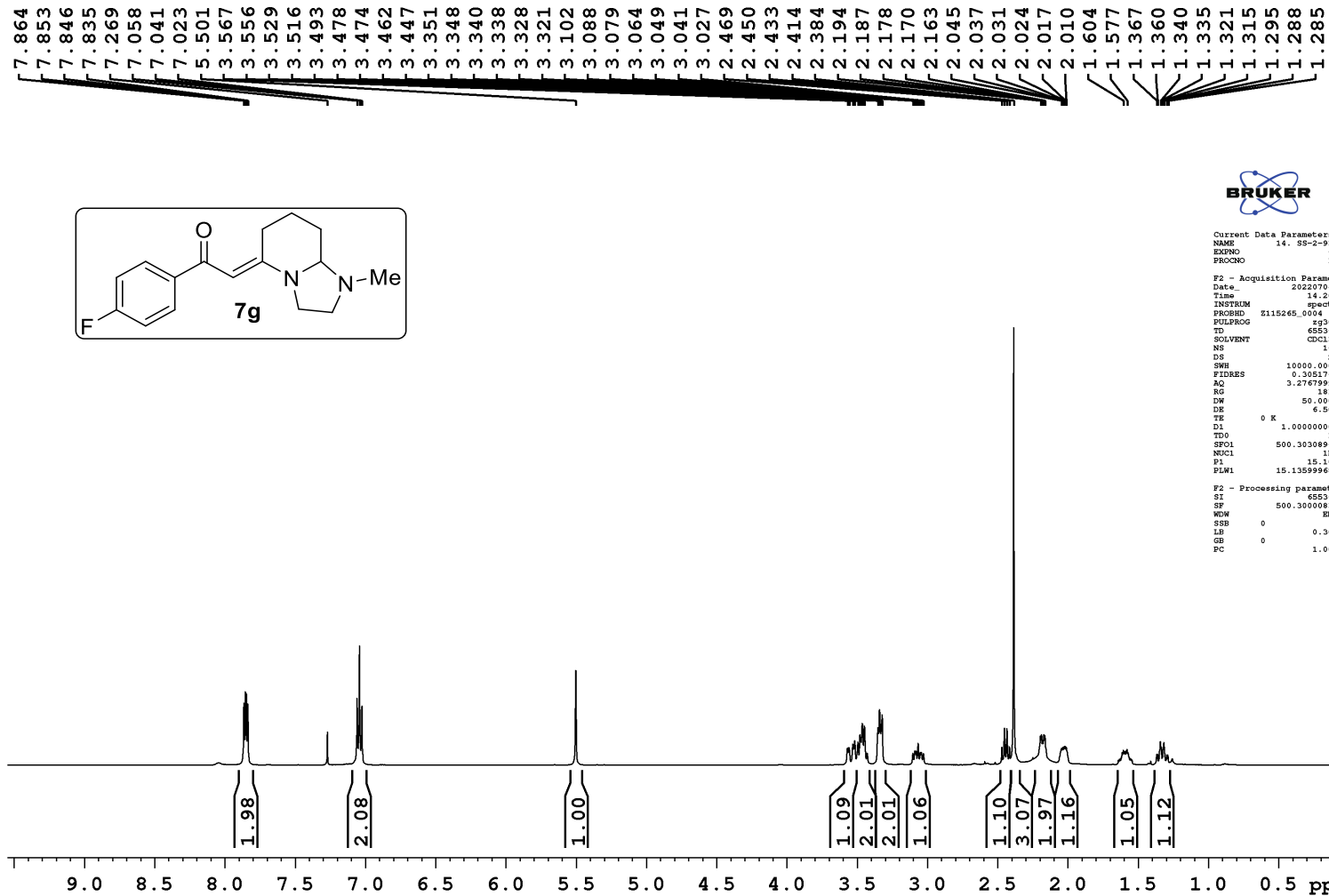
```
Current Data Parameters
NAME      19F spectra
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20231226
Time     16:23 h
INSTRUM  spect
PROBHD   E115245 0094 1
PULPROG  zgpg30p2
TD       131072
SOLVENT  CDCl3
NS       4
DS       4
SWH      113626.367 Hz
FIDRES   1.722392 Hz
AQ       0.5762168 sec
RG       724
SF       470.408 MHz
DE       6.50 usec
TE       300 K

D1       1.0000000 sec
d11      0.2000000 sec
D12      0.0002000 sec
TD0      0.0002000 sec
SFO1     470.6582192 MHz
NUC1     19F
P1       15.00 usec
P11      27.0000000 W
SFO2     500.2520015 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
P1A2     15.11533368 W
P1A12    0.55524009 W

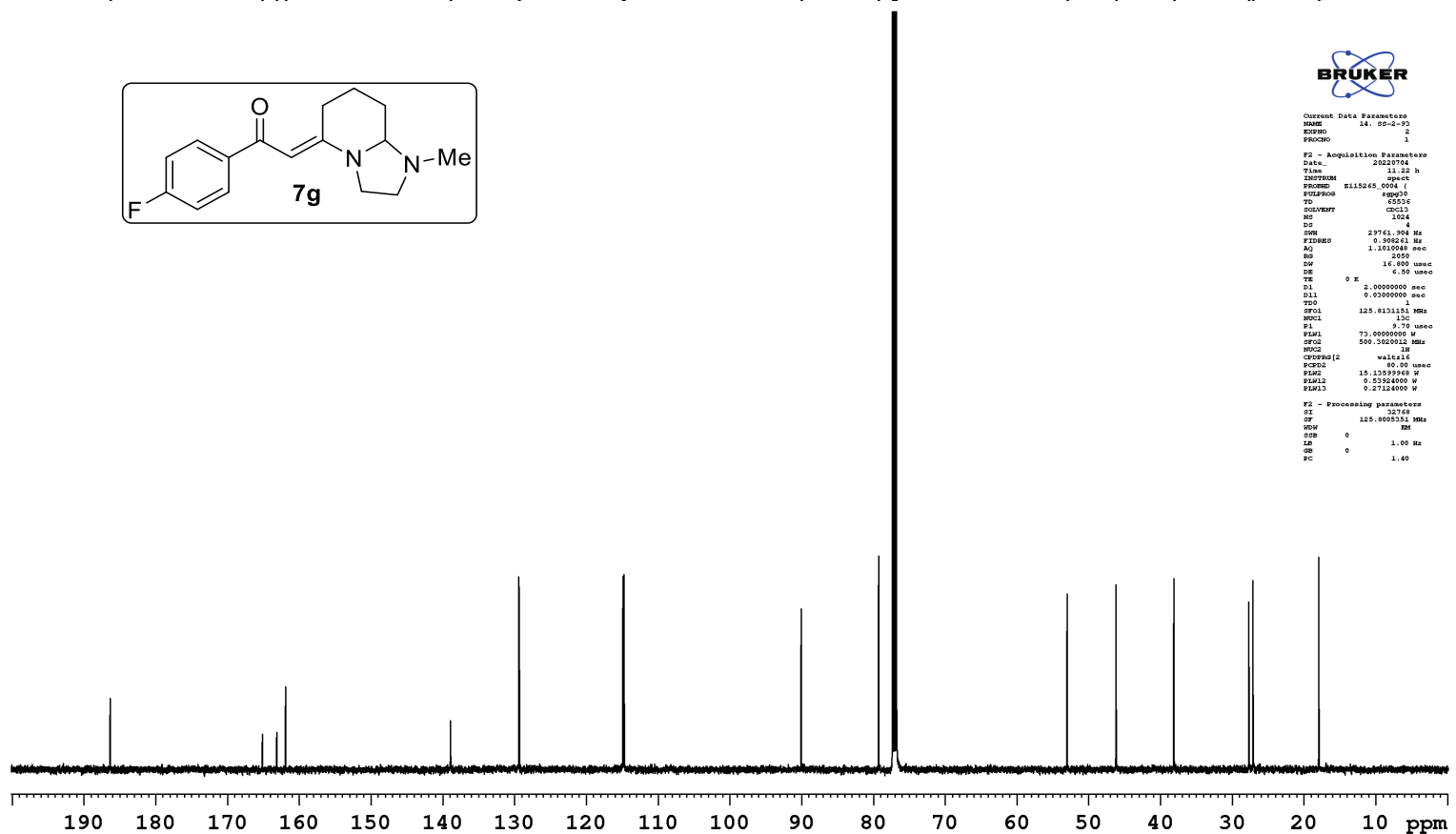
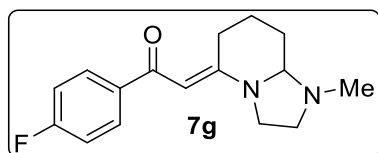
F2 - Processing parameters
SI       32768
SF       470.7652000 MHz
WDW      EM
SSB      0
GB       0
DE       0.30 Hz
SE       0
PC       1.00
```


ES-SS-2-93 re, 1H, CDCl3, 04-07-2022



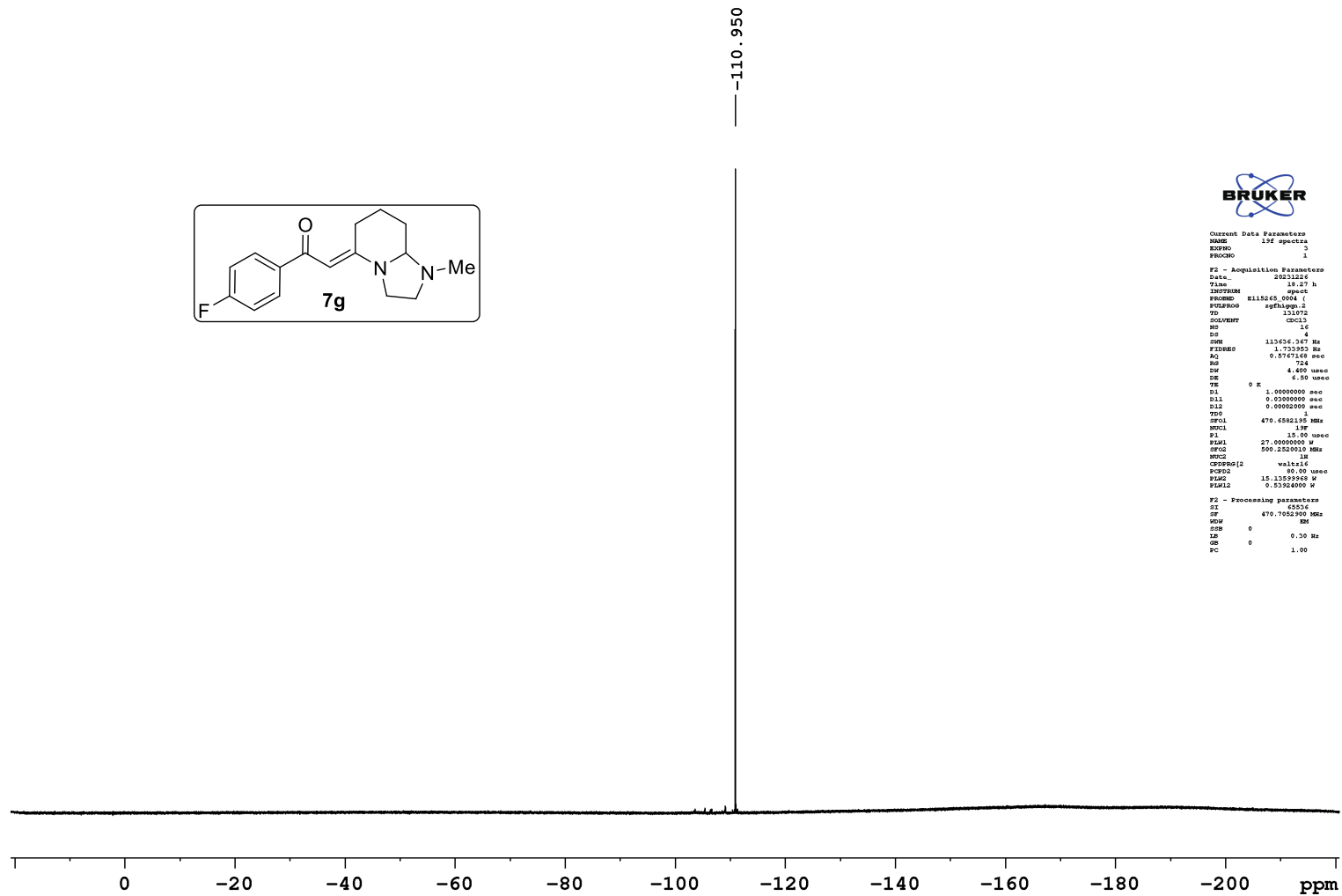
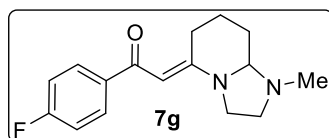
ES-SS-2-93, 13C, CDC13, 04-07-2022

— 186.295  
— 165.097  
— 163.113  
— 161.850  
— 138.904  
— 138.882  
— 129.366  
— 129.296  
— 114.864  
— 114.695  
— 90.014  
— 79.232  
— 77.276  
— 77.022  
— 76.768  
— 52.969  
— 46.151  
— 38.086  
— 27.641  
— 27.067  
— 17.901



  
Current Data Parameters  
NAME 14-SS-2-93  
EXPNO 2  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220704  
Time 11:22 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 328  
DS 4  
SFO 29761.994 Hz  
FIDRES 0.988261 Hz  
AQ 1.102048 sec  
RG 2050  
DM 14.900 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
D11 0.2000000 sec  
TD0 1  
SFO1 125.813151 MHz  
NUC1 13C  
PC1 150 usec  
P1 1.70 usec  
P1M1 70.0000000 W  
SFO2 500.302012 MHz  
NUC2 1H  
PCP2 18 usec  
P2M2 18.1359948 W  
P1M2 0.53264000 W  
P1M3 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.805511 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-2-93\_19F\_CDC13\_26-12-2023

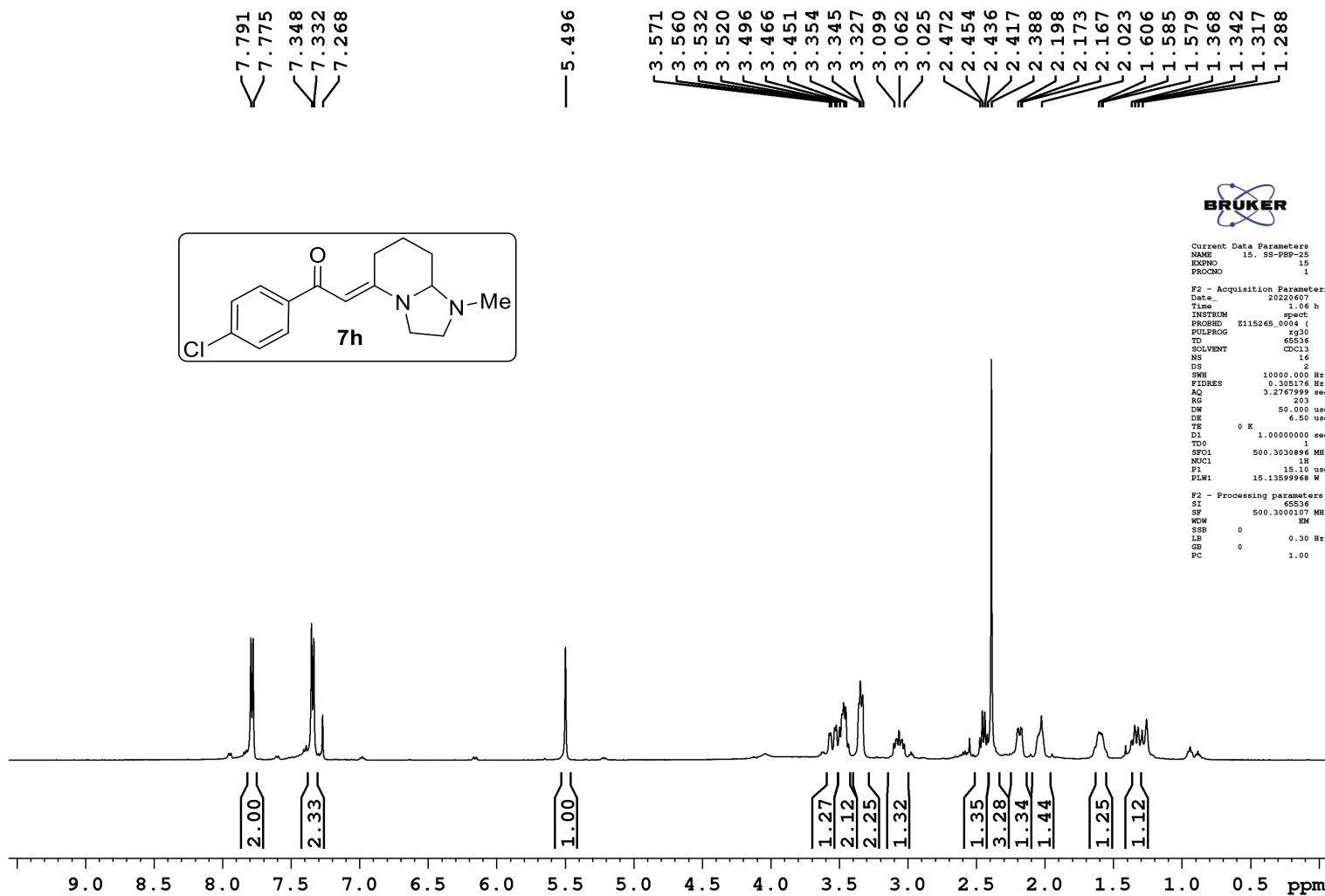
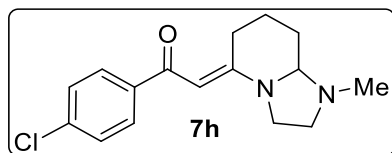


```
Current Data Parameters
NAME      19f spectra
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20231226
Time      16:27 h
INSTRUM   spect
PROBHD    E115245.0048 (
PULPROG   zgpg30p2
TD        133072
SOLVENT   CDCl3
NS        4
DS        4
SFR       115626.367 Hz
FIDRES    1.722950 Hz
AQ         0.5767168 sec
RG         724
DE         4.400 usec
TE         0 K
D1         1.0000000 sec
d11        0.0000000 sec
D12        0.0002000 sec
TD0        0.0002000 sec
SFO1       470.6582195 MHz
NUC1       13C
P1         15.00 usec
PL11       27.0000000 W
SFO2       500.2520010 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     60.00 usec
PLM2       15.23529968 W
PLM12     0.53324000 W

F2 - Processing parameters
SI         65536
SF         470.7682000 MHz
WDW        0
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

ES-SS-PBP-25, 1H, CDC13, 06-06-2022

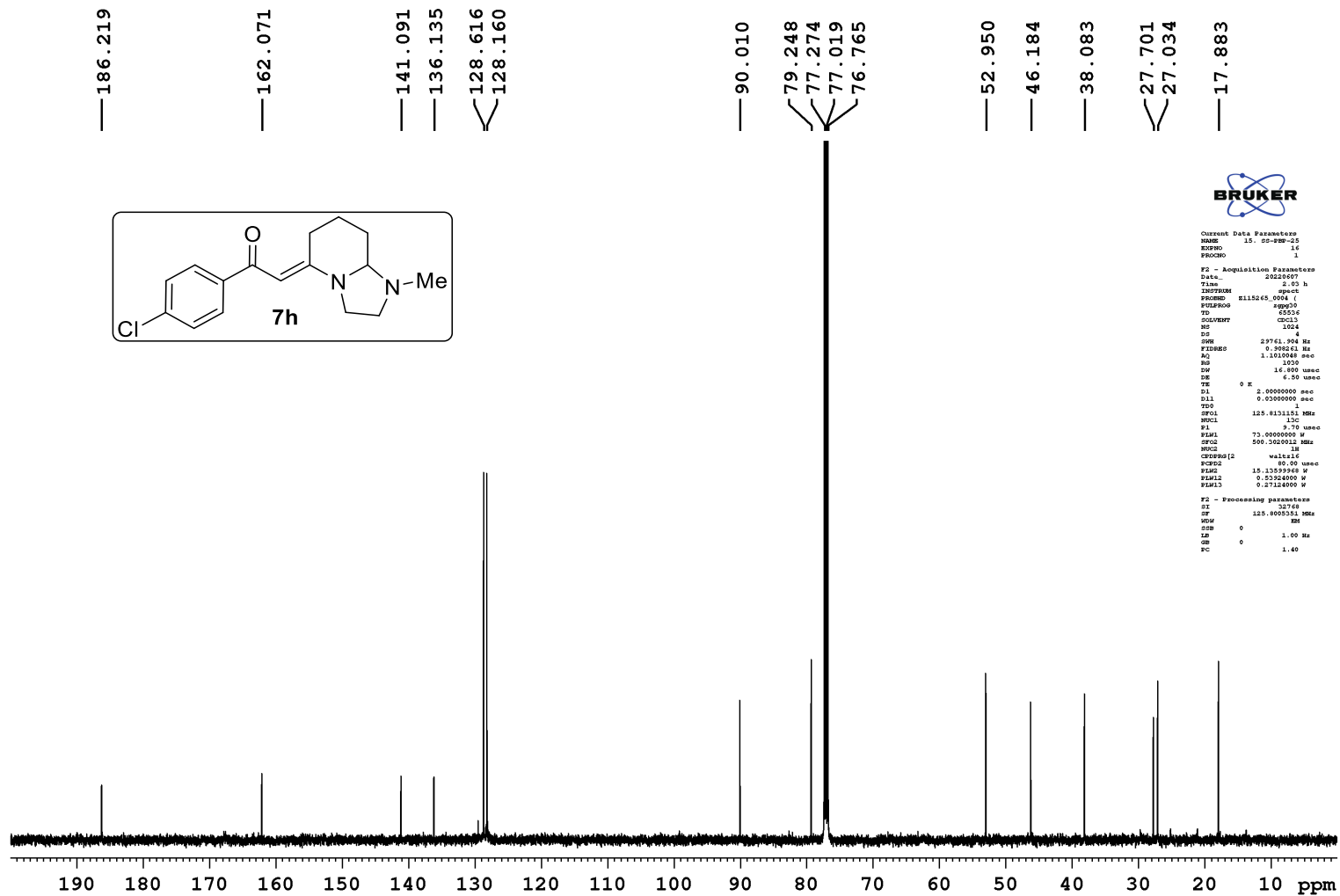


Current Data Parameters  
NAME 15. SS-PBP-25  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220607  
Time 1.06 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLN1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.3000107 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-PBP-25, 13C, CDC13, 06-06-2022

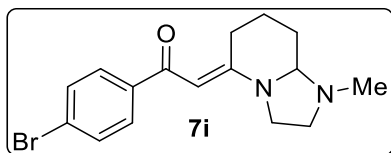


Current Data Parameters  
NAME 15\_50-PBP-25  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220601  
Time 08:07  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 4  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.398261 MHz  
AQ 1.101068 sec  
RG 4028  
DM 14.800 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
S1 0.2000000 sec  
TD0 1  
SFO1 125.8131151 MHz  
NUC1 13C  
PC1 3.70 usec  
P1 1.70 usec  
P1P1 70.0000000 W  
SFO2 500.3020112 MHz  
NUC2 1H  
CROSSP2 18  
PCP2 80.00 usec  
P2 18.1335948 W  
P1P2 0.5324400 W  
P1P3 0.2712400 W  
F2 - Processing parameters  
SI 32768  
SF 125.8055151 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



ES-SS-2-80, 1H, CDC13, 03-06-2022

7.723  
7.706  
7.510  
7.492  
7.269  
5.487  
3.566  
3.554  
3.529  
3.517  
3.490  
3.475  
3.469  
3.461  
3.456  
3.445  
3.349  
3.346  
3.338  
3.335  
3.325  
3.318  
3.098  
3.084  
3.075  
3.060  
3.045  
3.037  
2.467  
2.448  
2.431  
2.412  
2.384  
2.196  
2.189  
2.180  
2.171  
2.165  
2.047  
2.040  
2.033  
2.026  
2.014  
1.605  
1.600  
1.593  
1.590  
1.583  
1.578  
1.571  
1.343  
1.337  
1.332  
1.317  
1.312  
1.306  
1.292  
1.288



Current Data Parameters  
NAME 16-SS-2-80  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220603  
Time 21:15 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 161  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.1359996 W

F2 - Processing parameters  
SI 65536  
SF 500.3000086 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-2-80, 13C, CDC13, 03-06-2022

—186.272

—162.109

—141.558

—131.136

—128.864

—124.615

—89.939

—79.265

—77.285

—77.031

—76.777

—52.967

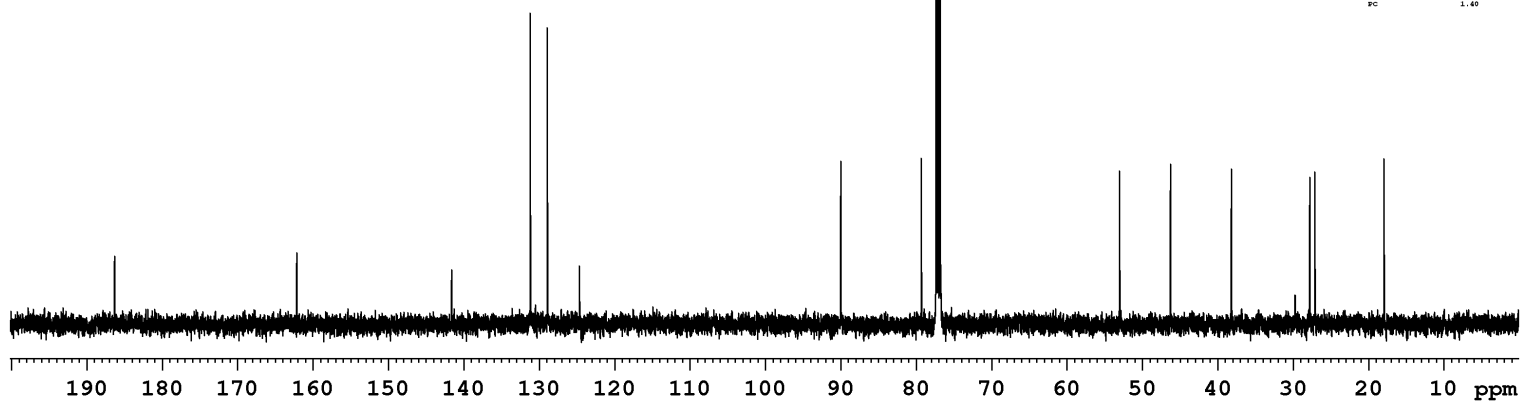
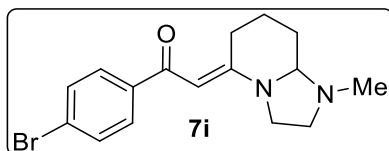
—46.206

—38.108

—27.723

—27.053

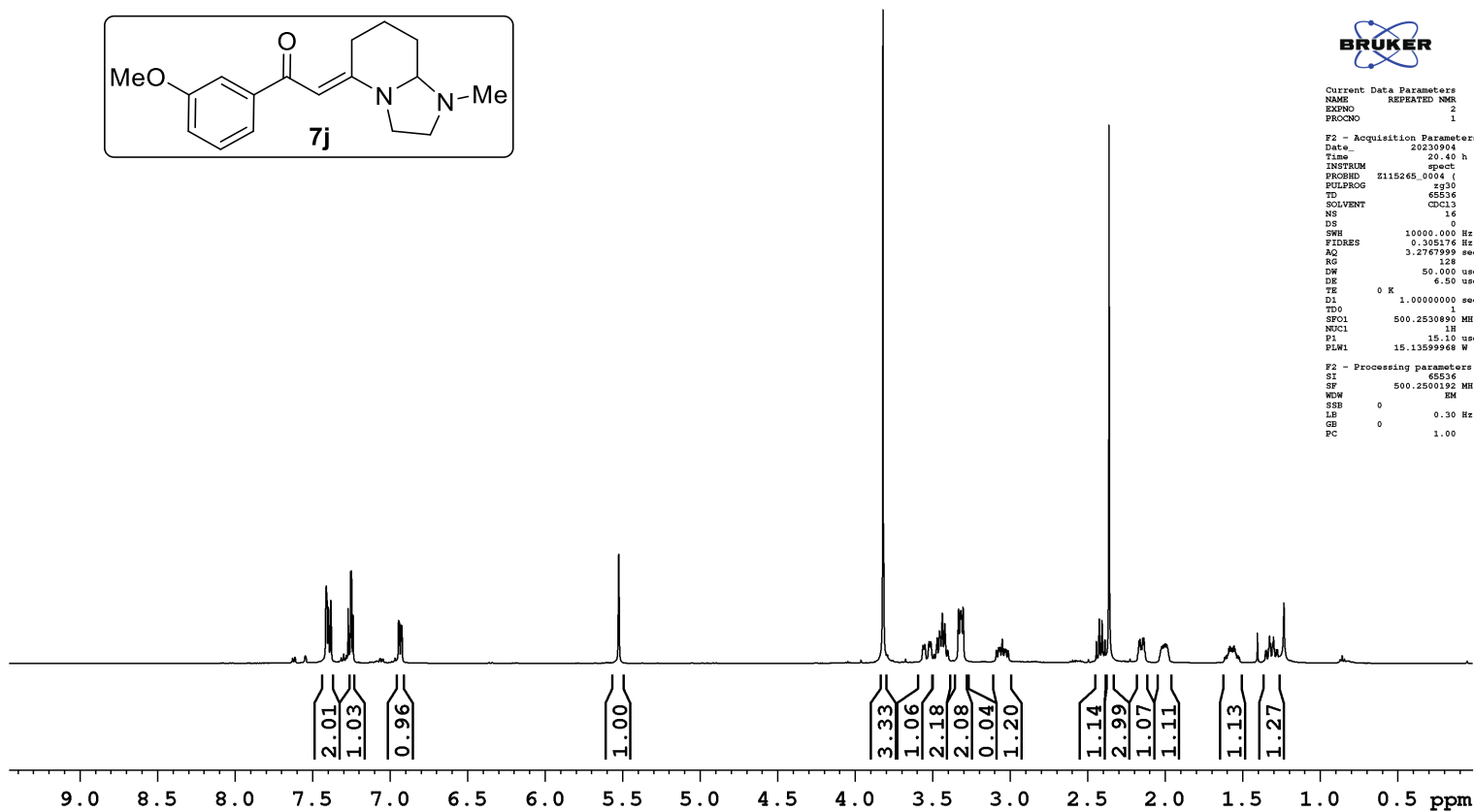
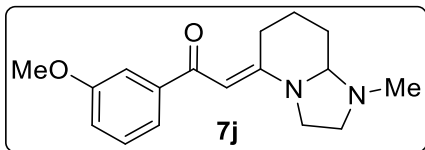
—17.880



