Supporting Information

Unconventional Synthetic Pathway of Alkynyl Sulfonium Ylides with Aromatic Acid Anhydrides Leading to the Formation of Sulfonium Diacylmethylide Frameworks

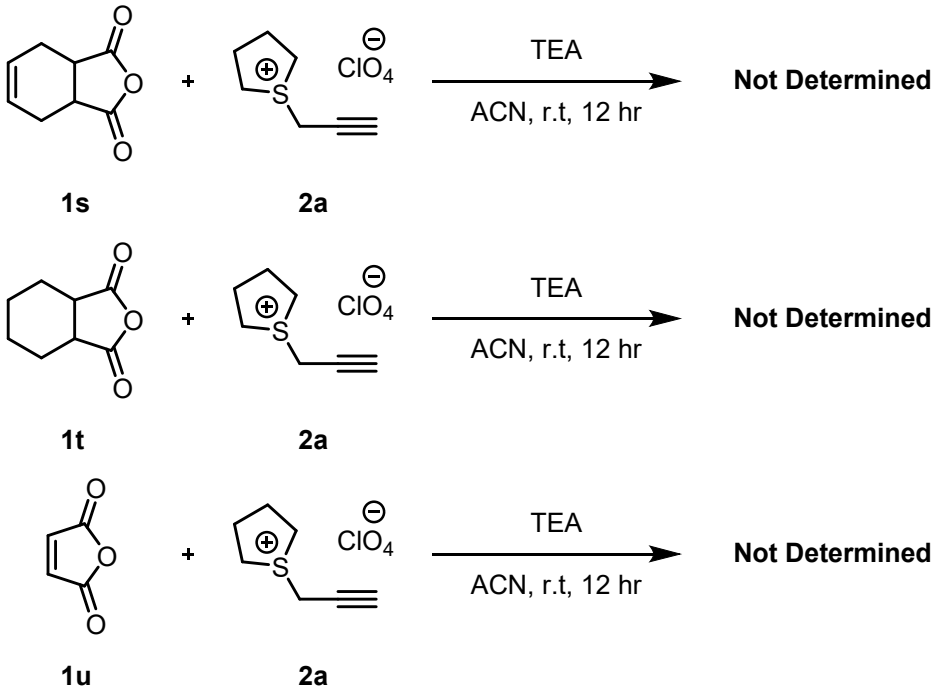
Evonne Liu, Lavanya Chandrasekar, Bo-Xuan Pan, Yun-Zhen Hsieh and Wei-Min Liu*

Department of Chemistry, Fu Jen Catholic University, New Taipei City 24205, Taiwan (R.O.C.)