```
Current Data Parameters
NAME      16-SS-2-80
EXPNO    13
PROCNO   1
F2 - Acquisition Parameters
Date_    20220603
Time     21.09 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  cdcl3
NS        256
DS        4
SFO      29761.994 MHz
FIDRES   0.988261 Hz
AQ        1.102068 sec
RG         912
DM         16.800 usec
DE         6.50 usec
TE        300.2 K
D1        2.0000000 sec
d11       0.2000000 sec
TD0       1
SFO1     125.813151 MHz
NUC1      13C
PC1       150 usec
P1        1.70 usec
P1M1     70.0000000 W
SFO2     500.302012 MHz
NUC2      1H
PC2       18 usec
P2M2     411.115 W
PCPD2    80.00 usec
P1M2     16.1359948 W
P1M12    0.53924000 W
P1M13    0.27124000 W
F2 - Processing parameters
SI        32768
SF        125.805511 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

ES-SS-2-89R\_1H\_CDCl3\_04-09-2023

7.413  
7.411  
7.406  
7.396  
7.381  
7.269  
7.253  
7.247  
7.238  
6.944  
6.943  
6.939  
6.937  
6.928  
6.926  
6.923  
6.921  
5.524  
3.819  
3.560  
3.549  
3.522  
3.511  
3.469  
3.455  
3.436  
3.421  
3.331  
3.321  
3.317  
3.313  
3.302  
3.064  
3.049  
2.442  
2.423  
2.406  
2.387  
2.361  
2.167  
2.160  
2.152  
2.143  
2.136  
2.022  
2.015  
2.008  
2.001  
1.994  
1.987  
1.581  
1.577  
1.559  
1.554  
1.325  
1.320  
1.306  
1.300

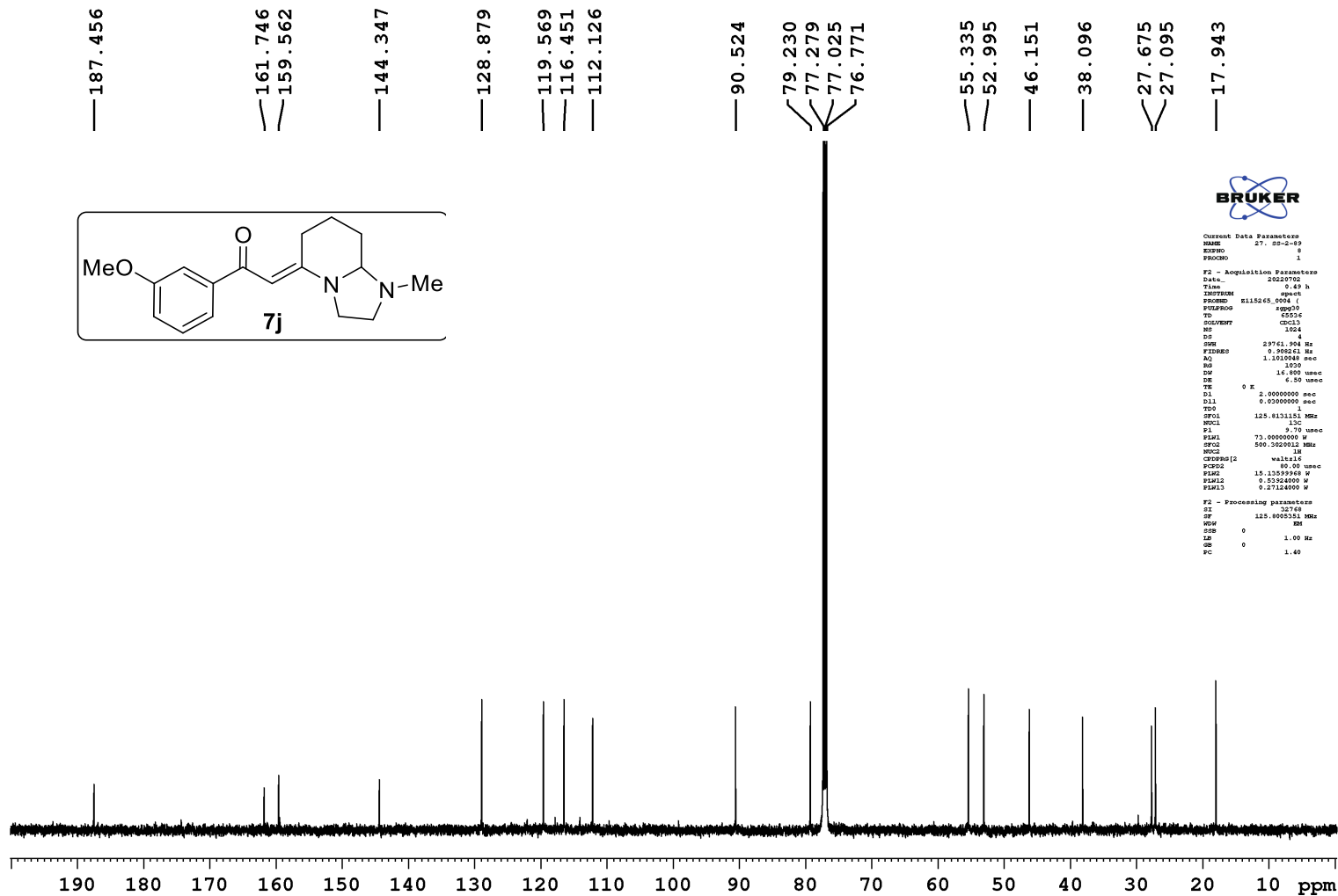
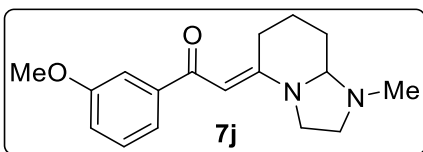


Current Data Parameters  
NAME REPEATED NMR  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230904  
Time 20.40 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 128  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLN1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500192 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

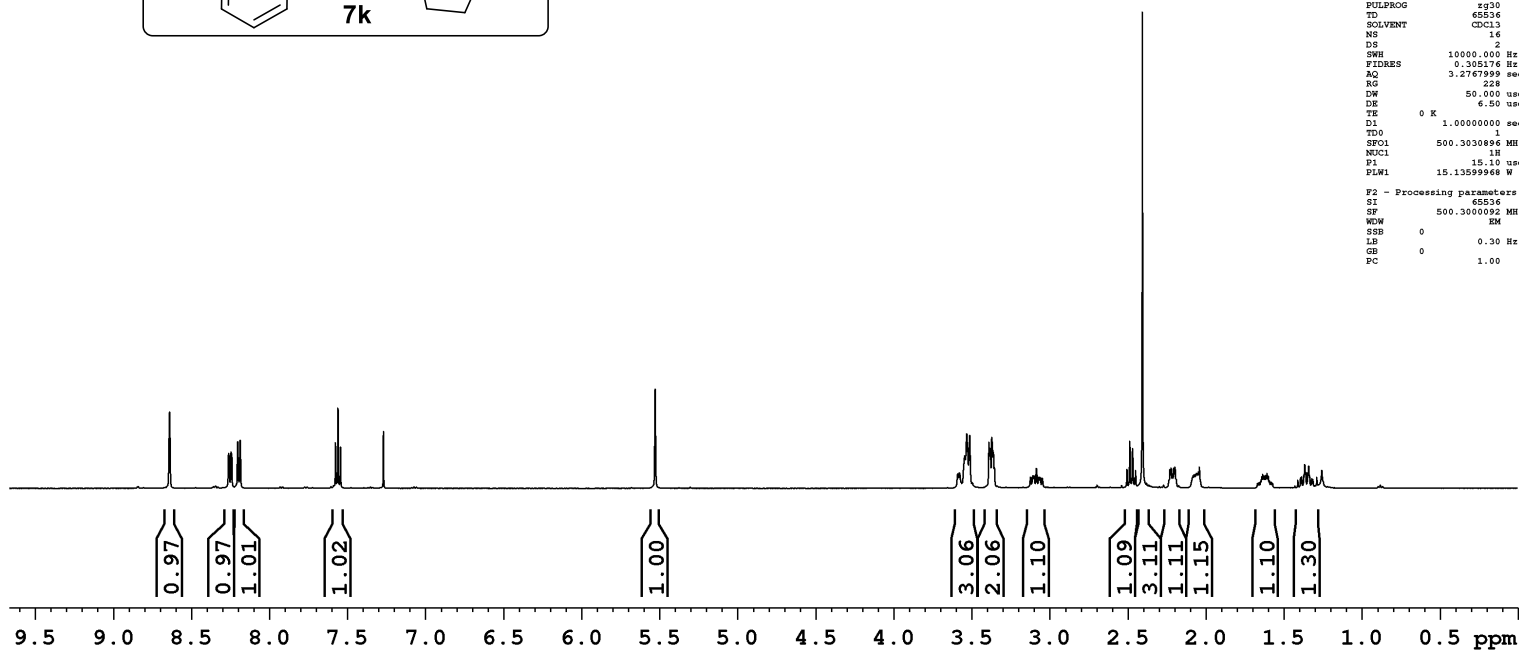
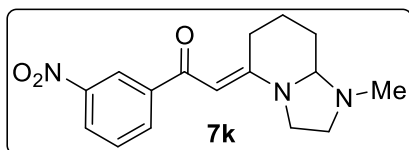
ES-SS-2-89, 13C, CDC13, 01-07-2022



Current Data Parameters  
NAME 27-SS-2-89  
EXPNO 8  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20220702  
Time 0.49 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdc13  
NS 4  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.988261 Hz  
AQ 1.101068 sec  
RG 4028  
DM 14.800 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
D11 0.2000000 sec  
TD0 1  
SFO1 125.8131511 MHz  
NUC1 13C  
PC1 1.70 usec  
P1 150.0000000 W  
SFO2 500.3020212 MHz  
NUC2 1H  
PCP2 80.00 usec  
P2 15.1359948 W  
P1P2 0.53264000 W  
P1P3 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.8055151 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-2-85, 1H, CDC13, 04-06-2022

8.639  
8.261  
8.244  
8.202  
8.187  
7.576  
7.560  
7.544  
7.269  
5.528  
3.589  
3.577  
3.544  
3.531  
3.512  
3.389  
3.383  
3.371  
3.361  
3.354  
3.122  
3.108  
3.100  
3.085  
3.070  
3.061  
2.505  
2.486  
2.469  
2.450  
2.406  
2.229  
2.222  
2.204  
2.197  
2.080  
2.073  
2.066  
2.059  
2.053  
2.046  
2.040  
1.641  
1.634  
1.629  
1.623  
1.619  
1.612  
1.607  
1.600  
1.385  
1.372  
1.365  
1.360  
1.346  
1.340  
1.334  
1.288



Current Data Parameters  
NAME 24-SS-2-85  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220604  
Time 19:19 h  
INSTRUM spect  
PROBRD Z115245.004 f  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 228  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.300092 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-2-85, 13C, CDC13, 04-06-2022

— 184.282

— 163.126

— 148.081

— 144.324

— 133.229

— 129.089

— 124.607

— 121.971

— 89.593

— 79.341

— 77.272

— 77.018

— 76.764

— 52.874

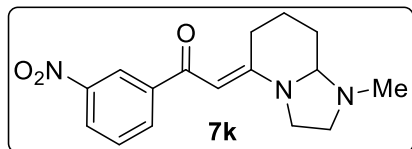
— 46.388

— 38.071

— 27.915

— 26.915

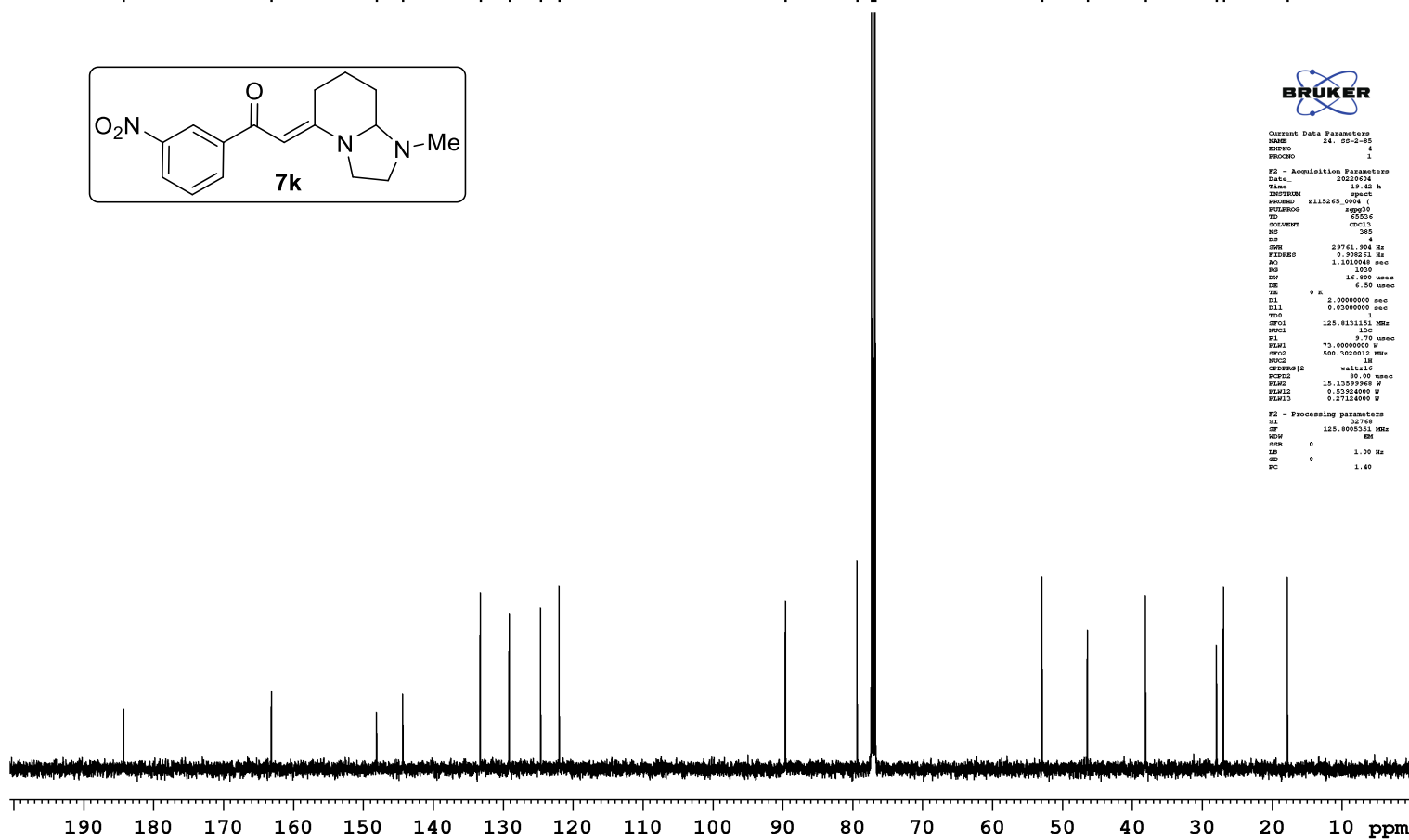
— 17.774



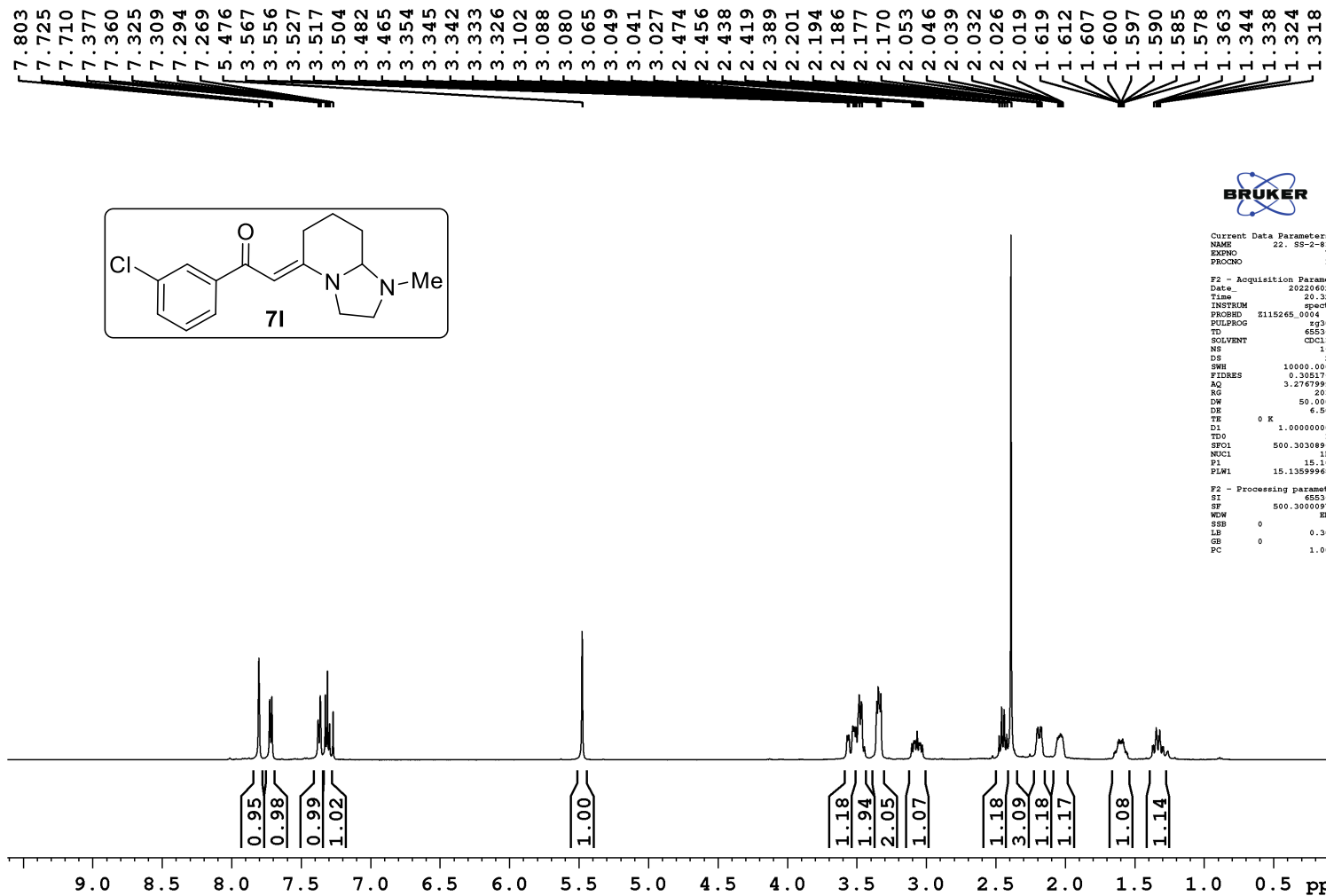
```
Current Data Parameters
NAME      24_05-2-85
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20220604
Time      13:42 h
INSTRUM   spect
PROBHD    E115245.0064 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         345
DS         4
SWH        29761.904 Hz
FIDRES    0.390261 Hz
AQ         1.3137048 sec
RG         1020
DQ         16.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
d11        0.0000000 sec
TDS        125.8131151 MHz
SFO1       125.8131151 MHz
NUC1        13C
P1         8.75 usec
PL1        70.0000000 W
SFO2       500.0000125 MHz
NUC2        1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PL2        15.1250000 W
PL12       0.52324000 W
PL13       0.27124000 W

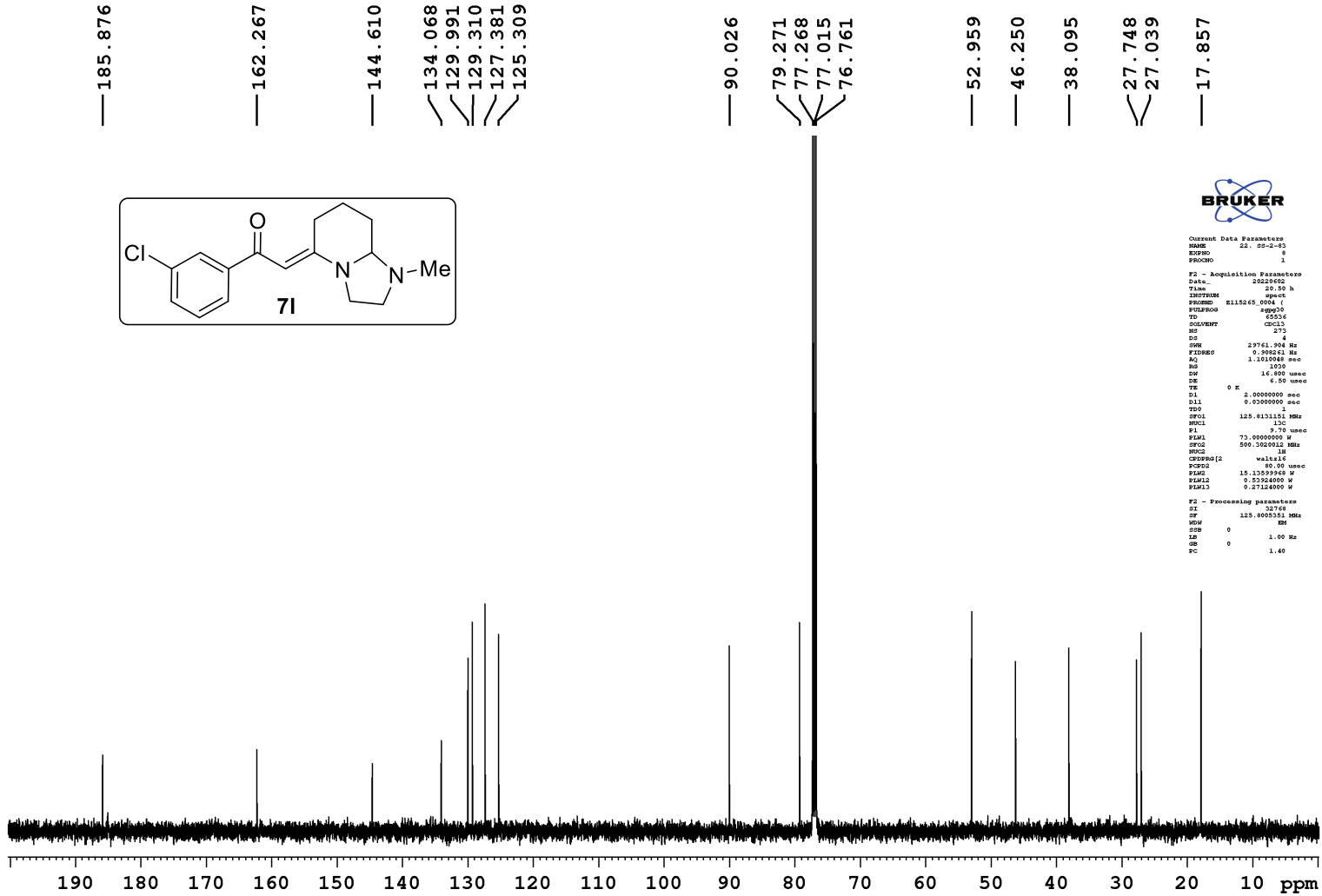
F2 - Processing parameters
SI         32743
SF         125.8005151 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```



ES-SS-2-83, 1H, CDC13, 02-06-2022



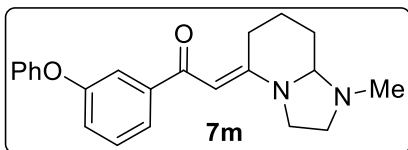
ES-SS-2-83, 13C, 02-06-2022





ES-SS-2-87, 1H, CDC13, 12-06-2022

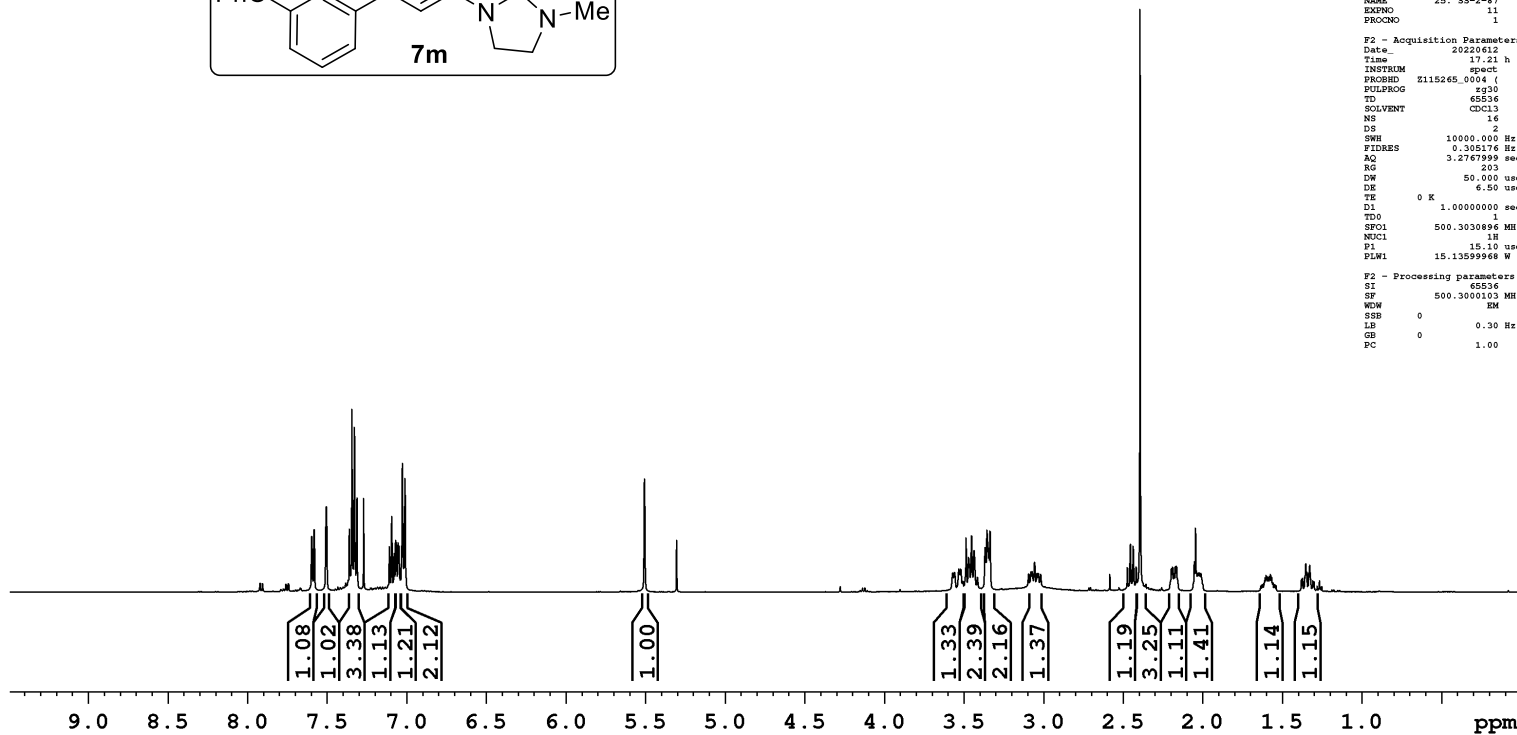
7.579  
7.507  
7.503  
7.499  
7.358  
7.342  
7.327  
7.310  
7.268  
7.106  
7.092  
7.077  
7.068  
7.066  
7.063  
7.061  
7.052  
7.050  
7.047  
7.025  
7.010  
5.504  
3.568  
3.557  
3.529  
3.518  
3.484  
3.468  
3.449  
3.433  
3.364  
3.362  
3.353  
3.350  
3.341  
3.334  
3.077  
3.068  
3.053  
2.470  
2.452  
2.434  
2.415  
2.391  
2.194  
2.187  
2.169  
2.162  
2.050  
2.042  
2.023  
2.017  
2.009  
1.350  
1.345  
1.330  
1.325



Current Data Parameters  
NAME 25. SS-2-87  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220612  
Time 17.21 h  
INSTRUM spect  
PROCNO 2115245\_004 ( )  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.3030896 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.3000103 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



ES-SS-2-87, 13C, CDC13, 13-06-2022

— 186.854

— 161.951  
— 157.257  
— 157.084

— 144.786

— 129.744  
— 129.309  
— 123.216  
— 122.132  
— 120.654  
— 118.854  
— 117.729

— 90.424

— 79.194  
— 77.303  
— 77.049  
— 76.794

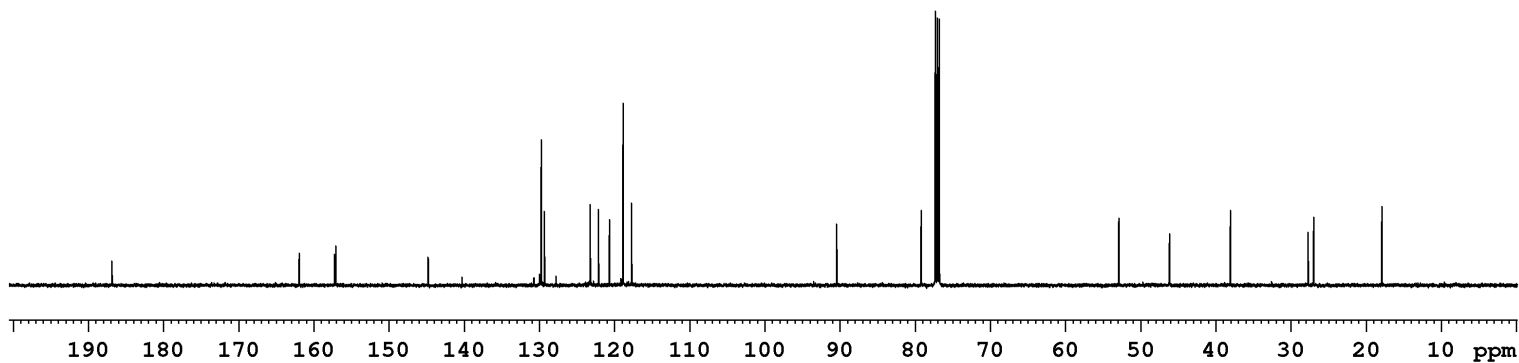
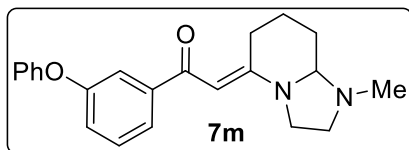
— 52.896

— 46.141

— 38.043

— 27.698  
— 26.967

— 17.894

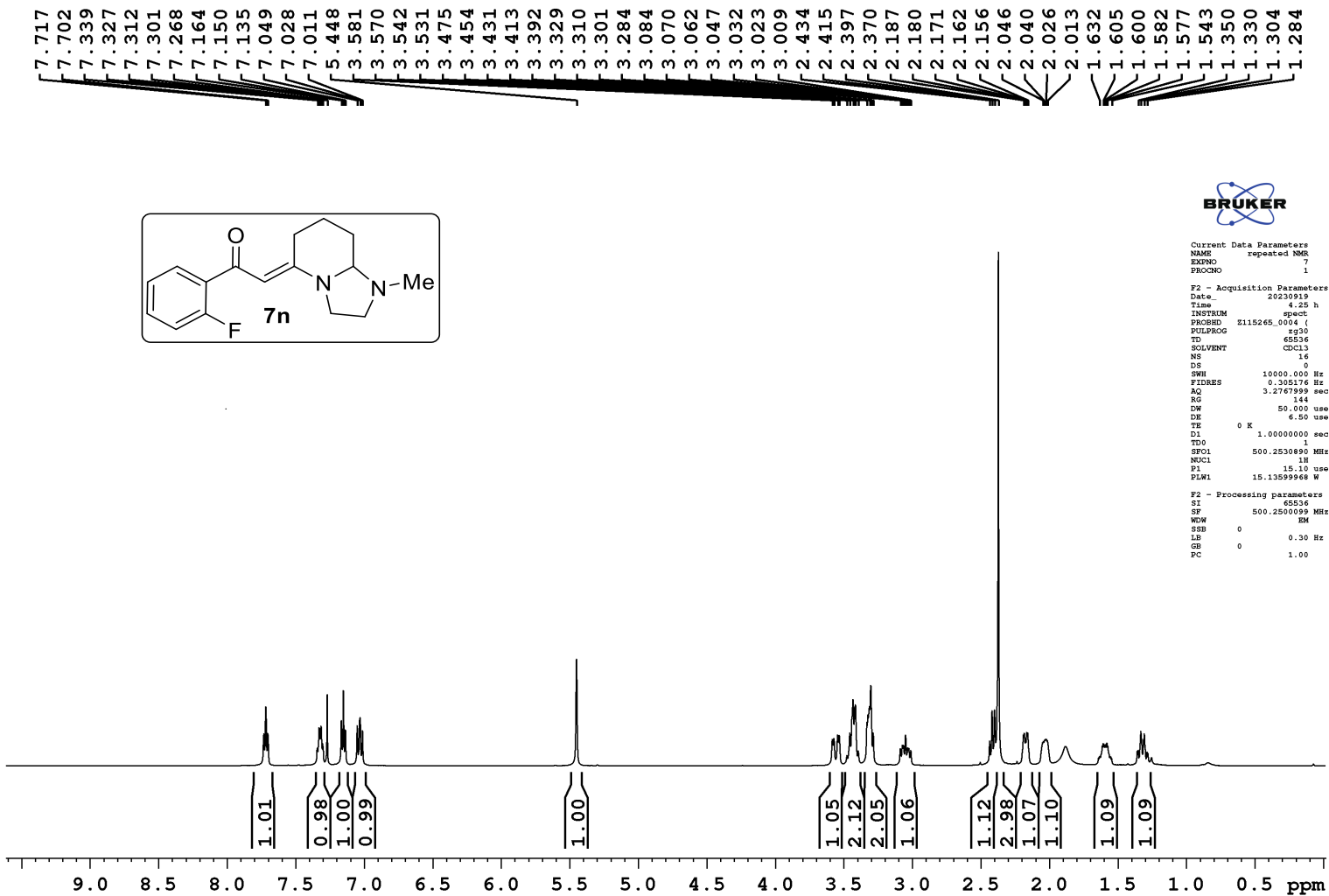


```
Current Data Parameters
NAME      25-06-2-87
EXPNO    3
PROCNO   1

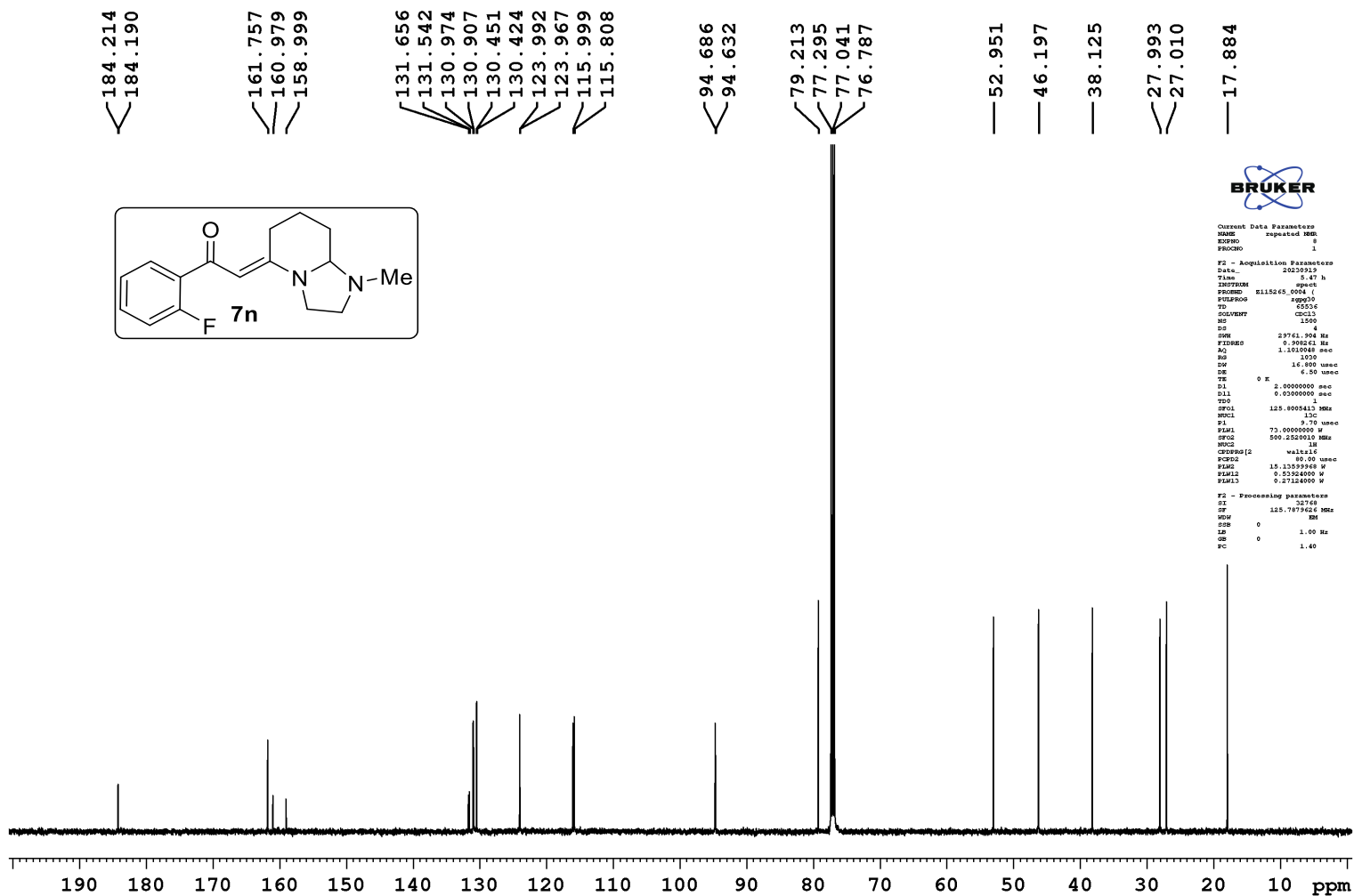
F2 - Acquisition Parameters
Date_    20220611
Time     23.13 h
INSTRUM  spect
PROBHD   BBO4 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       330
DS       4
SFO     29761.994 MHz
FIDRES   0.986261 MHz
AQ       1.101068 sec
RG       4028
DM       16.800 usec
DE       6.50 usec
TE       300 K
D1       2.0000000 sec
d11      0.2000000 sec
TD0      1
SFO1     125.8151511 MHz
NUC1      13C
PC1       150 usec
P1        1.70 usec
P1M1     70.0000000 MHz
SFO2     500.1362612 MHz
NUC2      1H
PC2M1    18
PC2M2    18
SFO3     400.1419111 MHz
PC3M1    80.00 usec
P3M1     16.1359948 MHz
P3M2     0.53264000 MHz
P3M3     0.27124000 MHz

F2 - Processing parameters
SI       32768
SF       125.8005151 MHz
WDW      EM
SSB      0
LB       1.00 MHz
GB       0
PC       1.40
```

ES-SS-pbp-27r\_1H\_CDCl3\_19-09-2023

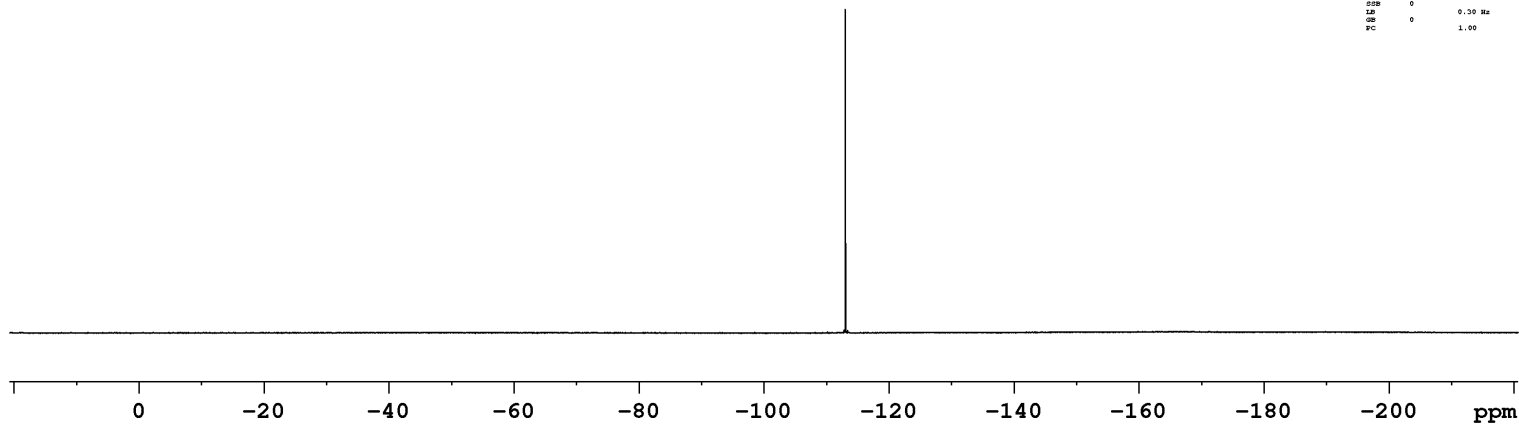
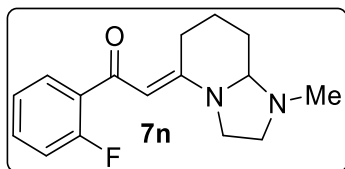


ES-SS-pbp-27r\_13C\_CDC13\_19-09-2023



Current Data Parameters  
NAME repeated 166  
EXPNO 8  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20230913  
Time 0.47 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65534  
SOLVENT cdc13  
NS 3200  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.988241 Hz  
AQ 1.102048 sec  
RG 1028  
DM 14.800 umsec  
DE 6.50 umsec  
TE 300 K  
D1 2.0000000 sec  
S11 0.0200000 sec  
TD0 1  
SFO1 125.805411 MHz  
NUC1 13C  
PC1 150 umsec  
P1 1.70 umsec  
P1M1 73.0000000 W  
SFO2 500.132010 MHz  
NUC2 1H  
PCP2 80.00 umsec  
P2M 18.1335948 W  
P1M2 0.53244000 W  
P1M3 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.7679424 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

---113.002



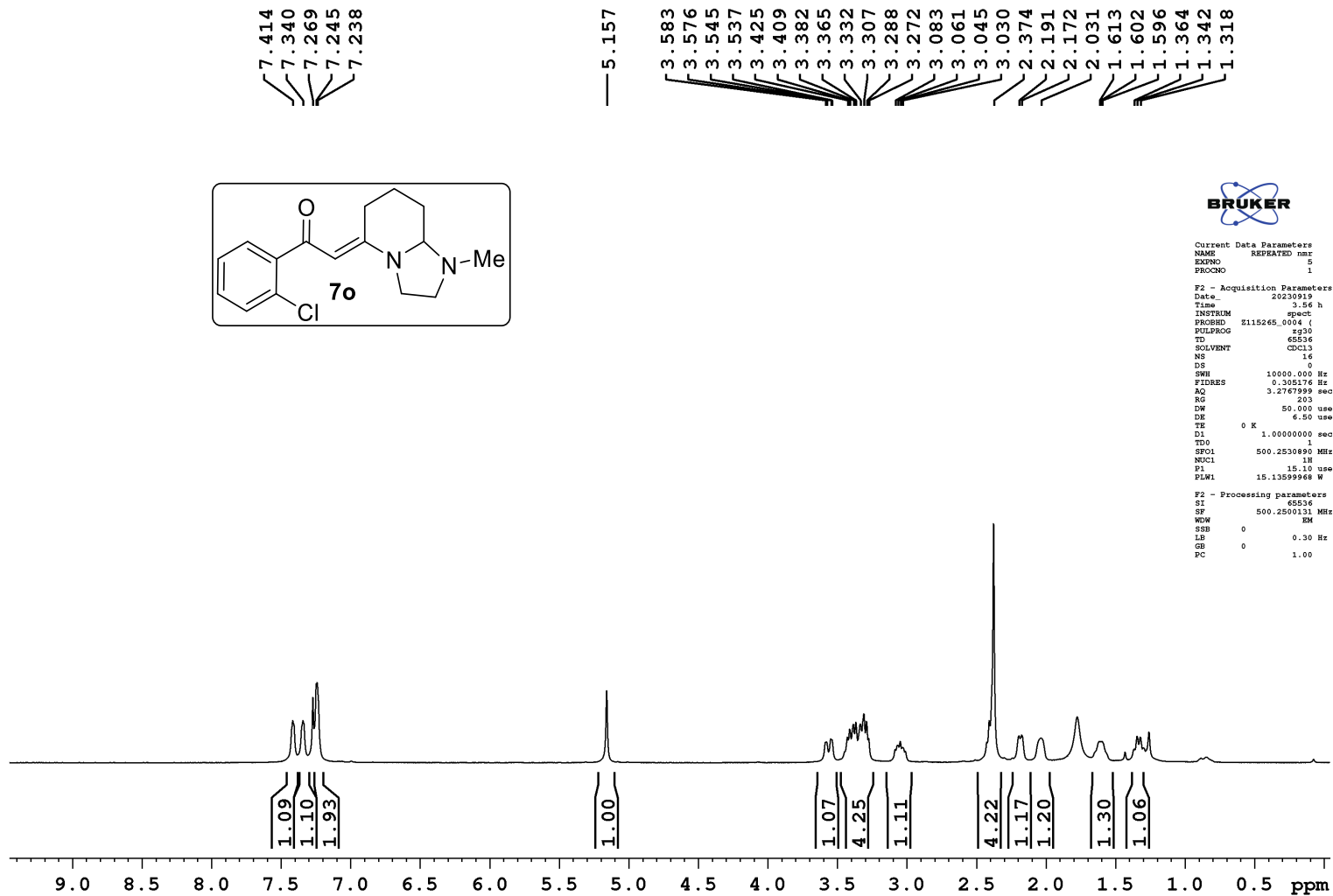
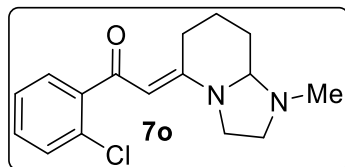
Current Data Parameters  
NAME 13F spectra  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231226  
Time 15:35 h  
INSTRUM spect  
PROBHD 1H5265.004 (1  
PULPROG zgpg30p2  
TD 131072  
SOLVENT cdcl3  
NS 4  
DS 4  
SFO 113.626367 Hz  
FIDRES 1.753952 Hz  
AQ 0.2767168 sec  
RG 724  
DM 4.800 usec  
DE 6.50 usec  
TE 300 K

D1 1.0000000 sec  
D12 0.0200000 sec  
D13 0.0002000 sec  
TD0  
SFO1 470.6582195 MHz  
NUC1 19F  
P1 15.00 usec  
PL1 27.0000000 W  
SFO2 500.2520019 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLA2 15.13539968 W  
PL12 0.53524000 W

F2 - Processing parameters  
SI 6554  
SF 470.7052700 MHz  
WDW 0  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-2-84R\_1H\_CDC13\_19-09-2023

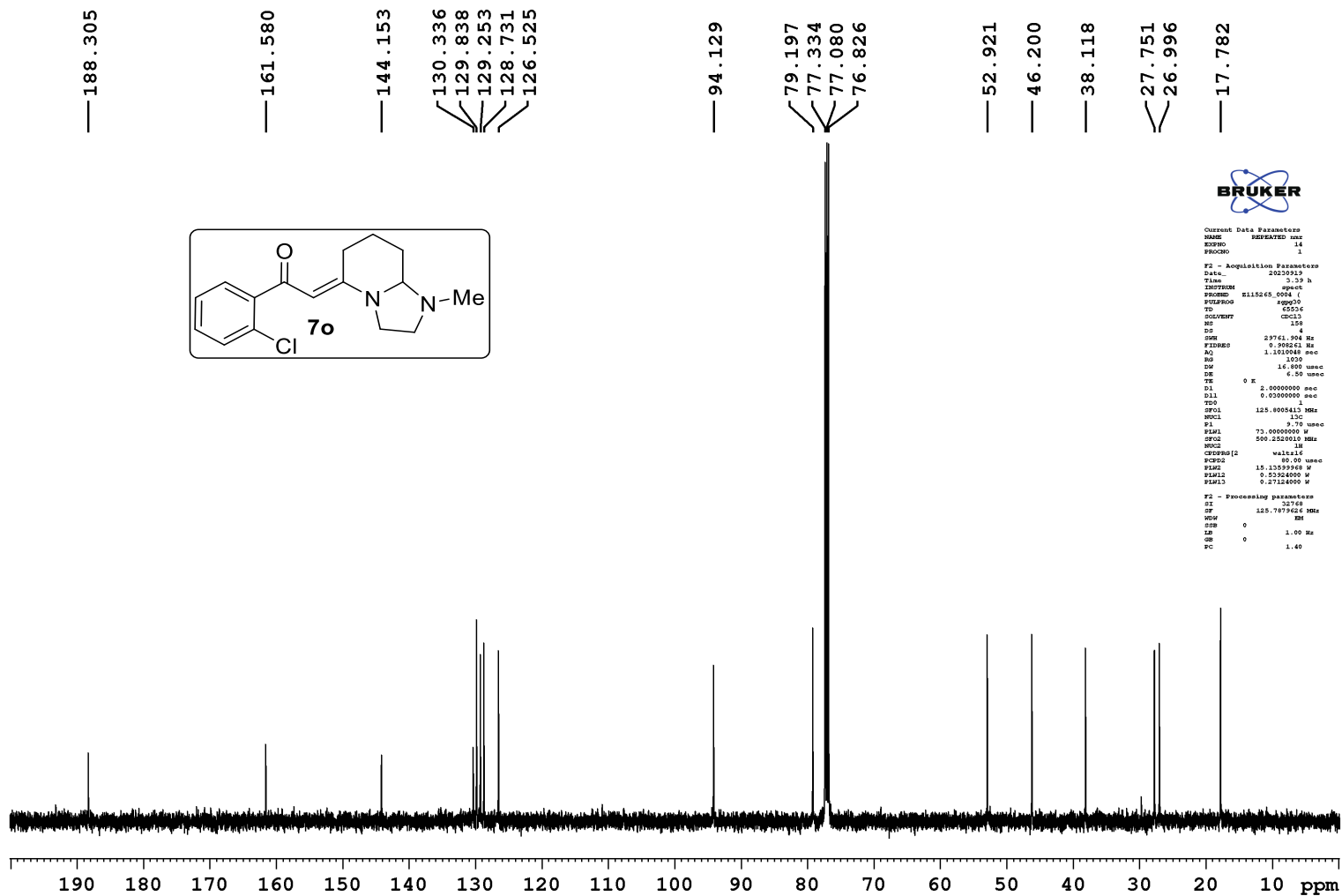


Current Data Parameters  
NAME REPEATED.nmr  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230919  
Time 3.56 h  
INSTRUM spect  
PROBHD Z115265.0004 ( eg30  
PULPROG gms36  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.274799 sec  
RG 203  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500131 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

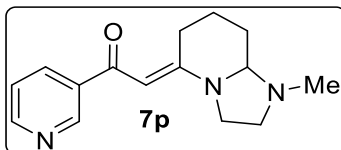
ES-SS-2-84 R\_13C\_CDCl3\_19-09-2023