Email: 133797@mail.fju.edu.tw

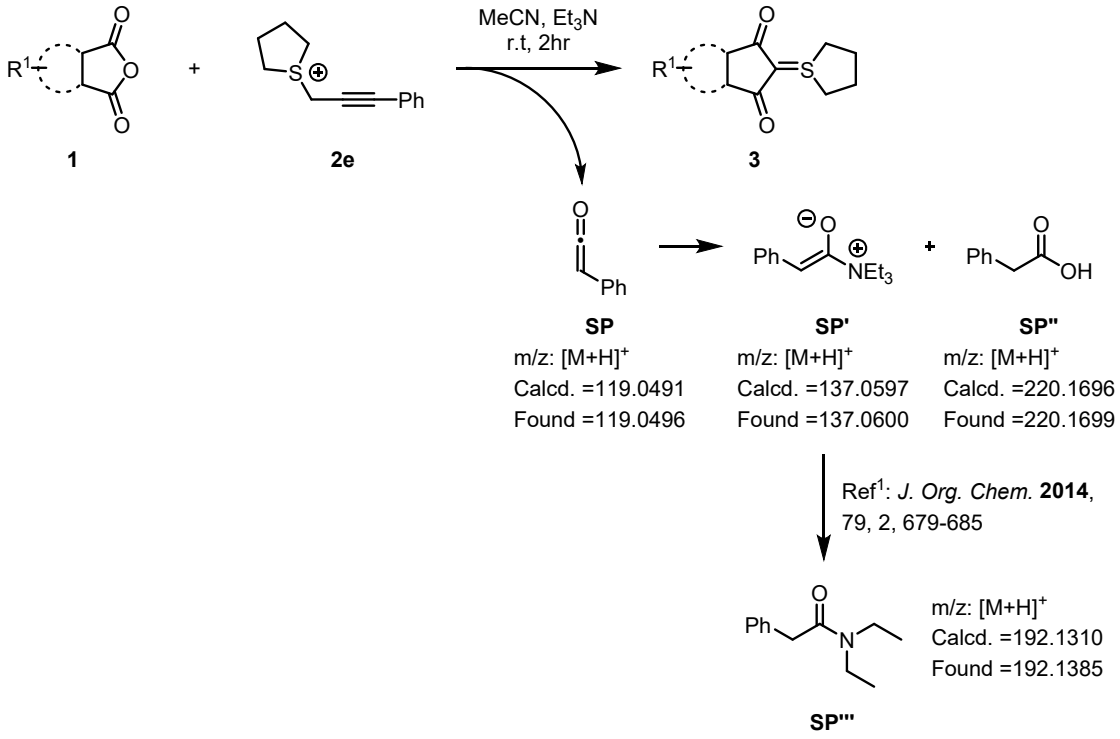
Table of Contents

1. Scheme S1. Reaction of cyclic non-aromatic acid anhydrides

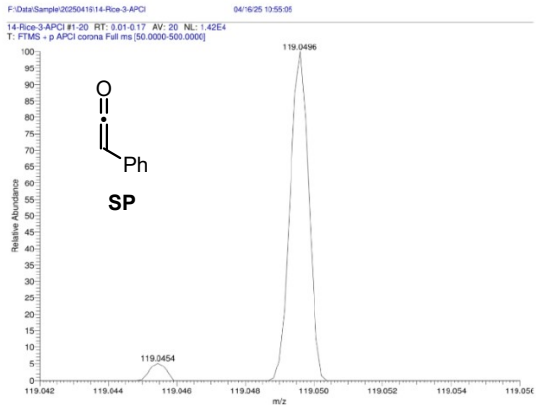


2. Figure S1. *In situ* HRMS analysis

(A)



(B)



F:\Data\Sample\20250416\14-Rice-3-APCI 04/16/25 10:55:05

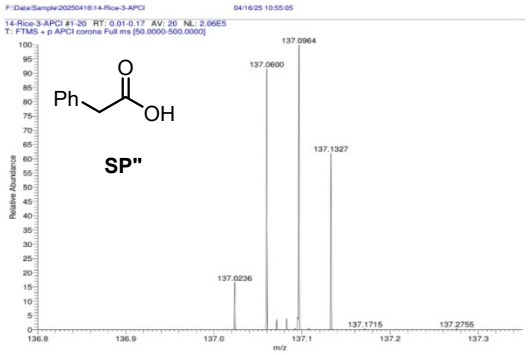
14-Rice-3-APCI#1-20 RT: 0.01-0.17 AV: 20
T: FTMS + p APCI corona Full ms [50.0000-500.0000]
m/z= 119.0420-119.0560

Isotope	Min	Max
N-14	0	0
O-16	1	1
C-12	8	8
H-1	0	60
Cl-35	0	1
Ar-40	0	1
Na-23	0	1
Br-79	0	1
S-32	0	1

Charge 1
Mass tolerance 500.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
119.0496	14260.6	100.00	119.0491	3.75	C_8H_7O

(C)



F:\Data\Sample\20250416\14-Rice-3-APCI 04/16/25 10:55:05

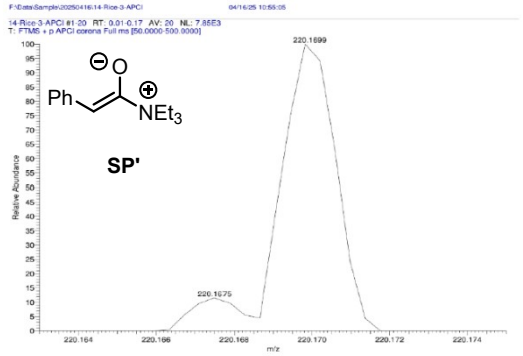
14-Rice-3-APCI#1-20 RT: 0.01-0.17 AV: 20
T: FTMS + p APCI corona Full ms [50.0000-500.0000]
m/z= 137.0438-137.0864