```
Current Data Parameters
NAME          REPEATED 4x
EXPNO        1
PROCNO       1
F2 - Acquisition Parameters
Date_        20230913
Time         3.33 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           4
DS           4
SFO          29761.994 MHz
FIDRES       0.986261 MHz
AQ           1.1010768 sec
RG           4028
DM           14.800 usec
DE           6.50 usec
TE           0 K
D1           2.0000000 sec
S11         0.0200000 sec
TD0         1
SFO1        125.8054113 MHz
NUC1         13C
PC1         150 usec
P1          1.70 usec
P1M1        73.0000000 W
SFO2        500.1320120 MHz
NUC2         1H
CPDPRG2     waltz16
PCPD2       80.00 usec
P2M1        15.1335948 W
P2M2        0.53264000 W
P2M3        0.27124000 W
F2 - Processing parameters
SI           32768
SF           125.7679624 MHz
WDW         EM
SSB         0
LB           1.00 Hz
GB           0
PC           1.40
```

ES-SS-2-88 R\_1H\_CDC13\_19-09-2023

9.007  
 8.587  
 8.578  
 8.119  
 8.103  
 7.309  
 7.299  
 7.293  
 7.284  
 7.269



5.471

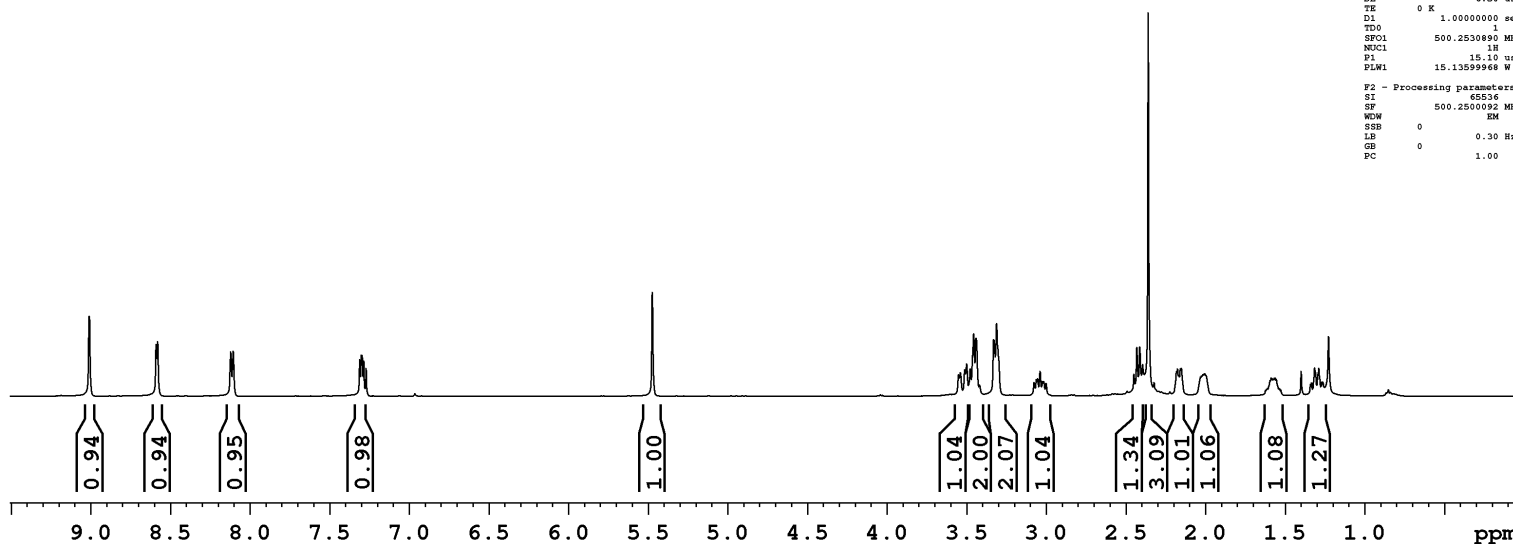
3.548  
 3.537  
 3.509  
 3.497  
 3.453  
 3.438  
 3.328  
 3.310  
 3.074  
 3.052  
 3.036  
 3.013  
 2.998  
 2.447  
 2.428  
 2.411  
 2.392  
 2.357  
 2.180  
 2.173  
 2.156  
 2.149  
 2.029  
 1.995  
 1.592  
 1.564  
 1.559  
 1.553  
 1.338  
 1.312



Current Data Parameters  
 NAME REPEATED NMR  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230919  
 Time 2.06 h  
 INSTRUM spect  
 PROBRD Z115245.004 /  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.276789 sec  
 RG 90.5  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TDO 1  
 SFOL 500.2530890 MHz  
 NUC1 1H  
 P1 15.10 usec  
 PLW1 15.13599968 W

F2 - Processing parameters  
 SI 65536  
 SF 500.2500092 MHz  
 NCM RM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





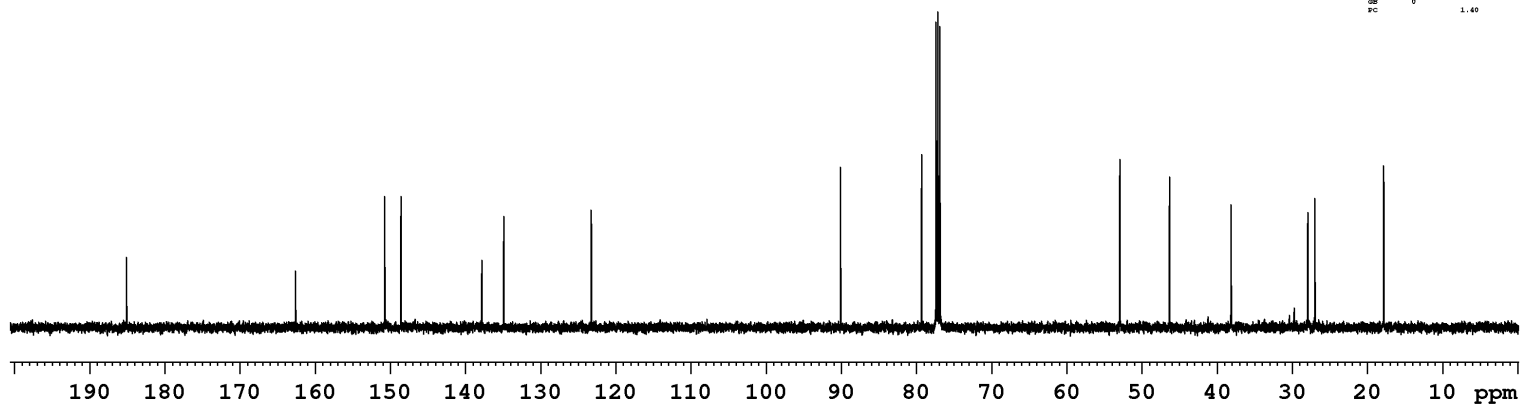
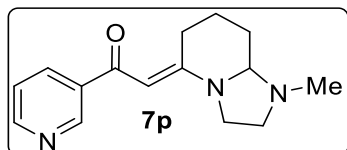
ES-SS-2-88 R\_13C\_CDCl3\_19-09-2023

—185.062  
—162.572  
—150.702  
—148.544  
—137.782  
—134.848  
—123.210

—90.045  
79.259  
77.339  
77.085  
76.831

—52.890  
—46.267  
—38.081

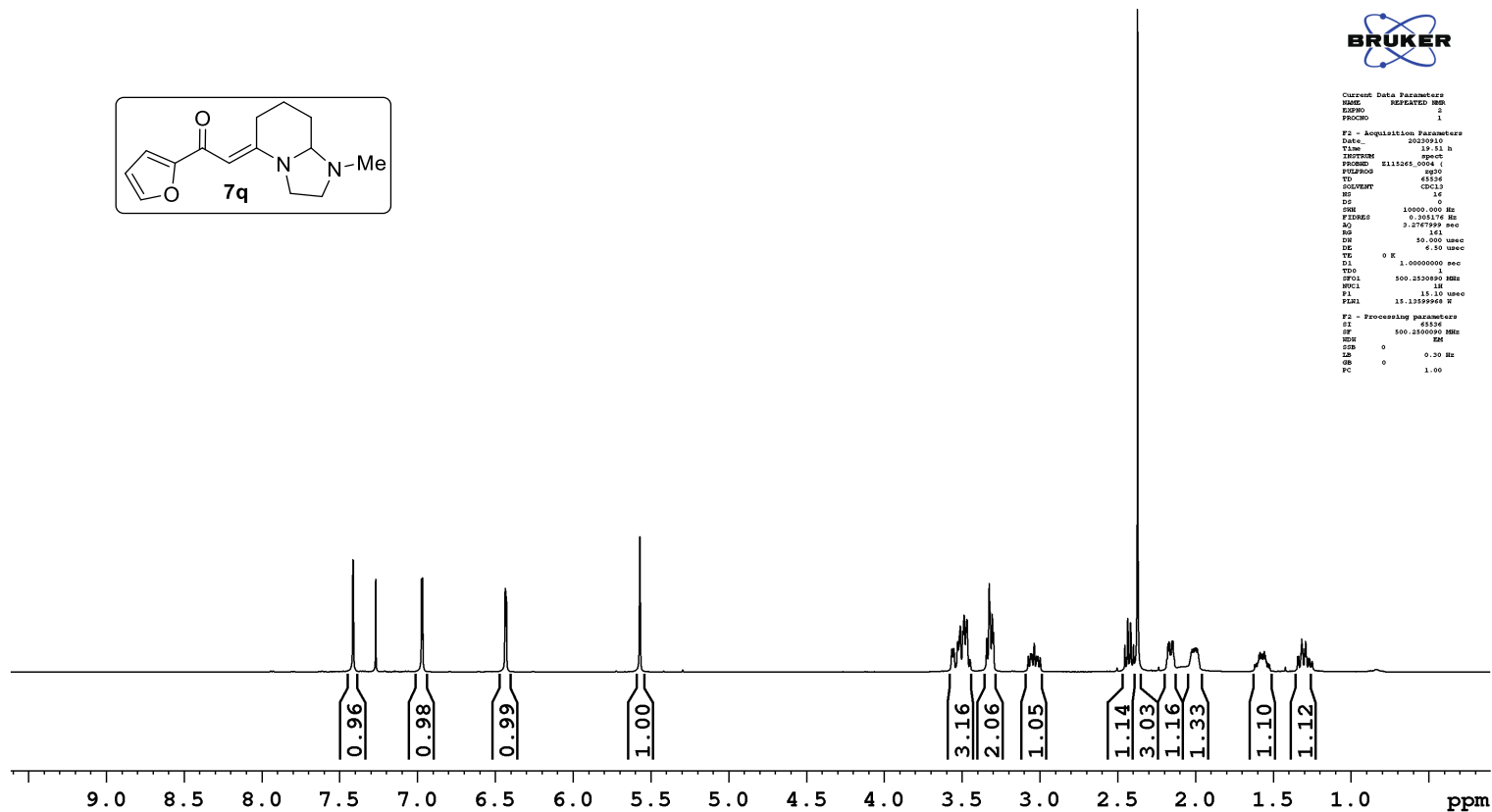
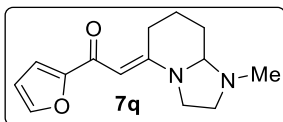
—27.864  
—26.934  
—17.766



```
Current Data Parameters
NAME      REPEATED NSD
EXPNO    13
PROCNO   1
F2 - Acquisition Parameters
Date_    20230913
Time     2.13 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS       6
DS       4
SFO     29761.994 MHz
FIDRES  0.398261 MHz
AQ       1.101068 sec
RG       3028
DM       14.900 usec
DE       6.50 usec
TE       300.2 K
D1       2.0000000 sec
d11      0.0200000 sec
TD0      1
SFO1     125.8054113 MHz
NUC1      13
PC1       150 usec
P1        3.70 usec
P1M1     73.00000000 W
SFO2     500.1320101 MHz
NUC2      1H
PC2       18
P2        14.14115
P2M2     80.00 usec
P2M1     18.13359948 W
P1M12    0.53264000 W
P1M13    0.27124000 W
F2 - Processing parameters
SI        32768
SF        125.7679424 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

ES-SS-2-91R\_1H\_CDCl3\_10-09-2023

7.414  
7.413  
7.268  
6.974  
6.973  
6.968  
6.966  
6.438  
6.434  
6.431  
6.428  
5.570  
3.564  
3.553  
3.526  
3.510  
3.494  
3.486  
3.468  
3.342  
3.339  
3.324  
3.320  
3.306  
3.297  
3.059  
3.050  
3.035  
2.452  
2.433  
2.416  
2.371  
2.175  
2.168  
2.160  
2.151  
2.144  
2.026  
2.021  
2.014  
2.007  
2.000  
1.994  
1.986  
1.981  
1.591  
1.584  
1.579  
1.572  
1.568  
1.561  
1.556  
1.549  
1.322  
1.315  
1.310  
1.296  
1.290



ES-SS-2-91R\_13C\_CDC13\_10-09-2023

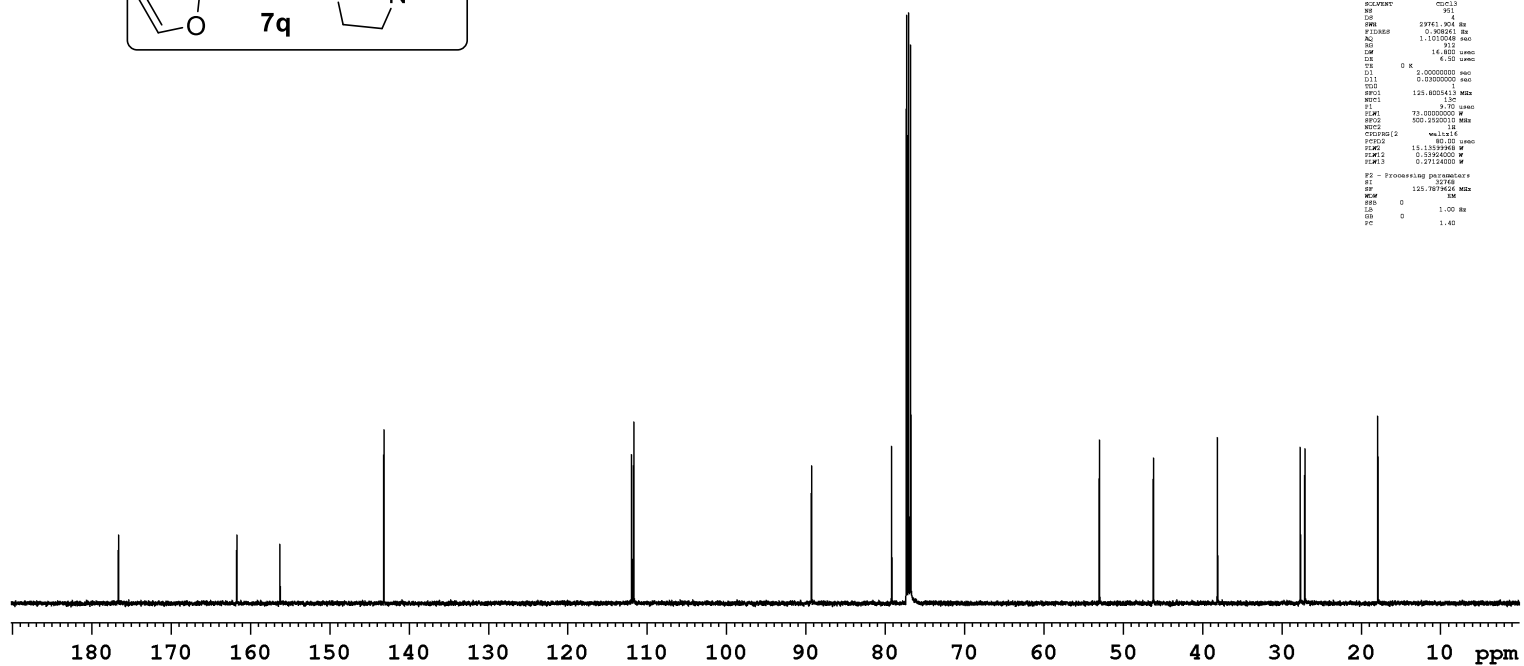
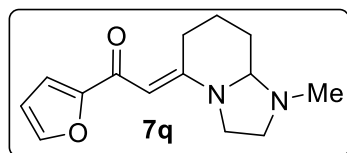
—176.622  
—161.697  
—156.287  
—143.175

<111.957  
<111.658

—89.265  
<79.175  
<77.295  
<77.041  
<76.786

—52.974  
—46.177  
—38.108

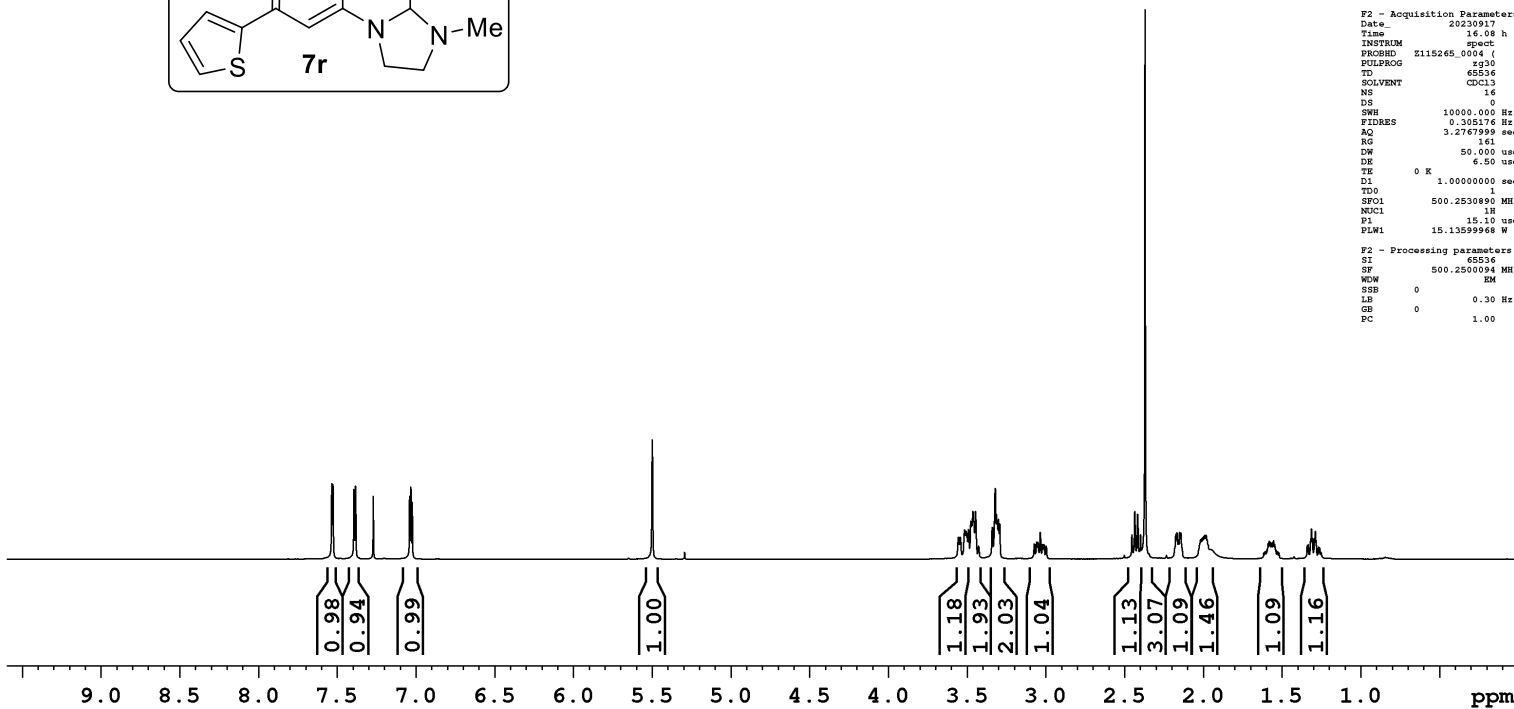
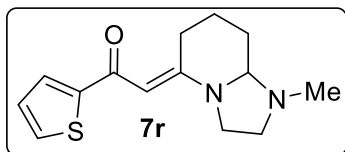
<27.654  
<27.078  
—17.883



```
Current Data Parameters
NAME: 815245_0004
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20230910
Time 20:44:5
INSTRUM spect
PROBHD 1H15245_0004
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 2741.064 Hz
FIDRES 0.000241 Hz
AQ 1.117058 sec
RG 512
SF 14.800 MHz
DE 0.8
TE 300.2 K
D1 2.0000000 sec
d11 0.0300000 sec
TDC
SFO1 125.805413 MHz
PC 8.70 sec
SFO2 31.0000000 MHz
SFO3 100.6200000 MHz
SFO4
PCPD1 16.12414 sec
SFO5 15.1339648 MHz
SFO6 0.2394000 MHz
SFO7 0.2318000 MHz
F2 - Processing parameters
SI 32768
SF 125.7673616 MHz
WDW EM
SSB 0
GB 0
PC 1.40
```

ES-SS-2-90R\_1H\_CDC13\_17-09-2023

7.531  
7.526  
7.524  
7.392  
7.390  
7.382  
7.380  
7.269  
7.038  
7.031  
7.029  
7.021  
5.497  
3.552  
3.541  
3.512  
3.502  
3.489  
3.474  
3.468  
3.461  
3.455  
3.444  
3.339  
3.336  
3.318  
3.311  
3.307  
3.298  
3.291  
3.047  
3.033  
2.451  
2.432  
2.415  
2.396  
2.367  
2.171  
2.164  
2.156  
2.147  
2.140  
2.014  
2.007  
2.000  
1.993  
1.987  
1.979  
1.974  
1.578  
1.573  
1.551  
1.317  
1.310  
1.305  
1.291  
1.285

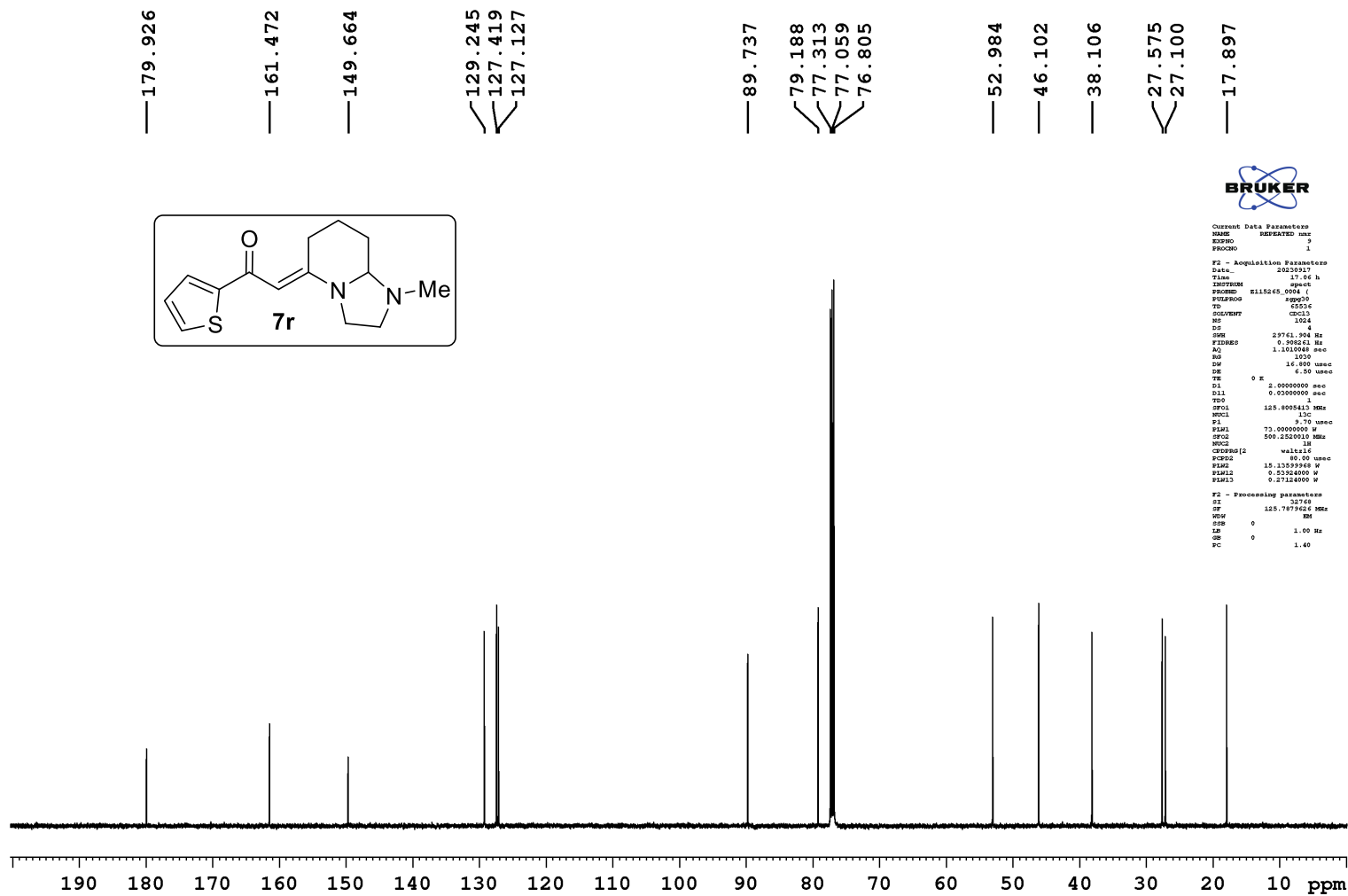


Current Data Parameters  
NAME REPEATED.nmr  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230917  
Time 16.08 h  
INSTRUM spect  
PROBRD Z115245.004 f  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 161  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

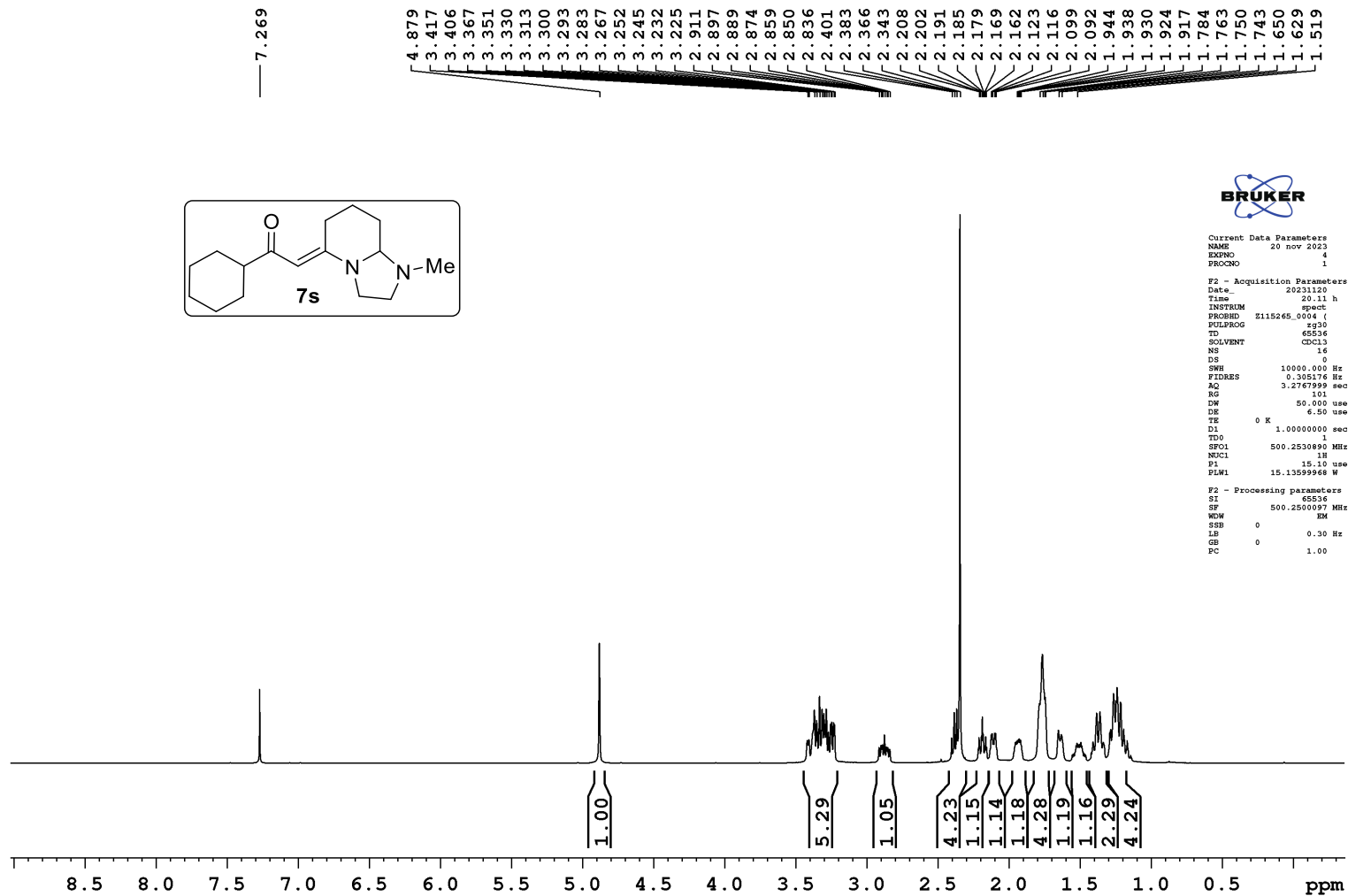
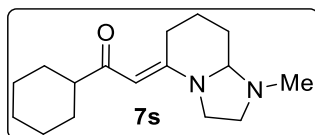
F2 - Processing parameters  
SI 65536  
SF 500.2500094 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-2-90R\_13C\_CDC13\_17-09-2023