Isotope	Min	Max
N-14	0	1
O-16	2	2
C-12	8	14
H-1	0	60
Cl-35	0	1
Ar-40	0	1
Na-23	0	1
Br-79	0	1
S-32	0	1

Charge 1
Mass tolerance 500.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
137.0600	192032.3	100.00	137.0597	1.83	$C_8H_9O_2$

(D)



F:\Data\Sample\20250416\14-Rice-3-APCI 04/16/25 10:55:05

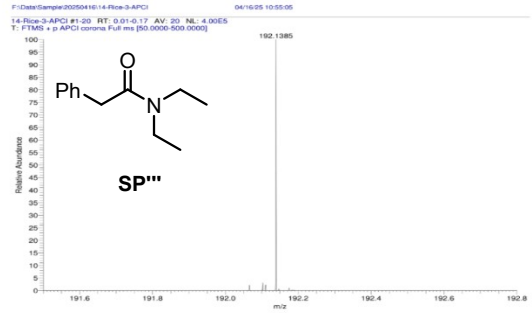
14-Rice-3-APCI#1-20 RT: 0.01-0.17 AV: 20
T: FTMS + p APCI corona Full ms [50.0000-500.0000]
m/z= 220.1630-220.1750

Isotope	Min	Max
N-14	1	1
O-16	1	1
C-12	14	14
H-1	0	60
Cl-35	0	1
Ar-40	0	1
Na-23	0	1
Br-79	0	1
S-32	0	1

Charge 1
Mass tolerance 500.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
220.1699	7976.1	100.00	220.1696	1.59	$C_{14}H_{22}ON$

(E)



F:\Data\Sample\20250416\14-Rice-3-APCI 04/16/25 10:55:05

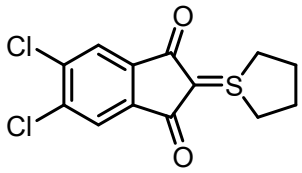
14-Rice-3-APCI#1-20 RT: 0.01-0.17 AV: 20
T: FTMS + p APCI corona Full ms [50.0000-500.0000]
m/z= 191.5000-192.8000

Isotope	Min	Max
N-14	1	1
O-16	1	1
C-12	12	12
H-1	0	60
Cl-35	0	1
Ar-40	0	1
Na-23	0	1
Br-79	0	1
S-32	0	1

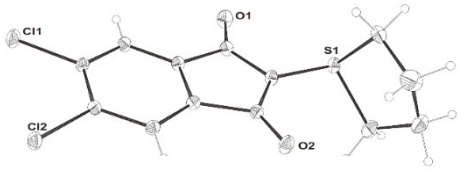
Charge 1
Mass tolerance 500.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
192.1385	399877.8	100.00	192.1383	1.32	$C_{12}H_{18}ON$

3. X-Ray Crystallographic Data of 3a



3a



CCDC: 2388736

Table 1. Crystal data and structure refinement for d24851.

Identification code	shelx	
Empirical formula	C13 H10 Cl2 O2 S	
Formula weight	301.17	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 10.4636(5) Å	α= 90°.
	b = 15.3707(7) Å	β= 114.6260(10)°.
	c = 8.6501(3) Å	γ = 90°.
Volume	1264.68(9) $Å^3$	
Z	4	
Density (calculated)	1.582 Mg/m^3	
Absorption coefficient	0.667 mm^{-1}	
F(000)	616	
Crystal size	0.260 x 0.150 x 0.120 mm^3	
Theta range for data collection	2.518 to 25.429°.	
Index ranges	-12<=h<=12, -18<=k<=18, -10<=l<=10	
Reflections collected	8338	
Independent reflections	2274 [R(int) = 0.0465]	
Completeness to theta = 25.242°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2274 / 2 / 163	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0259, wR2 = 0.0622	
R indices (all data)	R1 = 0.0276, wR2 = 0.0630	
Absolute structure parameter	0.03(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.297 and -0.189 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d24851. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7324(5)	3509(3)	9234(5)	49(1)
C(2)	8862(5)	3764(4)	9892(6)	66(1)
C(3)	9178(5)	4121(4)	8523(7)	72(2)
C(4)	8388(4)	3647(2)	6945(5)	40(1)
C(5)	5529(3)	4132(2)	5955(4)	28(1)
C(6)	4360(4)	3959(2)	4356(4)	30(1)
C(7)	3675(3)	4836(2)	3758(4)	25(1)
C(8)	2552(3)	5055(2)	2253(4)	29(1)
C(9)	2154(3)	5928(2)	2006(4)	27(1)
C(10)	2839(3)	6549(2)	3264(4)	26(1)
C(11)	3980(3)	6319(2)	4767(4)	28(1)
C(12)	4388(3)	5459(2)	4974(4)	25(1)
C(13)	5626(3)	5031(2)	6397(4)	27(1)
Cl(1)	808(1)	6235(1)	99(1)	40(1)
Cl(2)	2282(1)	7620(1)	2981(1)	37(1)
O(1)	3954(3)	3276(1)	3566(3)	42(1)
O(2)	6493(3)	5429(2)	7617(3)	38(1)
S(1)	6724(1)	3320(1)	6949(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for d24851.