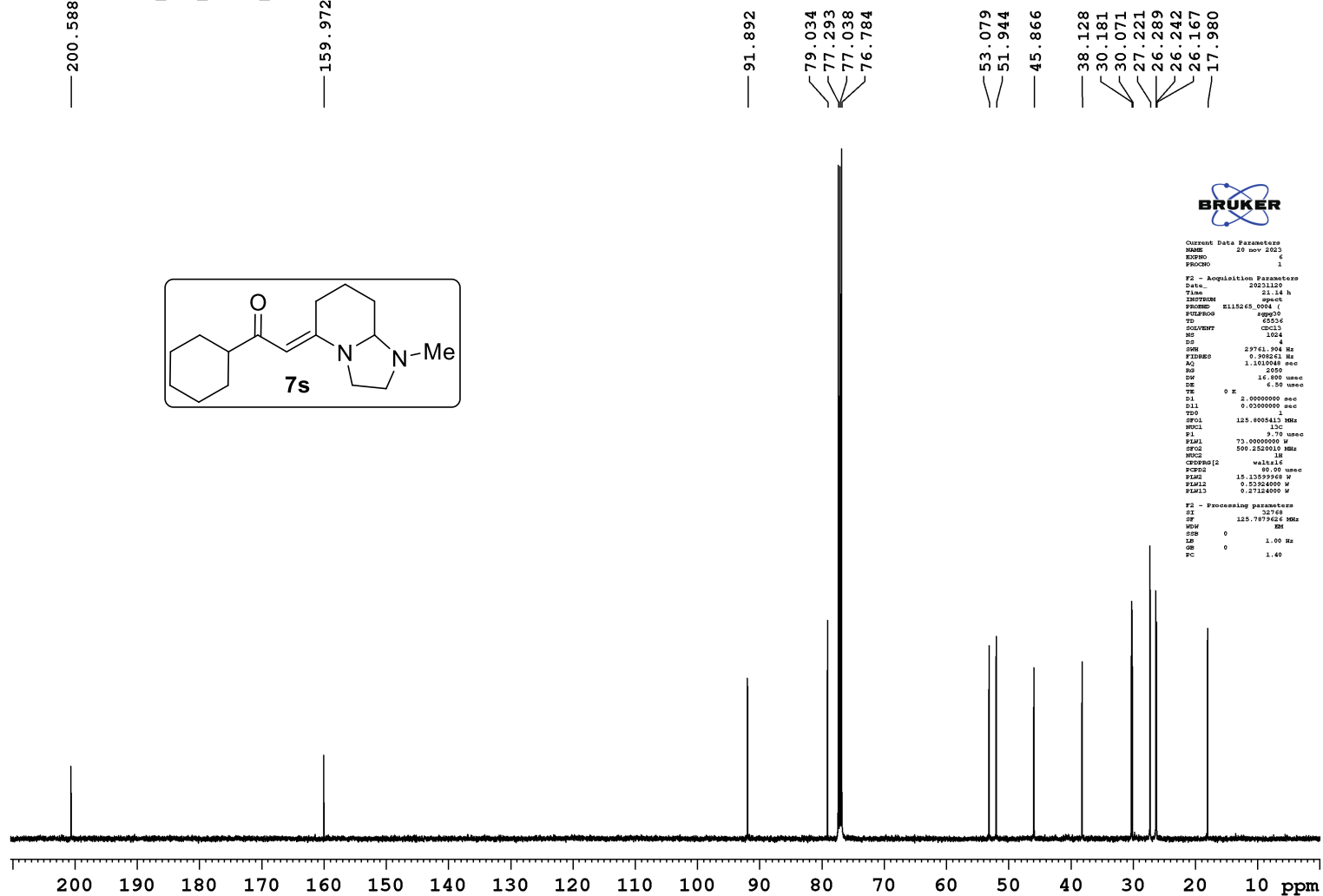


```
Current Data Parameters
NAME          REPEATED  hsc
EXPNO        1
PROCNO       1
F2 - Acquisition Parameters
Date_        20230917
Time         11.04 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           2048
DS           4
SFO          29761.994 MHz
FIDRES       0.988261 MHz
AQ           1.101068 sec
RG           4028
DM           14.800 usec
DE           6.50 usec
TE           300 K
D1           2.0000000 sec
d11          0.0200000 sec
TD0          1
SFO1         125.805411 MHz
NUC1         13C
PC1          150 usec
P1           1.50 usec
P1M1         73.0000000 W
SFO2         500.132010 MHz
NUC2         1H
PC2          18 usec
P2           18 usec
P2M2         15.1335948 W
P1M2         0.53264000 W
P1M3         0.27124000 W
F2 - Processing parameters
SI           32768
SF           125.7679624 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```

ES-SS-2-115\_1H\_CDC13\_20-11-2023



ES-SS-2-115\_13C\_CDC13\_20-11-2023

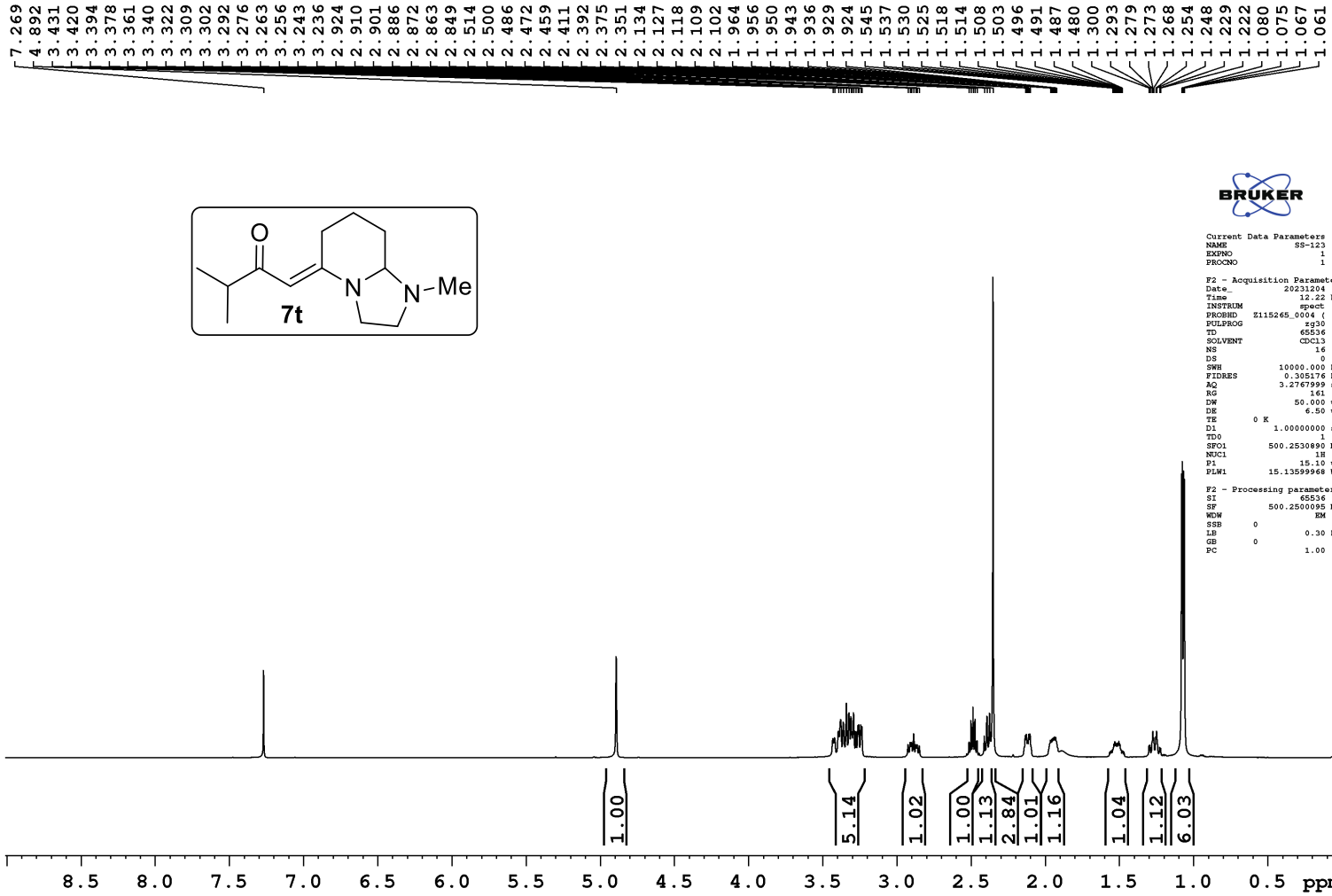


Current Data Parameters  
NAME 20 nov 2023  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231120  
Time 21:14 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdc13  
NS 4  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.986261 MHz  
AQ 1.102068 sec  
RG 1.2050  
DM 14.900 umsec  
DE 6.50 umsec  
TE 300 K  
D1 2.0000000 sec  
D11 0.0200000 sec  
TD0 1  
SFO1 125.905413 MHz  
NUC1 13C  
P1 3.70 umsec  
PCP1 73.0000000 W  
SFO2 500.132010 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 umsec  
P1M1 18.1359948 W  
P1M2 0.53244000 W  
P1M3 0.27124000 W

F2 - Processing parameters  
F2 32763  
SF 125.767962 MHz  
WDW EM  
SSB 0  
LB 1.00 MHz  
GB 0  
PC 1.40

ES-SS-2-123\_1H\_CDC13\_03-12-2023

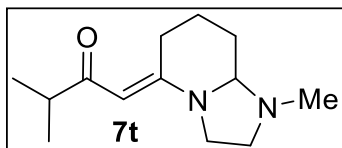




ES-SS-2-123\_13C\_CDC13\_03-12-2023

— 201.315

— 160.048



— 91.511

79.042

77.285

77.031

76.777

— 53.076

— 45.850

— 41.259

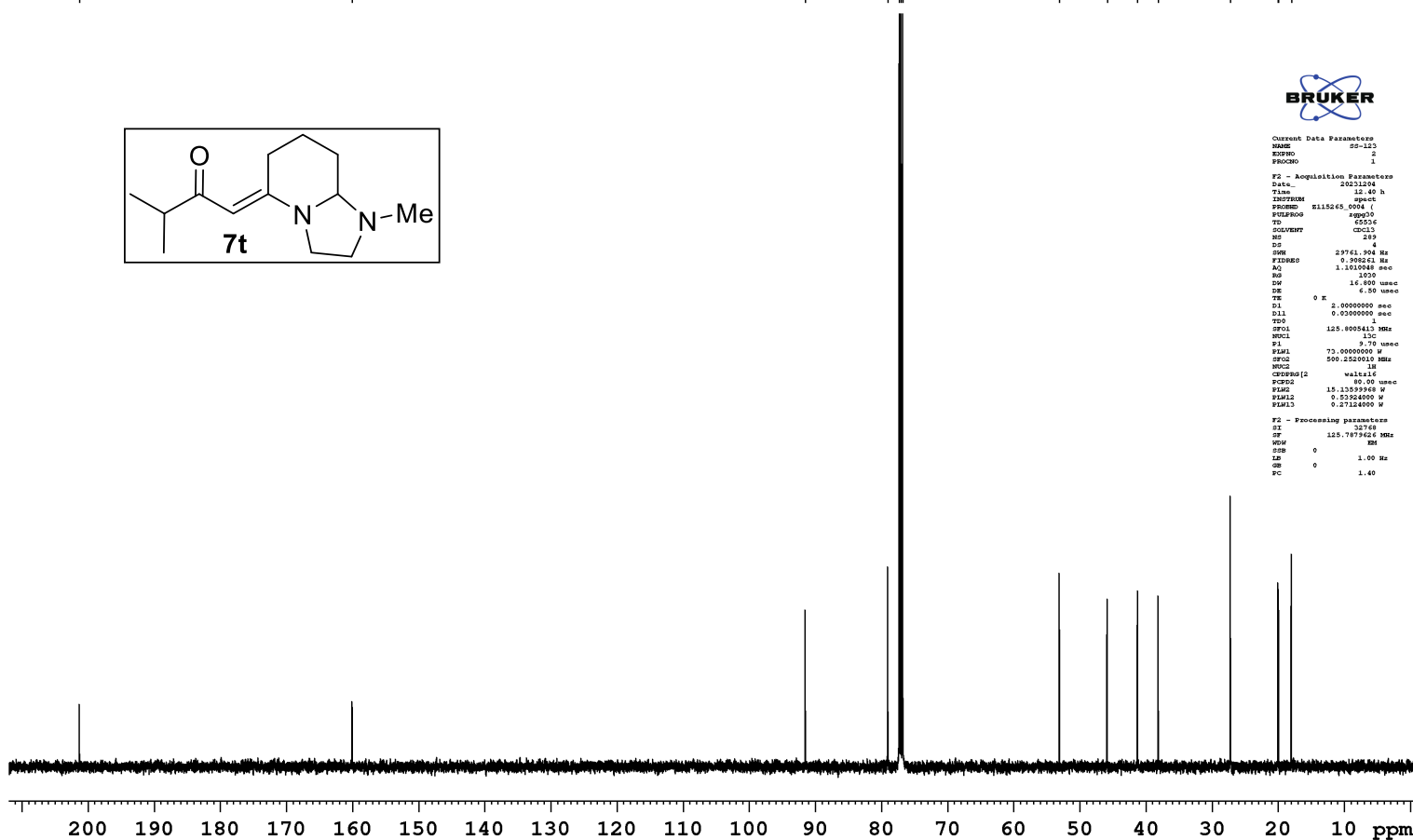
— 38.130

— 27.216

20.014

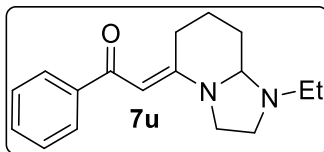
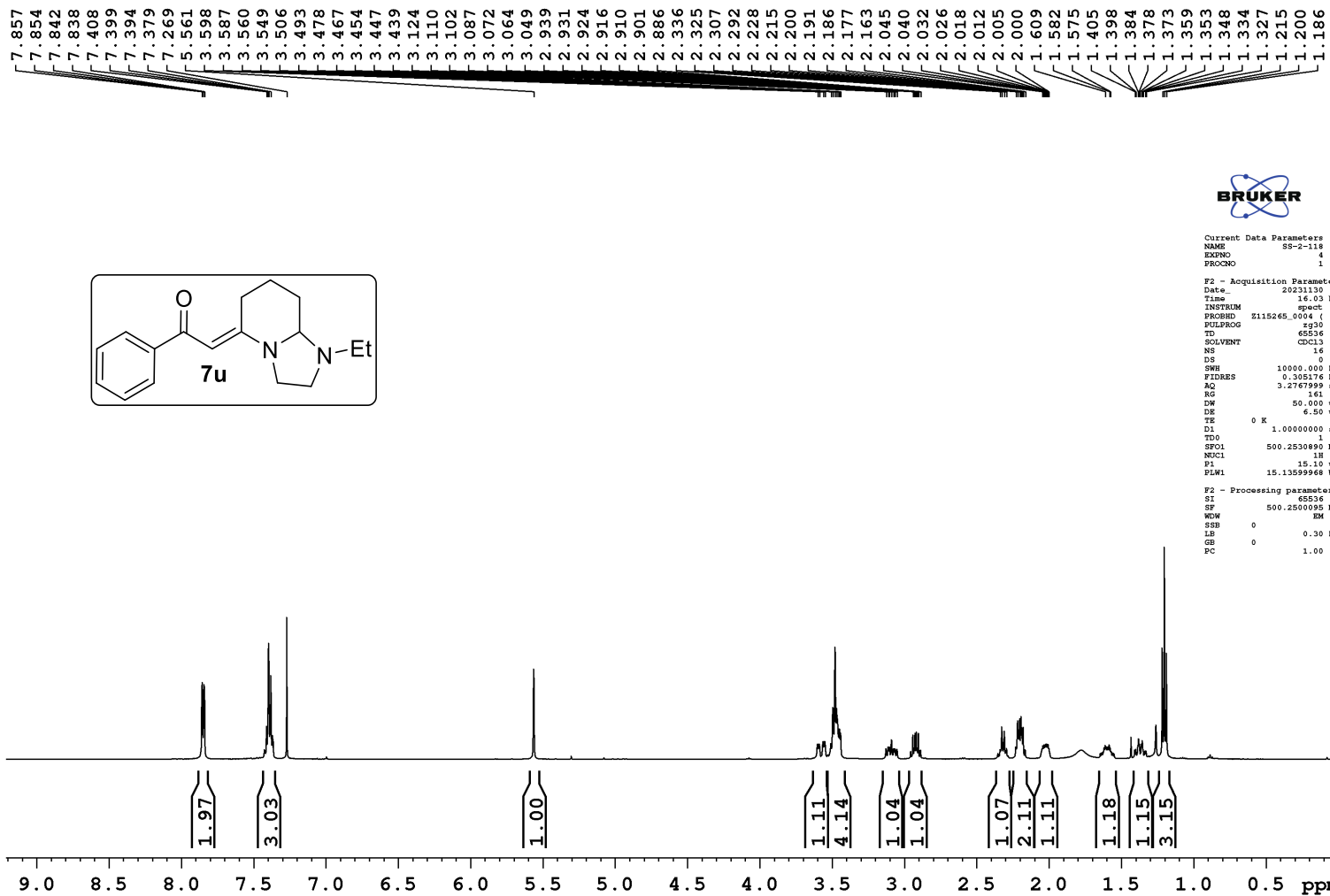
19.926

17.978



Current Data Parameters  
NAME ES-123  
EXPNO 2  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20231204  
Time 12:40 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 256  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.098261 MHz  
AQ 1.101068 sec  
RG 1028  
DM 14.808 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
D11 0.0200000 sec  
TD0 1  
SFO1 125.8054113 MHz  
NUC1 13C  
P1 1.70 usec  
PL1 0.0000000 W  
SFO2 500.1320120 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
P2 18.1335948 W  
PL2 0.5324400 W  
PL13 0.2712400 W  
F2 - Processing parameters  
F1 29761.994 MHz  
SFO 125.7679624 MHz  
NUC 13C  
SFO 500.1320120 MHz  
LQ 1.00 Hz  
GB 0  
PC 1.40

ES-SS-2-118\_1H\_CDC13\_30-11-2023



Current Data Parameters  
 NAME SS-2-118  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20231130  
 Time 16.03 h  
 INSTRUM spect  
 PROBRD Z115245.004 /  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.276789 sec  
 RG 161  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 500.2530890 MHz  
 NUC1 H  
 P1 15.10 usec  
 PLW1 15.13599968 W

F2 - Processing parameters  
 SI 65536  
 SF 500.2500095 MHz  
 NCM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ES-SS-2-118\_13C\_CDC13\_30-11-2023

187.792

161.596

142.813

130.130

127.995

127.189

90.455

77.281

77.027

76.773

49.765

46.072

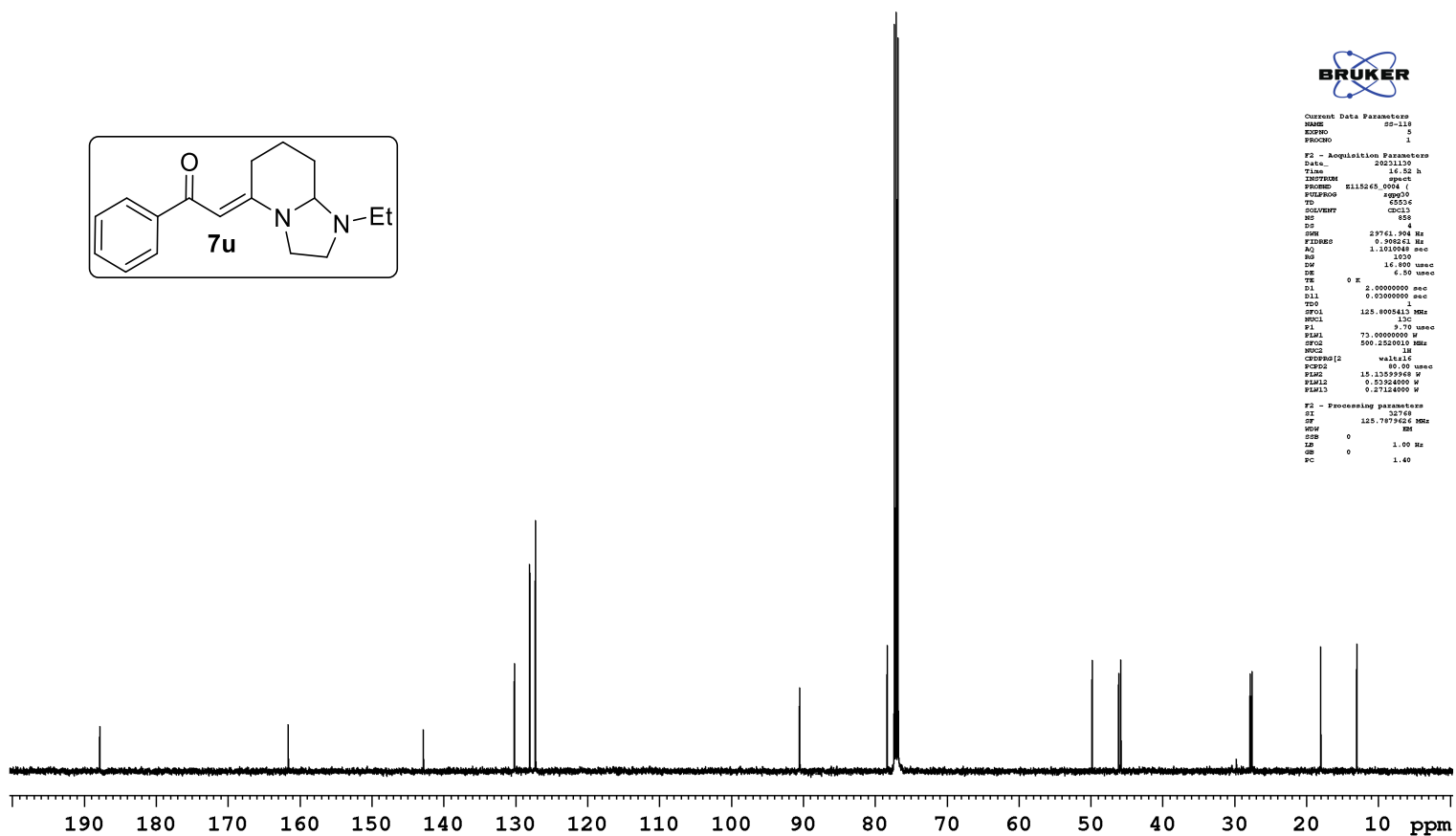
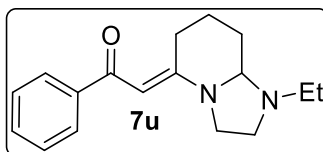
45.793

27.778

27.515

17.976

12.953

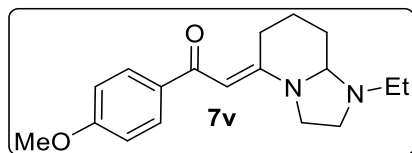


```
Current Data Parameters
NAME      ES-118
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20231130
Time     14:50 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  cdcl3
NS        4
DS        4
SFO      29761.994 MHz
FIDRES   0.988261 MHz
AQ        1.1010048 sec
RG         4028
DM         14.800 usec
DE         6.50 usec
TE        300 K
D1         2.0000000 sec
d11        0.0200000 sec
TD0        1
SFO1      125.8054113 MHz
NUC1       13C
PC1        150 usec
P1         1.0000000 sec
P1M1      73.00000000 W
SFO2      500.1300101 MHz
NUC2       1H
PC2        18 usec
P2         0.00000000 sec
P2M2      15.13359948 W
P1M3      0.53264000 W
P1M13     0.27124000 W

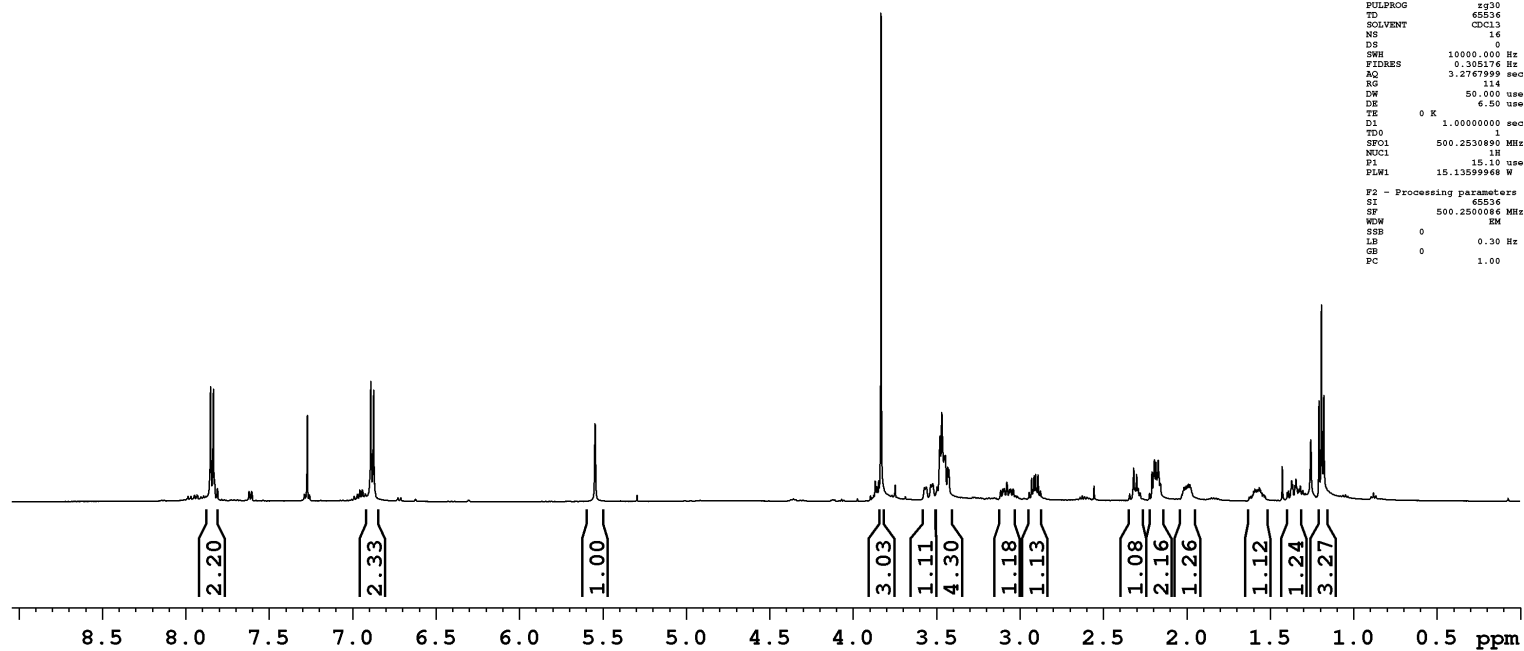
F2 - Processing parameters
SI         32768
SF         125.7679424 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-7-43\_1H\_CDC13\_22-12-2023



7.849  
7.832  
7.269  
6.889  
6.871

5.544  
3.830  
3.569  
3.559  
3.531  
3.520  
3.476  
3.466  
3.451  
3.444  
3.431  
3.423  
3.113  
3.099  
3.090  
3.076  
3.061  
3.052  
3.037  
2.942  
2.927  
2.918  
2.912  
2.904  
2.897  
2.889  
2.874  
2.339  
2.316  
2.308  
2.288  
2.289  
2.277  
2.206  
2.196  
2.192  
2.182  
2.168  
2.155  
2.145  
2.014  
1.623  
1.589  
1.562  
1.395

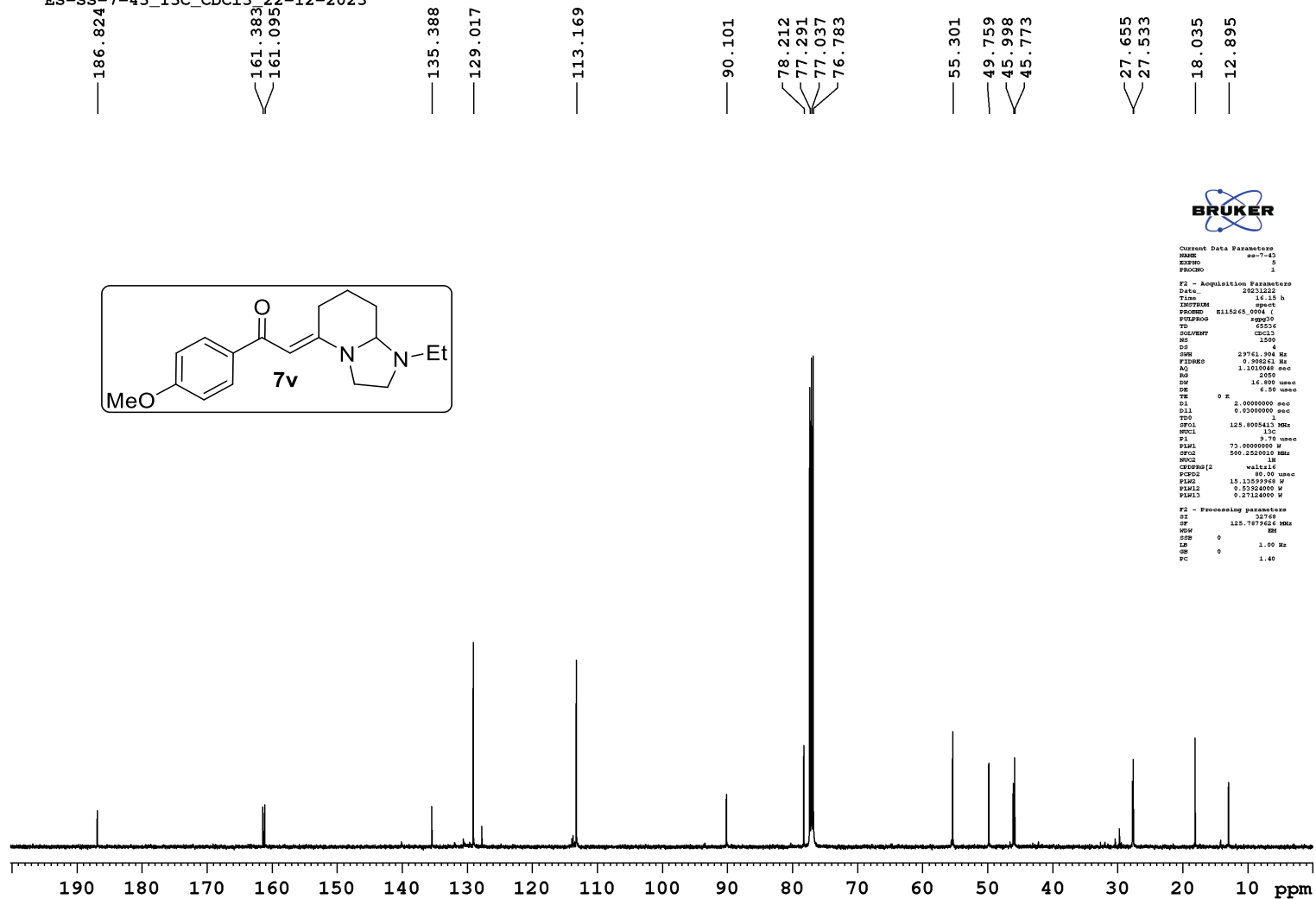


Current Data Parameters  
NAME es-7-43  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231222  
Time 14:54 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 114  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500086 MHz  
WDW EM  
SSB 0  
LP 0.30 Hz  
GB 0  
PC 1.00

ES-SS-7-43\_13C\_CDC13\_22-12-2023



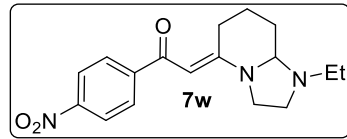
```
Current Data Parameters
NAME      #a-7-43
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20231222
Time     14:15 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SFO      29761.994 MHz
FIDRES   0.988261 MHz
AQ        1.101068 sec
RG         4056
DM         14.800 usec
DE         6.50 usec
TE        300 K
D1         2.0000000 sec
d11        0.0200000 sec
TD0        1
SFO1      125.8054113 MHz
NUC1       13C
PC1        150 usec
P1         1.70 usec
P1M1      73.00000000 W
SFO2      500.1320101 MHz
NUC2       1H
PC2M2     18 usec
P2M2     80.00 usec
P1M2     18.13359948 W
P1M12    0.53264000 W
P1M13    0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7679424 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-7-45\_1H\_CDCl3\_25-12-2023

8.147  
8.130  
7.880  
7.862  
7.202



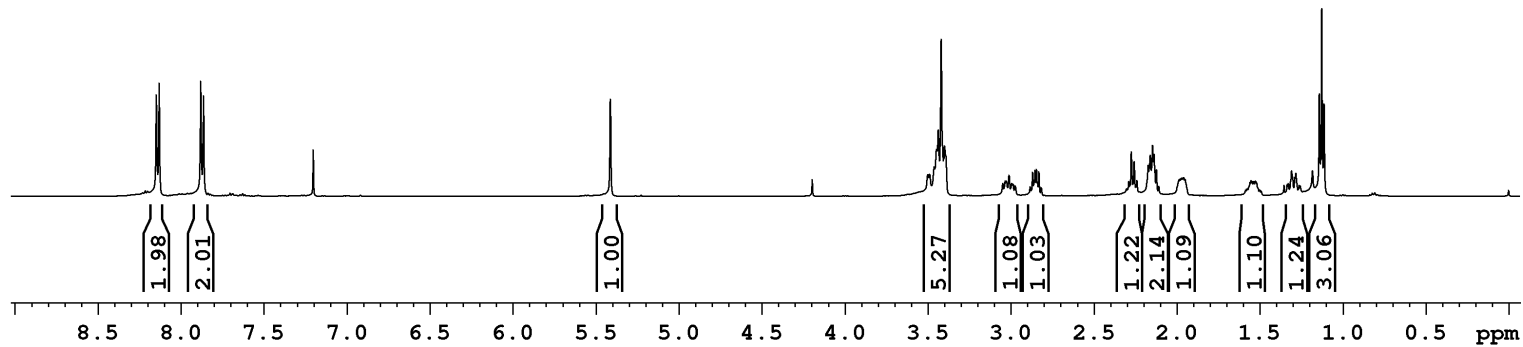
5.411  
3.499  
3.488  
3.460  
3.446  
3.435  
3.418  
3.403  
3.397  
3.391  
3.047  
3.032  
3.024  
3.009  
2.994  
2.986  
2.867  
2.852  
2.844  
2.829  
2.287  
2.272  
2.255  
2.239  
2.171  
2.158  
2.145  
2.135  
2.121  
2.107  
1.984  
1.977  
1.957  
1.949  
1.585  
1.550  
1.544  
1.546  
1.489  
1.333  
1.306  
1.281



Current Data Parameters  
NAME REPEAT  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231225  
Time 14.02 h  
INSTRUM spect  
PROCNO Z115265\_0004 ( )  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.275799 sec  
RG 114  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2500431 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500431 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



ES-ss-7-45\_13C\_CDC13\_25-12-2023

— 184.829  
— 163.143  
— 148.603  
— 148.496

— 128.006  
— 123.319

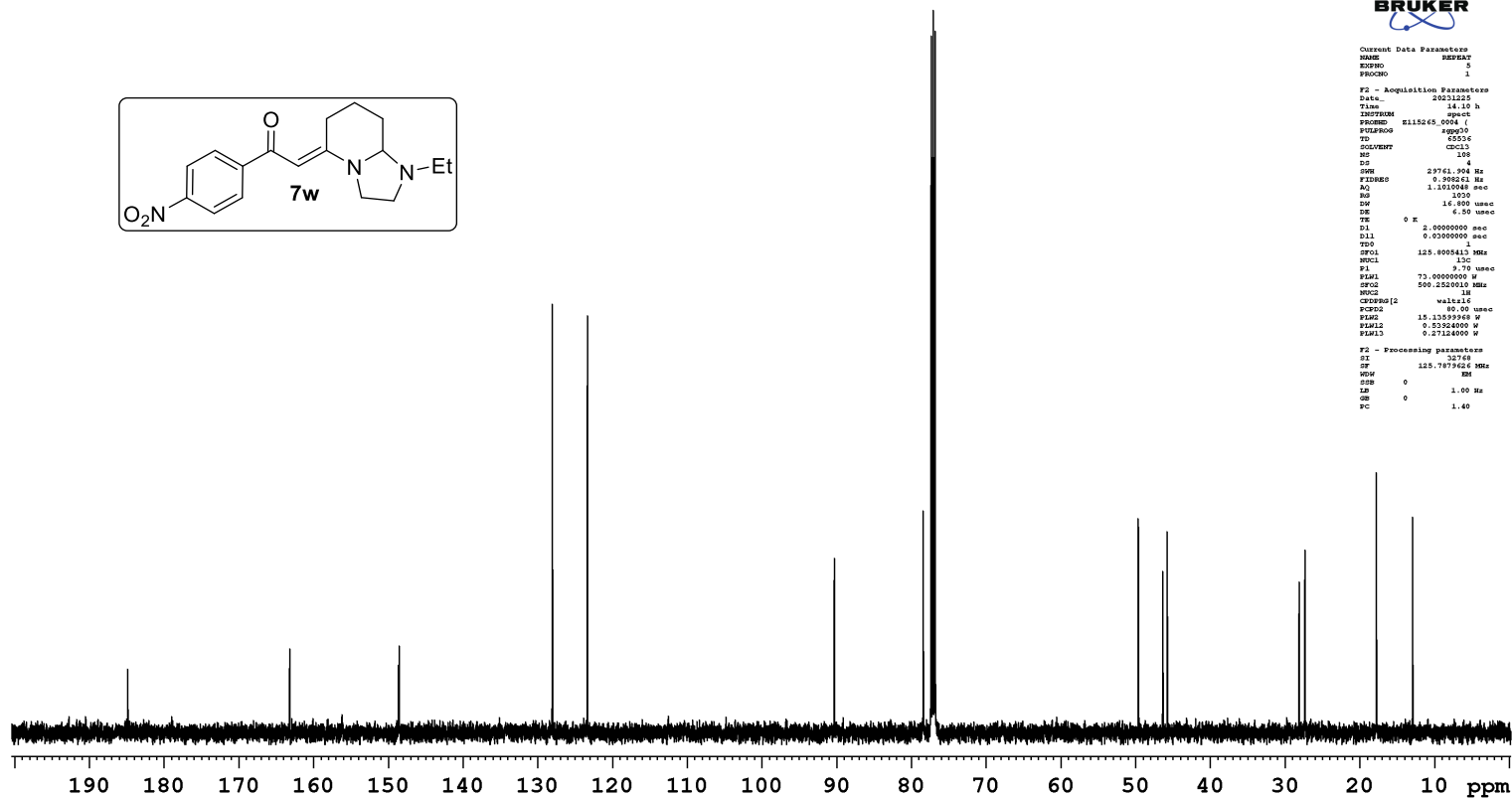
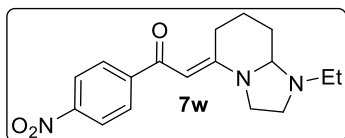
— 90.282

— 78.378  
— 77.296  
— 77.042  
— 76.788

— 49.594  
— 46.320  
— 45.717

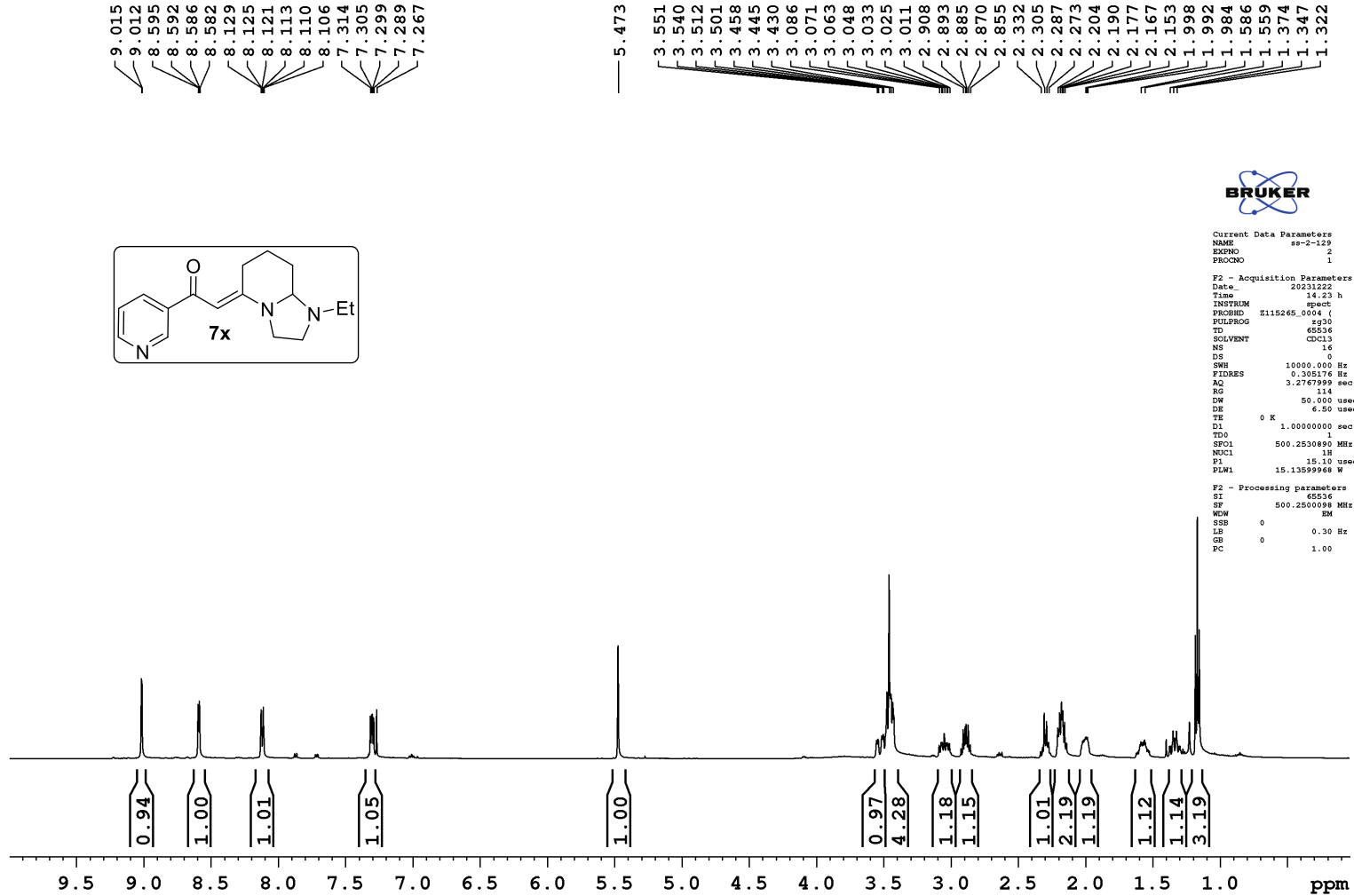
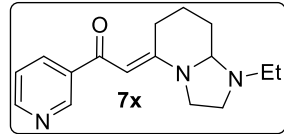
— 28.056  
— 27.300

— 17.739  
— 12.887



```
Current Data Parameters
NAME          REFNAME
EXPNO        2
PROCNO       1
F2 - Acquisition Parameters
Date_        20231220
Time         14.10 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           4
DS           4
SFO          29761.994 MHz
FIDRES       0.988261 Hz
AQ           1.101068 sec
RG           4028
DM           14.908 usec
DE           6.50 usec
TE           0 K
D1           2.0000000 sec
d12         0.0200000 sec
TD0          1
SFO1         125.805411 MHz
NUC1         13C
PC1          150 usec
P1           150 usec
P1P1         70.0000000 W
SFO2         500.132010 MHz
NUC2         1H
PCP2P2       18
P2P2P2       80.00 usec
P1P2         16.1335948 W
P1P12        0.53264000 W
P1P13        0.27124000 W
F2 - Processing parameters
SI           32768
SF           125.7679424 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```

ES-SS-2-129\_1H\_CDC13\_22-12-2023



Current Data Parameters  
 NAME es-2-129  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20231222  
 Time 14.23 h  
 INSTRUM spect  
 FREQHD Z115265.0004 ( MHz)  
 PULPROG zg30  
 TD 65536  
 SFO1 500.13559968  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.2757999 sec  
 RG 114  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 500.2500098 MHz  
 NUC1 1H  
 P1 15.10 usec  
 PLW1 15.13559968 W

F2 - Processing parameters  
 SI 65536  
 SF 500.2500098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



ES-SS-2-129\_13C\_CDCl3\_22-12-2023

184.990

162.550

150.613

148.502

137.847

134.895

123.208

90.047

78.292

77.323

77.068

76.814

49.627

46.210

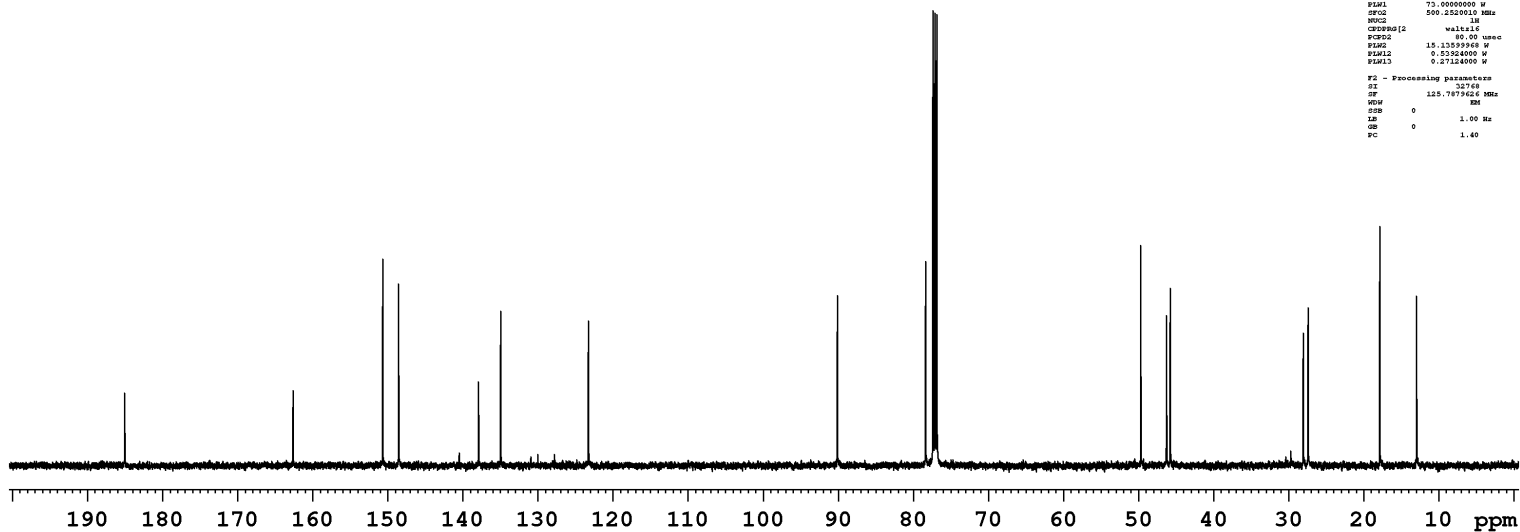
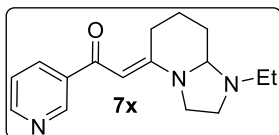
45.708

27.972

27.341

17.790

12.884



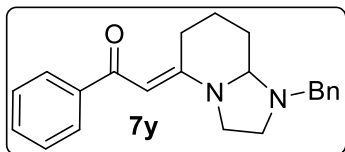
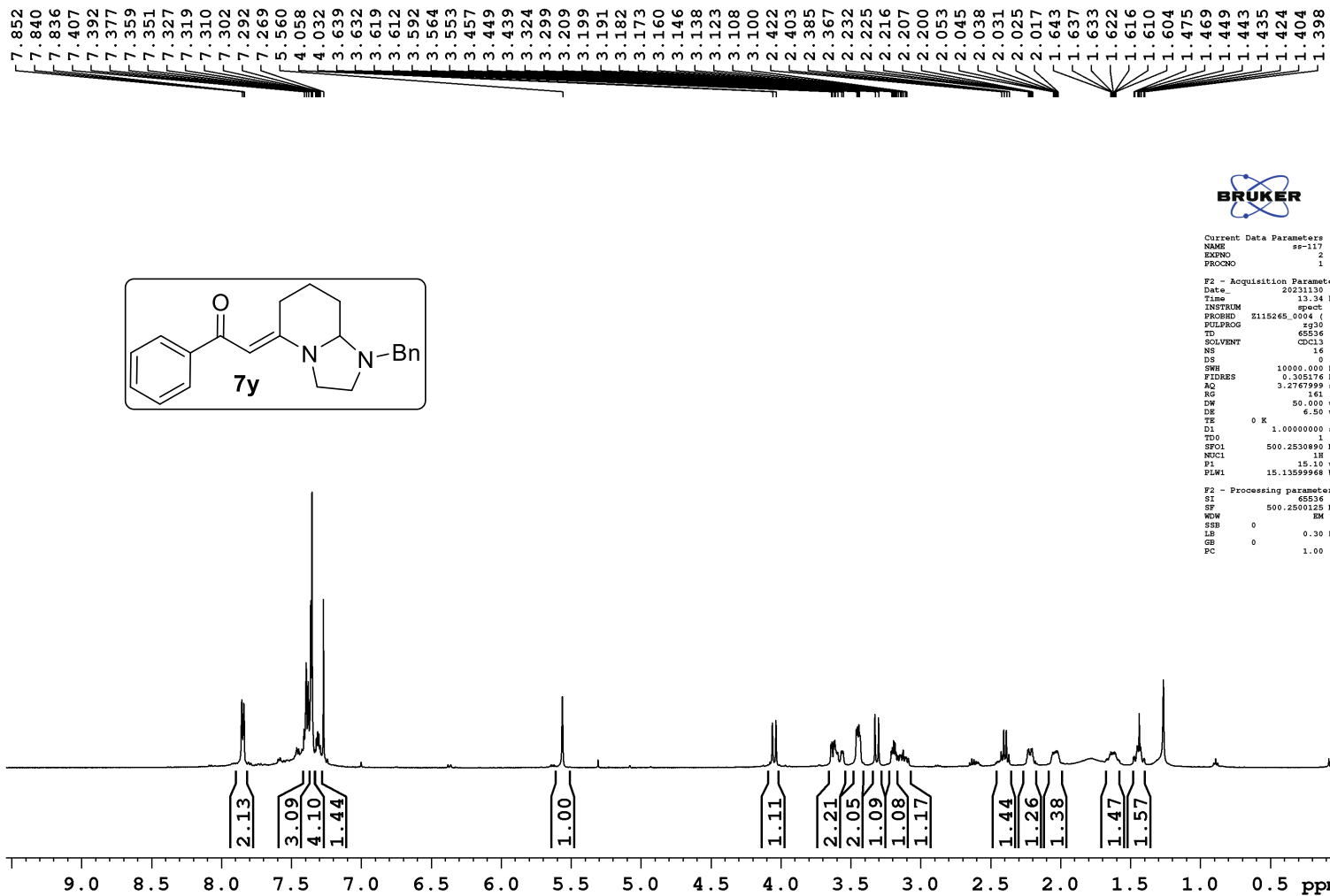
```

Current Data Parameters
NAME          #2-129
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_        20211222
Time         24.46 h
INSTRUM      spect
PROBHD       E115245.004 (
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           374
DS           4
SWH          29761.994 Hz
FIDRES      0.398241 Hz
AQ          1.102048 sec
RG           1020
DM          16.800 usec
DE           6.50 usec
TE           0 K
D1          2.0000000 sec
d11         0.0000000 sec
SFO1        125.8005413 MHz
TD0         150
SFO2        125.8005413 MHz
SF         125.8005413 MHz
NUC1         13C
P1          8.75 usec
PL1         0 dB
PL12        73.0000000 W
PL13        500.0000010 MHz
PL14        1H
CFOFFS12    0.1111111
PCPD2       80.00 usec
PL2         0 dB
PL22        15.1259990 W
PL23        0.53324000 W
PL24        0.27124000 W

F2 - Processing parameters
SI          32768
SF          125.7673624 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
SB          1.40
    
```

ES-SS-2-117\_1H\_CDC13\_29-11-2023

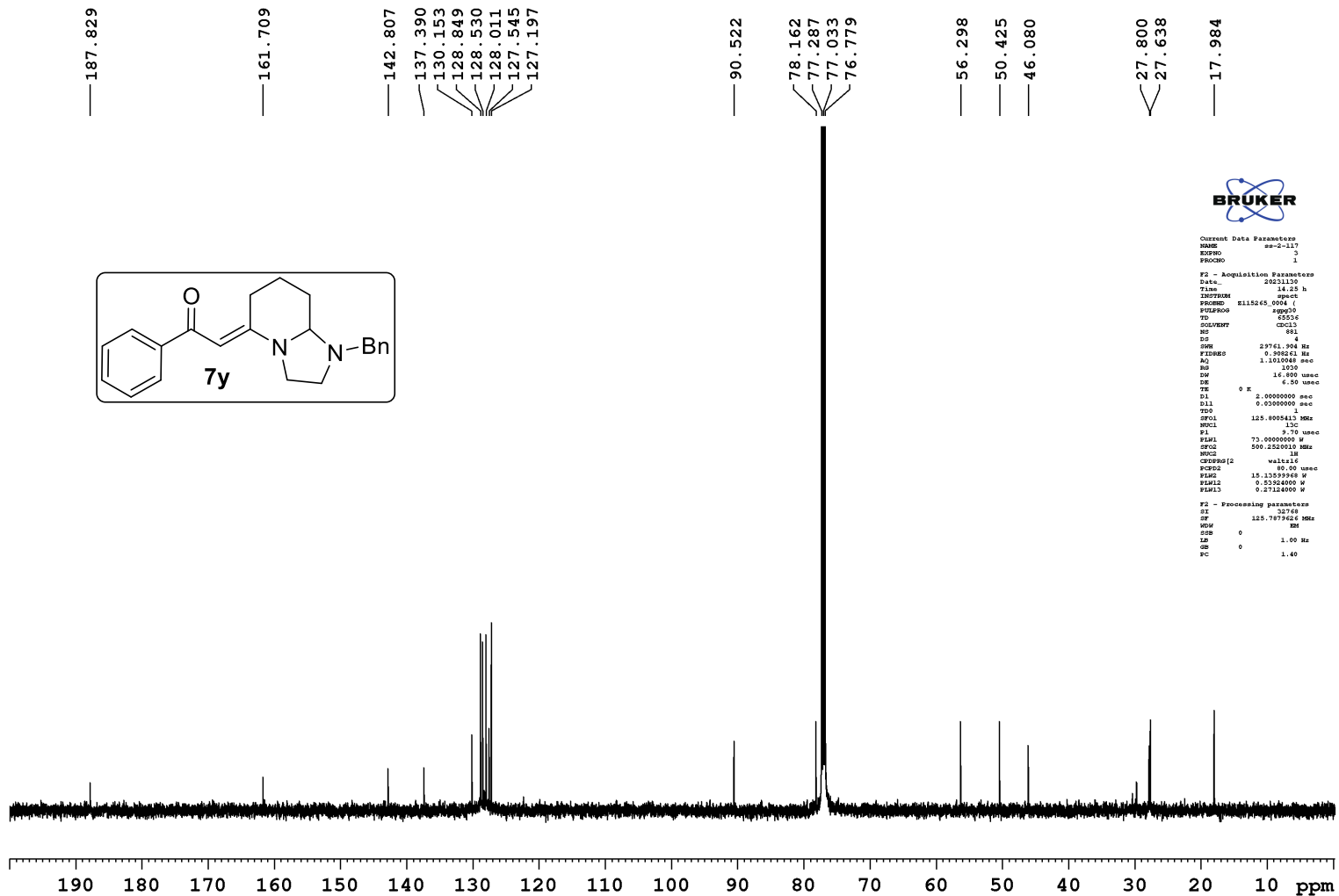


Current Data Parameters  
 NAME ss-117  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20231130  
 Time 13.34 h  
 INSTRUM spect  
 PROBRD Z115245.004 /  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.276789 sec  
 RG 161  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 500.2530890 MHz  
 NUC1 H  
 P1 15.10 usec  
 PLW1 15.1359946 W

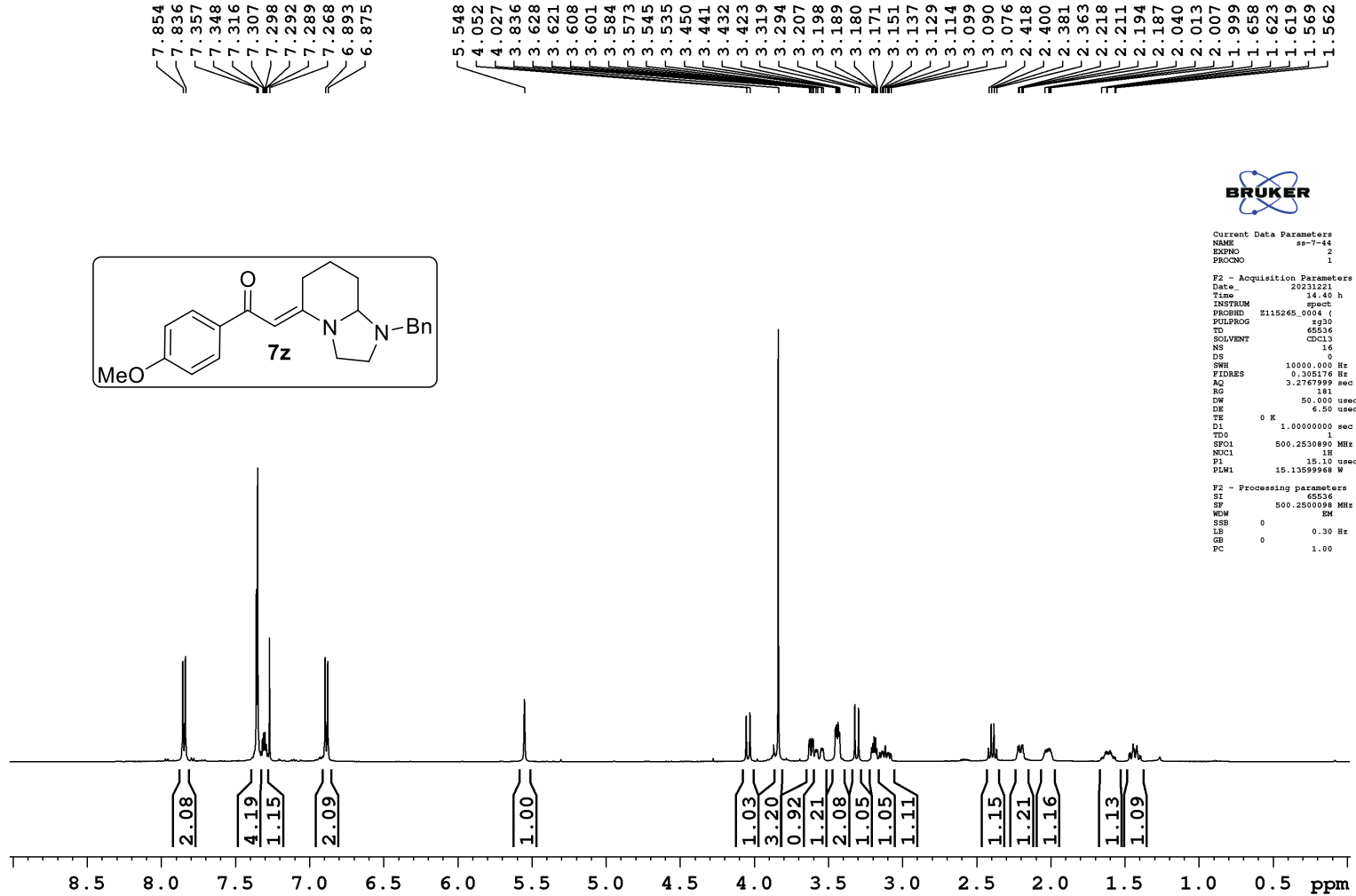
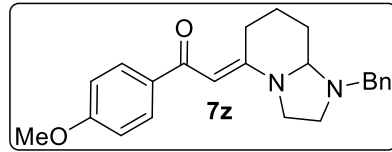
F2 - Processing parameters  
 SI 65536  
 SF 500.2500125 MHz  
 NCM RM  
 SSB 0  
 LP 0.30 Hz  
 GB 0  
 PC 1.00

ES-SS-2-117\_13C\_CDC13\_30-11-2023



Current Data Parameters  
NAME es-2-117  
EXPNO 3  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20231120  
Time 14:25 h  
INSTRUM spect  
PROBHD 1H15265.004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdc13  
NS 6  
DS 4  
SFO 29761.994 MHz  
FIDRES 0.398261 MHz  
AQ 1.101068 sec  
RG 4028  
CW 14.800 usec  
DE 6.50 usec  
TE 300 K  
D1 2.0000000 sec  
S11 0.0200000 sec  
TD0 1  
SFO1 125.805411 MHz  
NUC1 13C  
P1 150 usec  
PL1 0  
PL12 73.0000000 W  
SFO2 500.132010 MHz  
NUC2 1H  
SFO202 400.141615 MHz  
P202 80.00 usec  
PL2 18.1335948 W  
PL13 0.53264000 W  
PL13 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.767962 MHz  
WDW EM  
SSB 0  
LB 1.00 MHz  
GB 0  
PC 1.40

ES-SS-7-44\_1H\_CDCl3\_21-12-2023

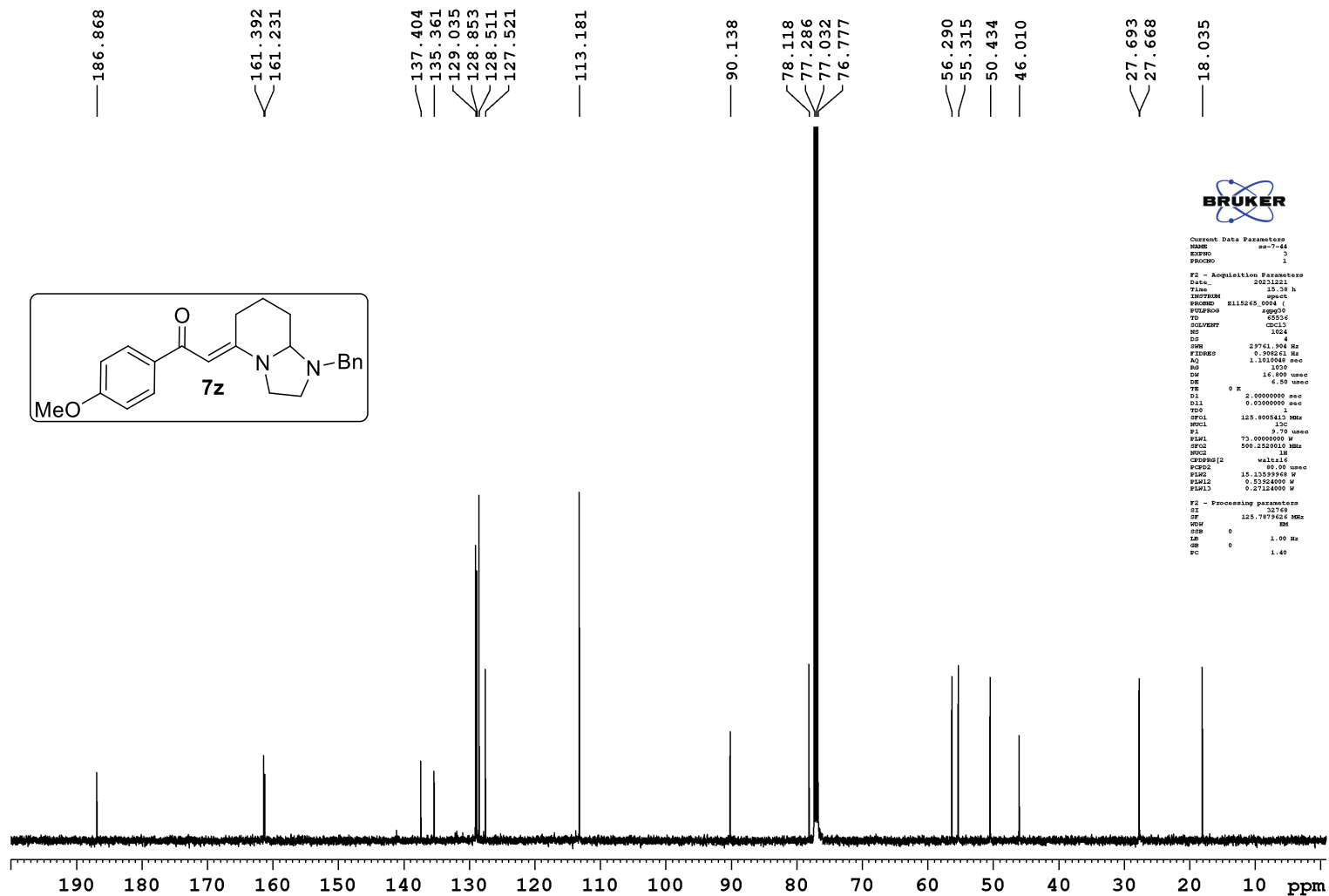
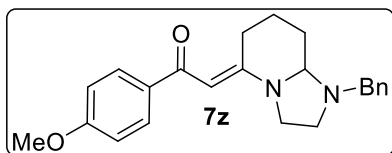


Current Data Parameters  
NAME ss-7-44  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231221  
Time 14.40 h  
INSTRUM spect  
PROBHD Z115265.0004 (   
PULPROG zg30  
TD 65536  
FIDRES 0.305176 Hz  
AQ 1.2757999 sec  
RG 181  
SW 10000.000 Hz  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.2757999 sec  
RG 181  
SW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

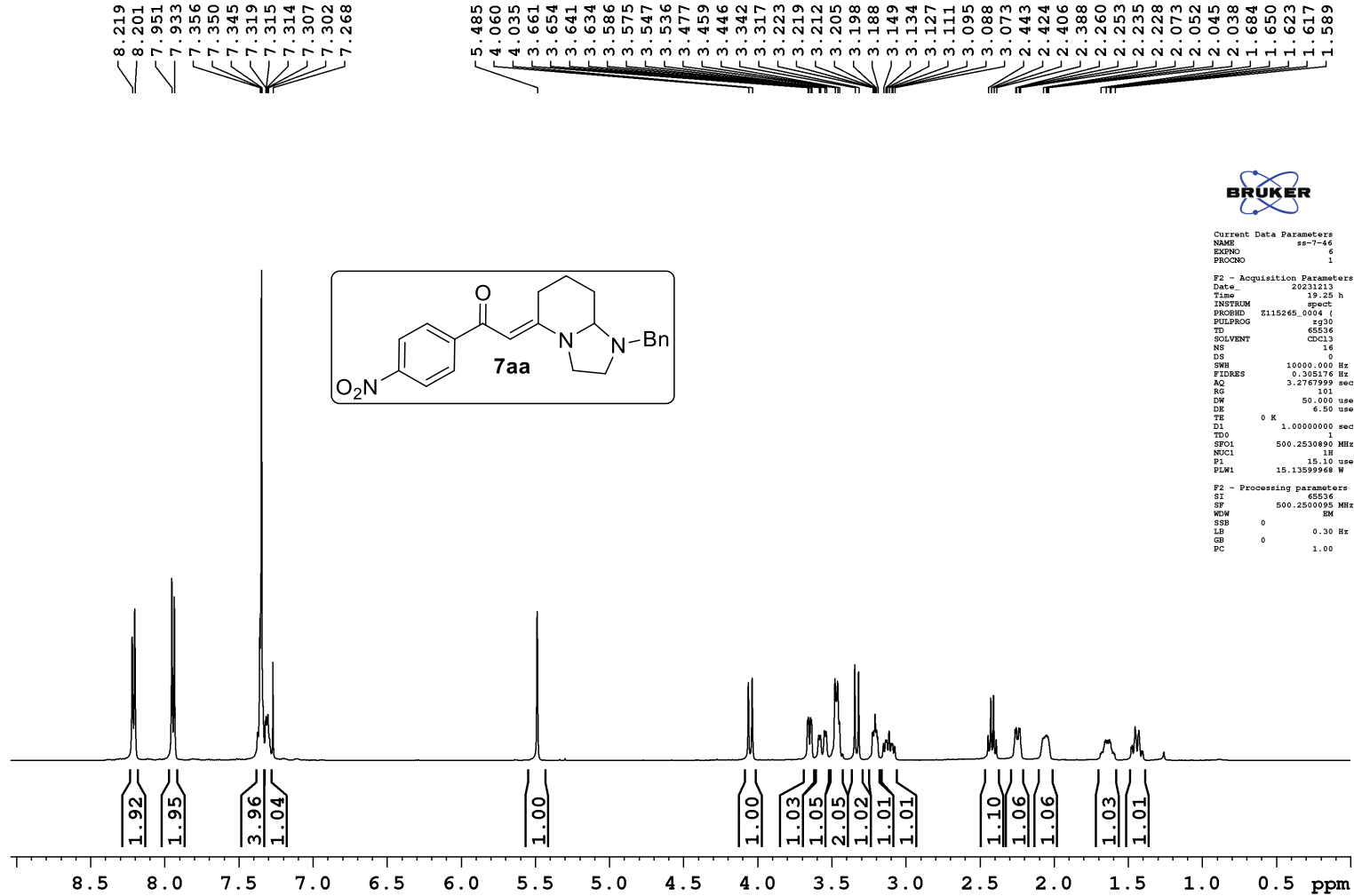
F2 - Processing parameters  
SI 65536  
SF 500.2500098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-7-44\_13C\_CDC13\_21-12-2023



Current Data Parameters  
NAME es-7-44  
EXPNO 3  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20211221  
Time 15:26 h  
INSTRUM spect  
PROBHD E115245.0054 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 1024  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.398241 Hz  
AQ 1.102048 sec  
RG 1020  
DM 16.800 usec  
DE 6.50 usec  
TE 0 K  
D1 2.0000000 sec  
d11 0.0000000 sec  
TDO 0  
SFO1 125.8005413 MHz  
NUC1 13C  
P1 8.75 usec  
PL1 73.0000000 W  
SFO2 500.1320101 MHz  
NUC2 1H  
CFO2R12 14111.6  
PCPD2 80.00 usec  
PL2 15.13259950 W  
PL12 0.53324000 W  
PL13 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.7679624 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-7-46\_1H\_CDC13\_13-12-2023

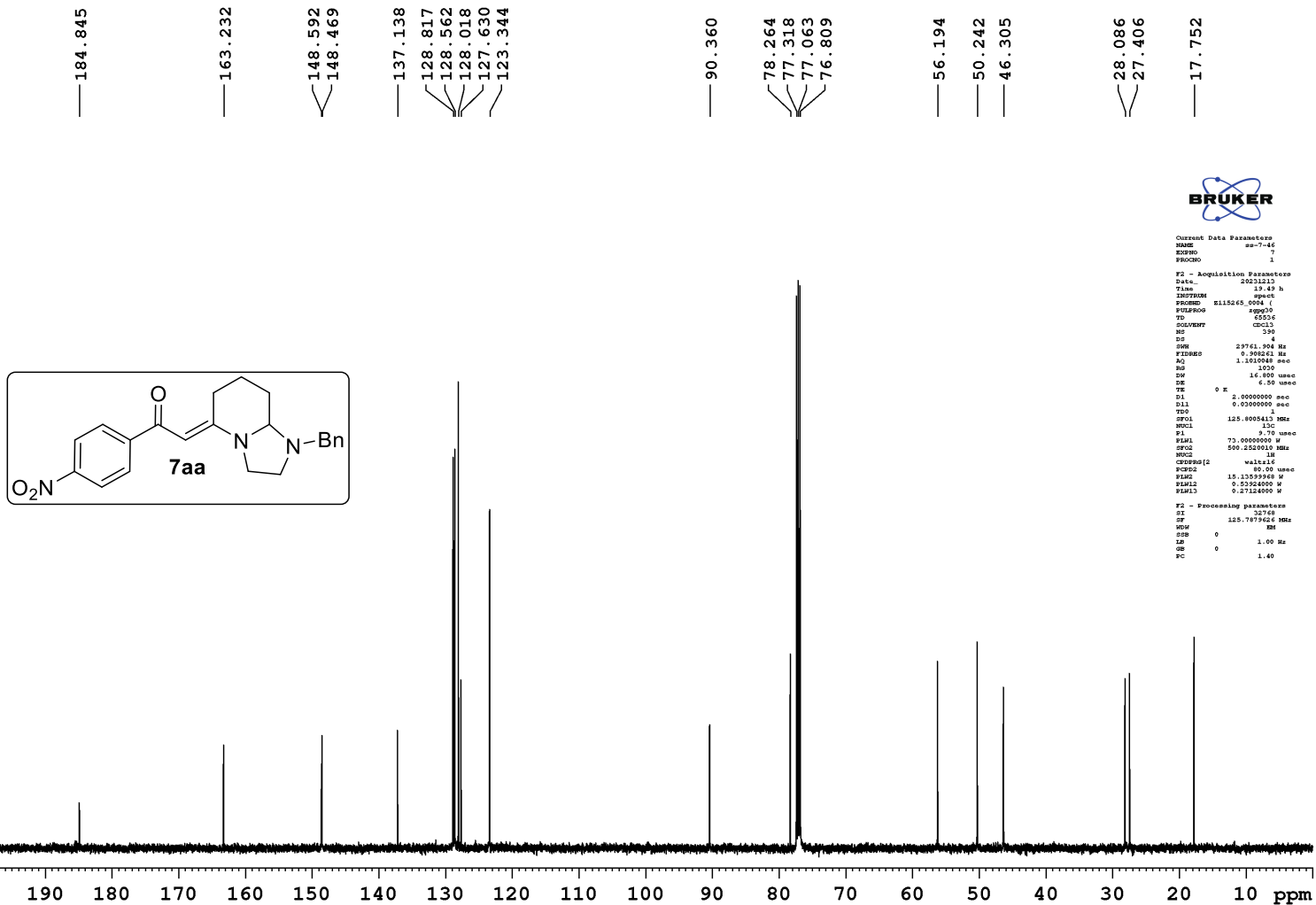


Current Data Parameters  
NAME ss-7-46  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231213  
Time 19.25 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276789 sec  
RG 101  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500995 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ES-SS-7-46\_13C\_CDC13\_13-12-2023

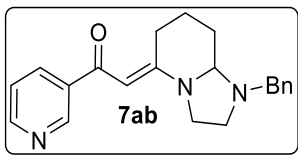
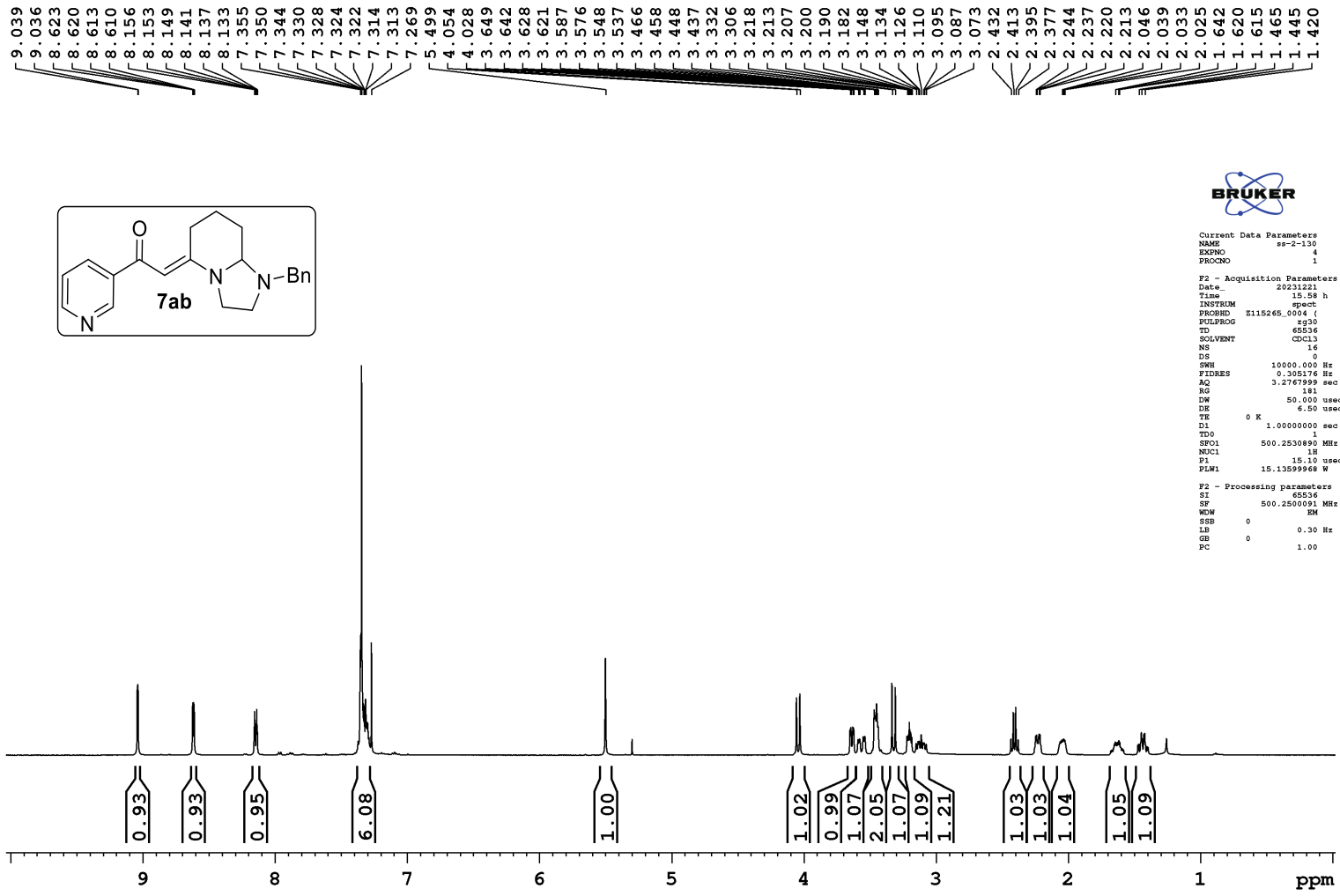


```
Current Data Parameters
NAME      #a-7-46
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20231213
Time     11:45 h
INSTRUM  spect
PROBHD   5mmBBO
PULPROG  zgpg30
TD        65536
SOLVENT  cdcl3
NS        4
DS        4
SFO      29761.994 MHz
FIDRES   0.988261 MHz
AQ        1.101068 sec
RG         4028
DM         16.800 usec
DE         6.50 usec
TE        300 K
D1        2.0000000 sec
d11       0.0200000 sec
TD0       125.8005413 MHz
SFO1      125.8005413 MHz
NUC1      13C
P1         150 usec
PL1        0 dB
PL12      73.0000000 dB
SFO2      500.1320101 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2     80.00 usec
PL2       18.1335948 dB
PL13      0.53264000 dB
PL14      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7679624 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

ES-SS-2-130\_1H\_CDC13\_21-12-2023



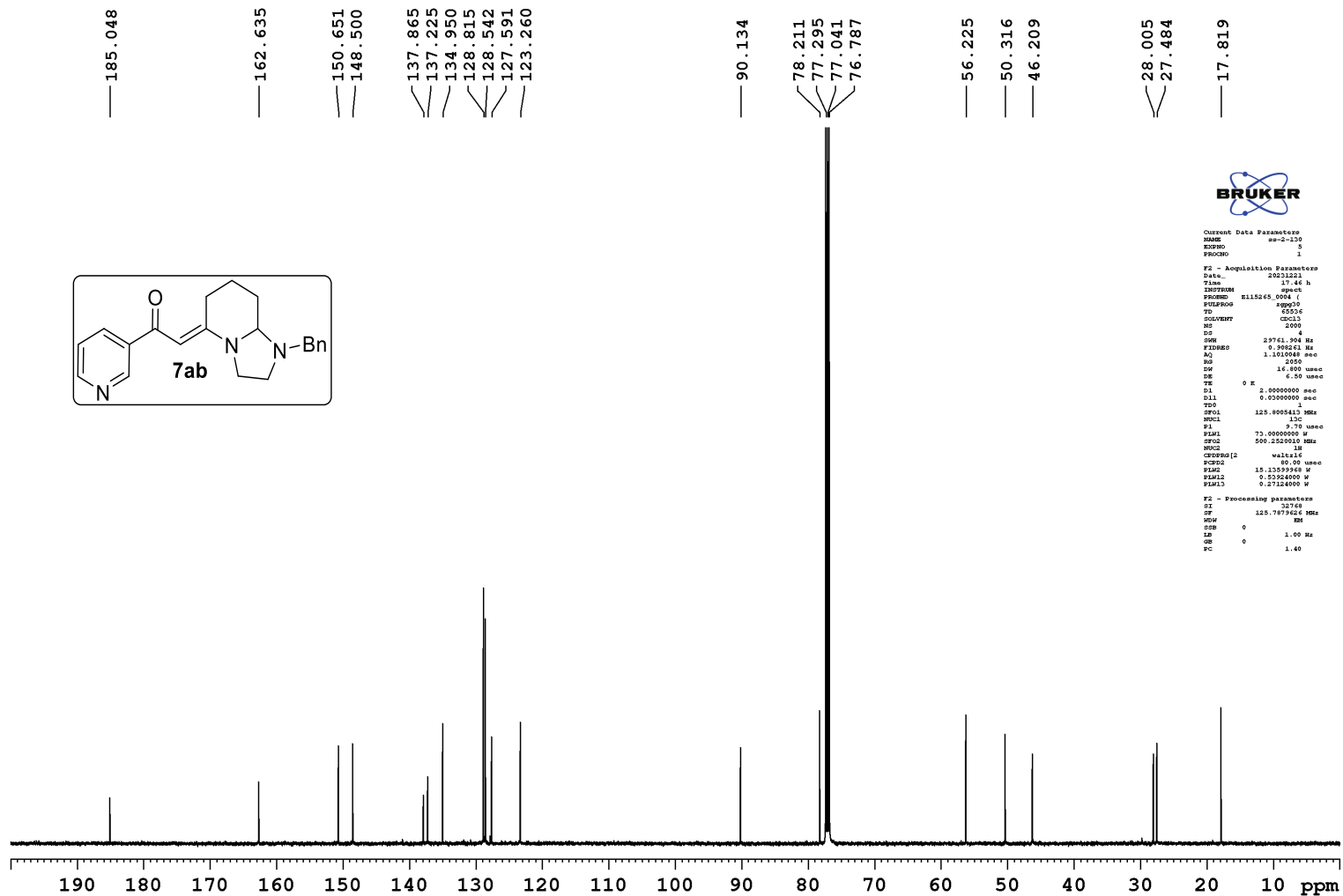
Current Data Parameters  
NAME ss-2-130  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231221  
Time 15.58 h  
INSTRUM spect  
PROBRD Z115245.004 /  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.276799 sec  
RG 181  
DW 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.2530890 MHz  
NUC1 1H  
P1 15.10 usec  
PLW1 15.13599968 W

F2 - Processing parameters  
SI 65536  
SF 500.2500091 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



ES-SS-2-130\_13C\_CDC13\_21-12-2023

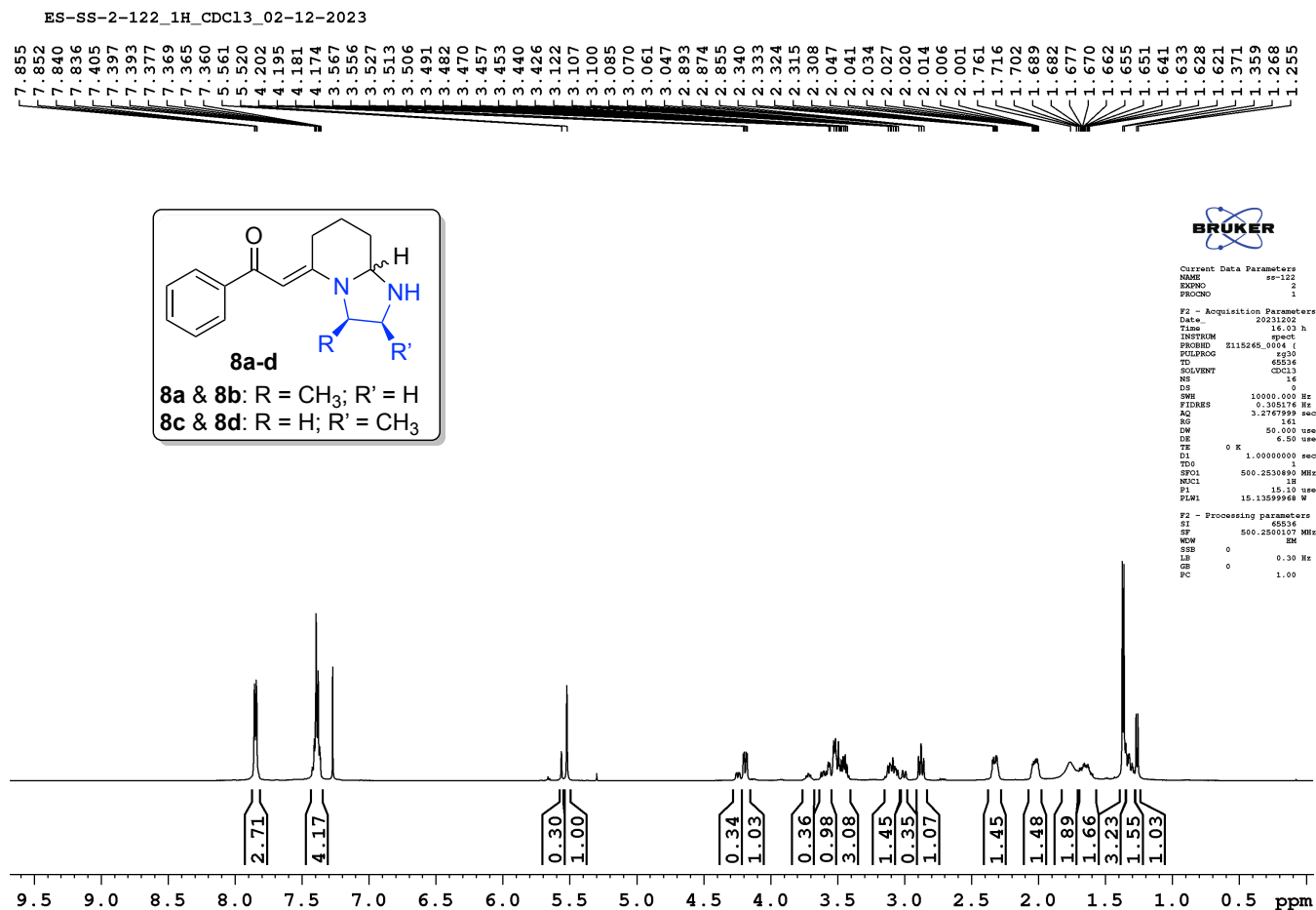


```
Current Data Parameters
NAME          es-2-130
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_        20231221
Time         11:46 h
INSTRUM      spect
PROBHD       5mmBBO
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           2000
DS           4
SFO          29761.994 MHz
FIDRES       0.988261 MHz
AQ           1.102068 sec
RG           2050
DM           16.900 usec
DE           6.50 usec
TE           300 K
D1           2.0000000 sec
d12         0.0200000 sec
TD0         1
SFO1        125.8054113 MHz
NUC1         13C
PC1         150 usec
P1          3.70 usec
P1M1        73.00000000 W
SFO2        500.1320101 MHz
NUC2         1H
CPDPRG2     waltz16
PCPD2       80.00 usec
P2M2        16.1359948 W
P1M2        0.53264000 W
P1M3        0.27124000 W

F2 - Processing parameters
SI           32768
SF           125.7679424 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```

**NMR Spectra of the product 8:** The  $^1\text{H}$  and NMR  $^{13}\text{C}$  spectra given below (pages 106 & 107) belong to an inseparable mixture of two products (two regioisomers OR a diastereomeric pair in the ratio ~3:1 (77:23)) of the four possible products **8a-d** obtained in the reaction of the MBH ketone **4a** with 1,2-diaminopropane (**2e**). **8a & 8b** and **8c & 8d** represent the possible diastereomeric pairs, defined by the relative stereochemistry of the ring junction.



ES-SS-2-122\_13C\_CDC13\_02-12-2023

187.854  
187.702

160.967  
160.949

142.742  
142.685

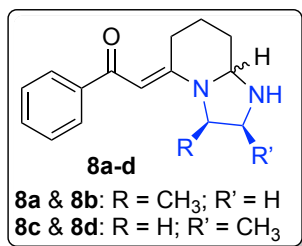
130.193  
130.139  
128.006  
127.174  
127.145

91.185  
90.718

77.292  
77.038  
76.784  
74.616  
71.215

54.693  
53.899  
52.462  
50.610

28.382  
28.252  
27.732  
27.392  
20.845  
18.993  
18.821  
18.408

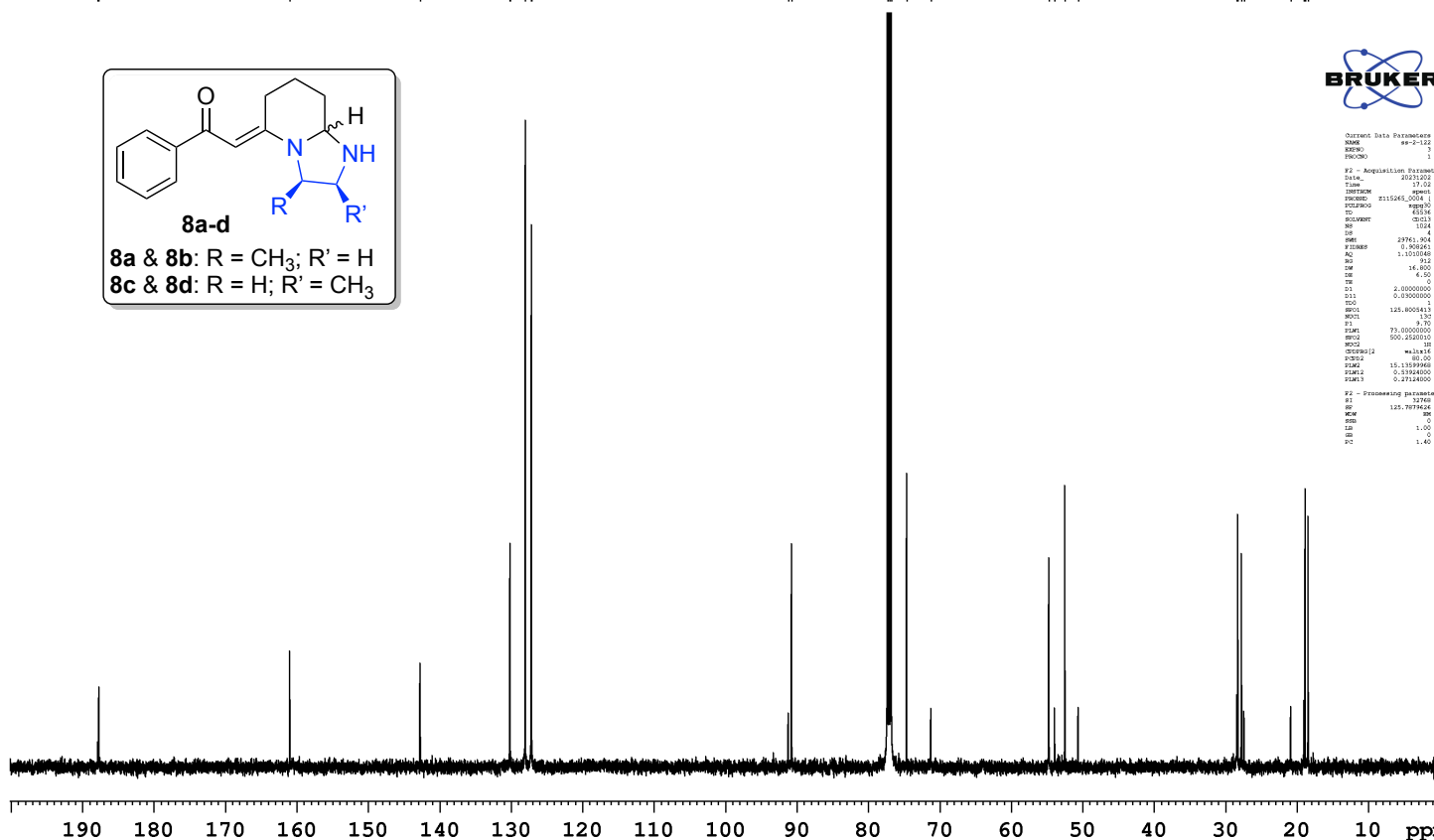


```

Current Data Parameters
NAME          **P-122
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_         20121202
Time          17:24
INSTRUM      spect
PROBHD       1H1246_0004 1
PULPROG      zgpg30
PC          6514
SOLVENT      CDCl3
DS           1514
DE           4
SWH          23741.504 Hz
FIDRES      0.30262 Hz
AQ          1.1010548 sec
RG           612
SF          14.600 MHz
AQ           4.50 sec
TE           300.2
D1           2.0000000 sec
D11          0.0300000 sec
D2           0.0300000 sec
D3           125.0006413 MHz
DELTA       1.32
PC          6514
SFO1        75.0000000 MHz
SFO2        500.1362610 MHz
SFO3        400.1463610 MHz
SFO4        101.6253610 MHz
SFO5        15.115399468 MHz
SFO6        0.331848000 MHz
SFO7        0.271400000 MHz

F2 - Processing parameters
SI           32768
SF          125.767424 MHz
WDW          EM
SS           0
LB           1.00 Hz
GB           0
PC          1.40
    
```

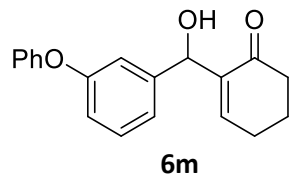


ES-SS-MBH-DY-08 R1\_1H\_CDC13\_18-09-2023

7.284  
7.268  
7.252  
7.232  
7.216  
7.200  
7.048  
7.036  
7.023  
6.970  
6.949  
6.934  
6.838  
6.825  
6.700  
6.692  
6.684  
— 5.446

— 3.439

2.400  
2.387  
2.373  
2.348  
2.337  
2.327  
2.317  
1.942  
1.929  
1.916

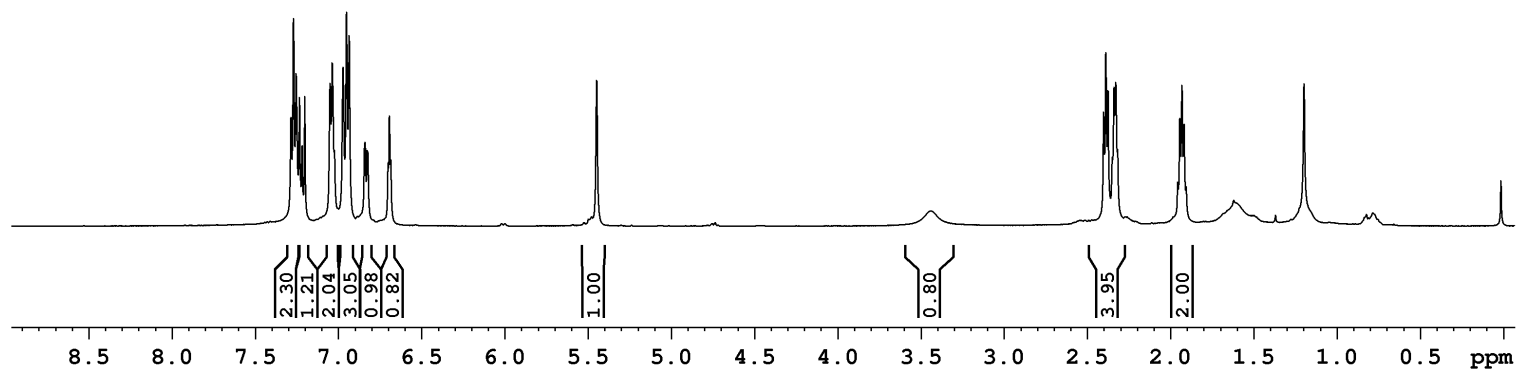


```

Current Data Parameters
NAME          ADDUCT
EXPNO        11
PROCNO       1

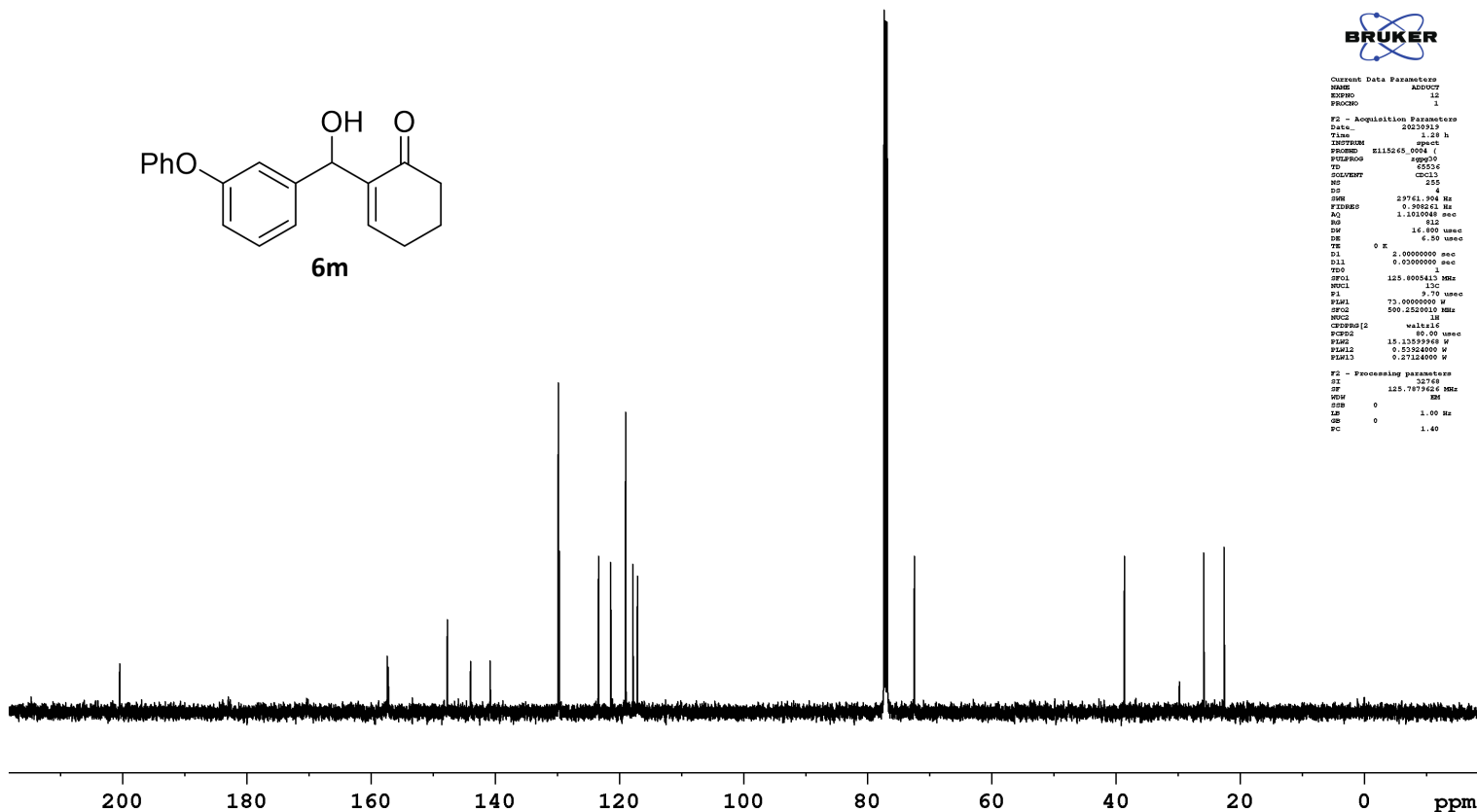
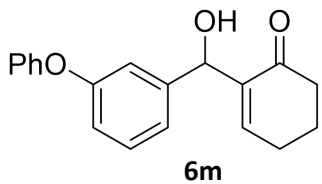
F2 - Acquisition Parameters
Date_         20230915
Time          1.12 h
INSTRUM      spect
PROBHD       H115265_0004 (
PULPROG      zgpg
TD           65536
SOLVENT      CDCl3
RG           16
DS           0
SHE         10000.000 Hz
FIDRES      0.305176 Hz
AQ          3.2767999 sec
RG          128
SW           50.000 usec
DE           6.50 usec
TE           0 K
D1          1.00000000 sec
TBD         1
SFO1        500.2530850 MHz
NUC1         1H
P1          15.10 usec
PL1         15.13599968 W

F2 - Processing parameters
SI           65536
SF          500.2500465 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
    
```



ES-SS-MBH-DY-08 R1\_13C\_CDC13\_18-09-2023

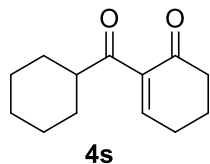
— 200.407  
— 157.313  
— 157.145  
— 147.628  
— 143.902  
— 140.743  
— 129.753  
— 129.630  
— 123.288  
— 121.314  
— 118.912  
— 117.746  
— 117.010  
— 77.300  
— 77.047  
— 76.792  
— 72.419  
— 38.568  
— 25.787  
— 22.499



Current Data Parameters  
NAME ADDUCT  
EXPNO 12  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20230912  
Time 1:28 h  
INSTRUM spect  
PROBHD E115245.004 L  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.398241 Hz  
AQ 1.102048 sec  
RG 811  
DM 16.400 usec  
DE 6.50 usec  
TE 0 K  
D1 2.0000000 sec  
S11 0.0000000 sec  
TPO 125.8005411 MHz  
NUC1 13C  
P1 8.75 usec  
PL1 73.0000000 W  
SFO2 500.1320101 MHz  
NUC2 1H  
CFO2R12 411.1111111  
PCPD2 80.00 usec  
PL2 15.13299900 W  
PL12 0.53324000 W  
PL13 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.7679214 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

ES-SS-7-40\_1H\_CDC13\_09-11-2023

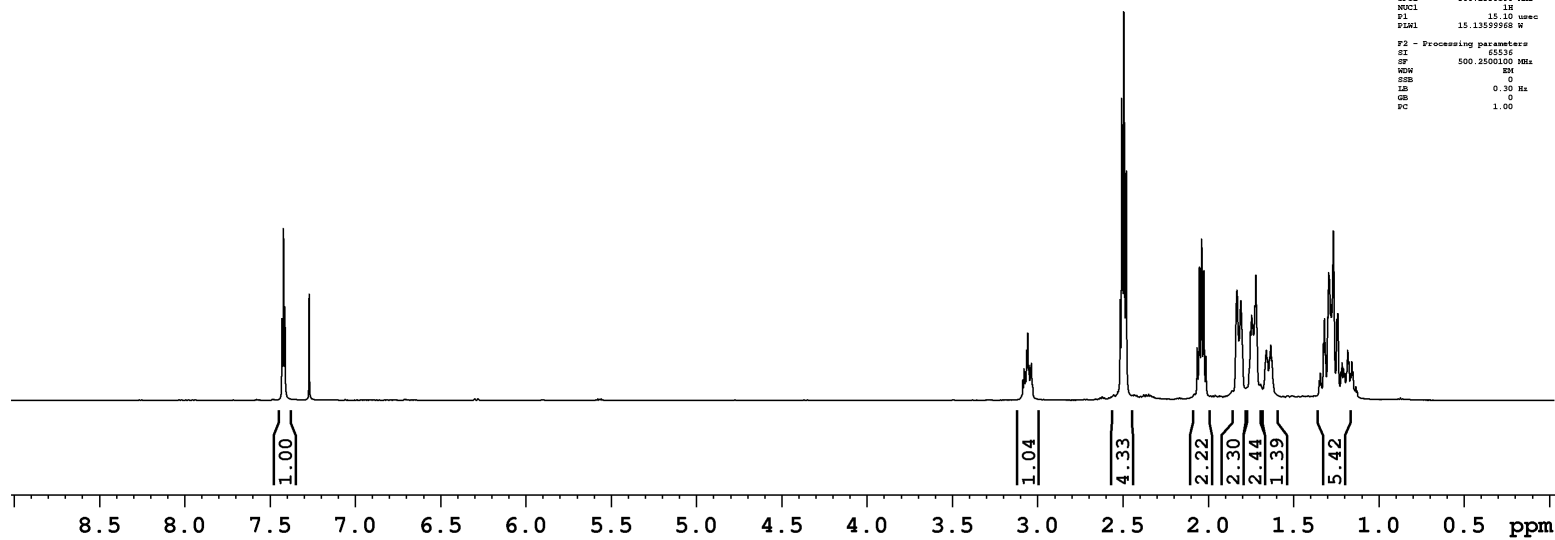
7.428  
7.419  
7.411  
7.269



3.077  
3.062  
3.055  
3.049  
3.040  
3.034  
2.513  
2.505  
2.493  
2.481  
2.478  
2.062  
2.050  
2.036  
2.023  
2.011  
1.828  
1.806  
1.750  
1.743  
1.737  
1.723  
1.718  
1.656  
1.637  
1.630  
1.623  
1.322  
1.316  
1.297  
1.291  
1.278  
1.273  
1.264  
1.243



Current Data Parameters  
NAME Ketone ss-7-40  
EXPRO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date 20231109  
Time 11:20 h  
INSTRUM spect  
PROCNO 2115265\_0004 (C  
PURPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SFR 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2767595 sec  
RG 101  
DH 50.000 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.2513650 MHz  
NUC1 1H  
P1 15.10 usec  
P1M1 15.13595968 W  
F2 - Processing parameters  
SI 65536  
SF 500.2500100 MHz  
WDW BM  
SSB 0  
IB 0.30 Hz  
GB 0  
PC 1.00



ES-SS-7-40\_13C\_CDC13\_09-11-2023

— 205.325

— 196.815

— 154.538

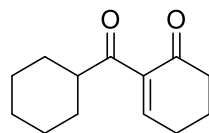
— 140.633

77.304  
77.050  
76.796

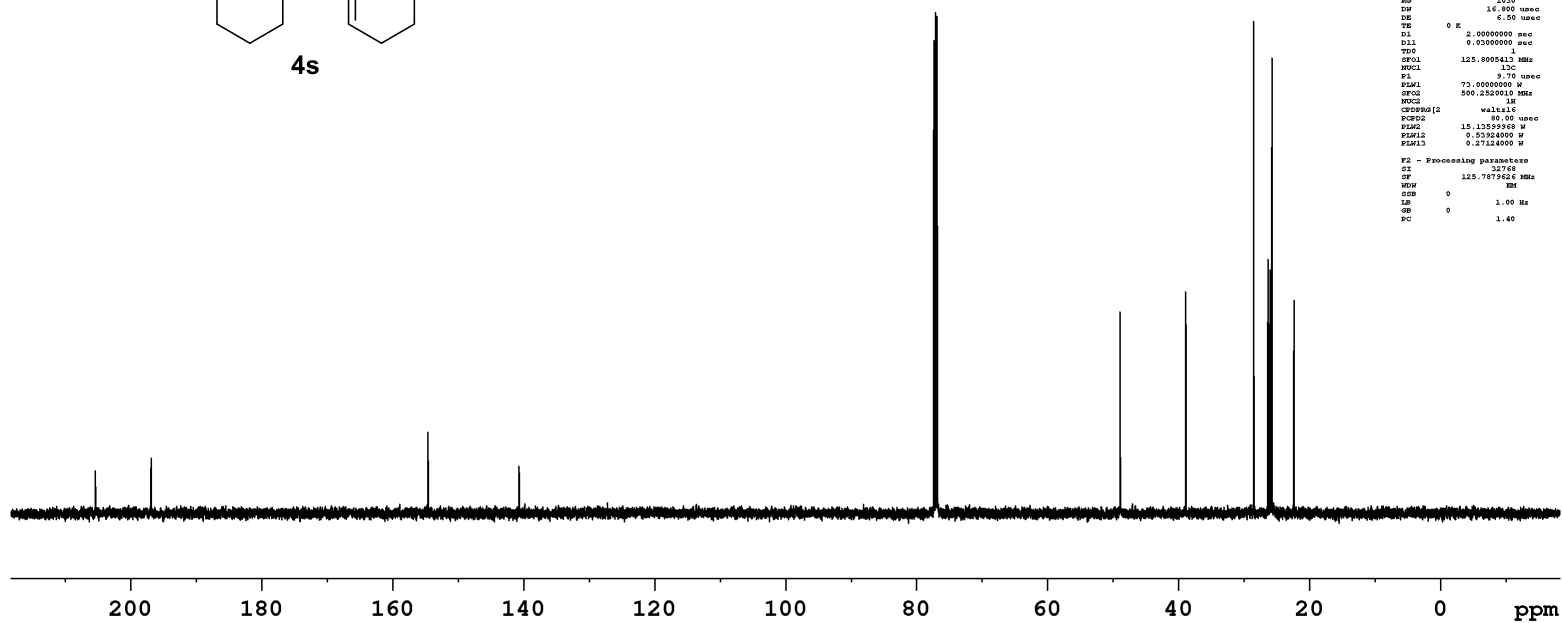
— 48.859

— 38.829

28.470  
26.259  
25.984  
25.676  
22.306



4s



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Current Data Parameters
NAME      ES-7-40
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20231109
Time      11.28 h
INSTRUM   spect
PROBHD    E1H2265.0004 (
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        40
DS        4
SWH        29761.904 Hz
FIDRES    0.998261 Hz
AQ         1.1010041 sec
RG         1020
DF         164.800 usec
DE         6.50 usec
TE         0 K
D1         2.0000000 sec
d11        0.0000000 sec
TDS        125.0005411 MHz
SFO1       125.0005411 MHz
NUC1       13C
P1         2.70 usec
PL1        75.0000000 W
SFO2       500.2520101 MHz
NUC2       1H
CPCPRG2    waltz16
PCPD2      60.00 usec
PLM2       15.1553968 W
PLM12      0.13324000 W
PLM13      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.7679626 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
```