C(1)-C(2)	1.518(7)
C(1)-S(1)	1.831(4)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.462(8)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.462(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-S(1)	1.813(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(13)	1.427(4)
C(5)-C(6)	1.438(4)
C(5)-S(1)	1.721(3)
C(6)-O(1)	1.229(4)
C(6)-C(7)	1.513(4)
C(7)-C(8)	1.384(4)
C(7)-C(12)	1.388(4)
C(8)-C(9)	1.395(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.399(4)
C(9)-Cl(1)	1.729(3)
C(10)-C(11)	1.395(4)
C(10)-Cl(2)	1.731(3)
C(11)-C(12)	1.378(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.515(4)
C(13)-O(2)	1.230(4)
C(2)-C(1)-S(1)	106.2(3)
C(2)-C(1)-H(1A)	110.5
S(1)-C(1)-H(1A)	110.5
C(2)-C(1)-H(1B)	110.5
S(1)-C(1)-H(1B)	110.5

H(1A)-C(1)-H(1B)	108.7
C(3)-C(2)-C(1)	110.8(4)
C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(2)	109.8(4)
C(4)-C(3)-H(3A)	109.7
C(2)-C(3)-H(3A)	109.7
C(4)-C(3)-H(3B)	109.7
C(2)-C(3)-H(3B)	109.7
H(3A)-C(3)-H(3B)	108.2
C(3)-C(4)-S(1)	107.8(3)
C(3)-C(4)-H(4A)	110.1
S(1)-C(4)-H(4A)	110.1
C(3)-C(4)-H(4B)	110.1
S(1)-C(4)-H(4B)	110.1
H(4A)-C(4)-H(4B)	108.5
C(13)-C(5)-C(6)	111.9(3)
C(13)-C(5)-S(1)	127.8(2)
C(6)-C(5)-S(1)	119.8(2)
O(1)-C(6)-C(5)	130.6(3)
O(1)-C(6)-C(7)	124.5(3)
C(5)-C(6)-C(7)	104.9(3)
C(8)-C(7)-C(12)	121.5(3)
C(8)-C(7)-C(6)	129.4(3)
C(12)-C(7)-C(6)	109.1(3)
C(7)-C(8)-C(9)	117.5(3)
C(7)-C(8)-H(8)	121.3
C(9)-C(8)-H(8)	121.3
C(8)-C(9)-C(10)	120.8(3)
C(8)-C(9)-Cl(1)	118.7(2)
C(10)-C(9)-Cl(1)	120.4(2)
C(11)-C(10)-C(9)	121.0(3)
C(11)-C(10)-Cl(2)	118.7(2)
C(9)-C(10)-Cl(2)	120.3(2)
C(12)-C(11)-C(10)	117.6(3)

C(12)-C(11)-H(11)	121.2
C(10)-C(11)-H(11)	121.2
C(11)-C(12)-C(7)	121.6(3)
C(11)-C(12)-C(13)	129.4(3)
C(7)-C(12)-C(13)	108.9(3)
O(2)-C(13)-C(5)	131.0(3)
O(2)-C(13)-C(12)	123.8(3)
C(5)-C(13)-C(12)	105.1(3)
C(5)-S(1)-C(4)	107.22(16)
C(5)-S(1)-C(1)	106.00(17)
C(4)-S(1)-C(1)	93.47(18)

Symmetry transformations used to generate equivalent atoms:

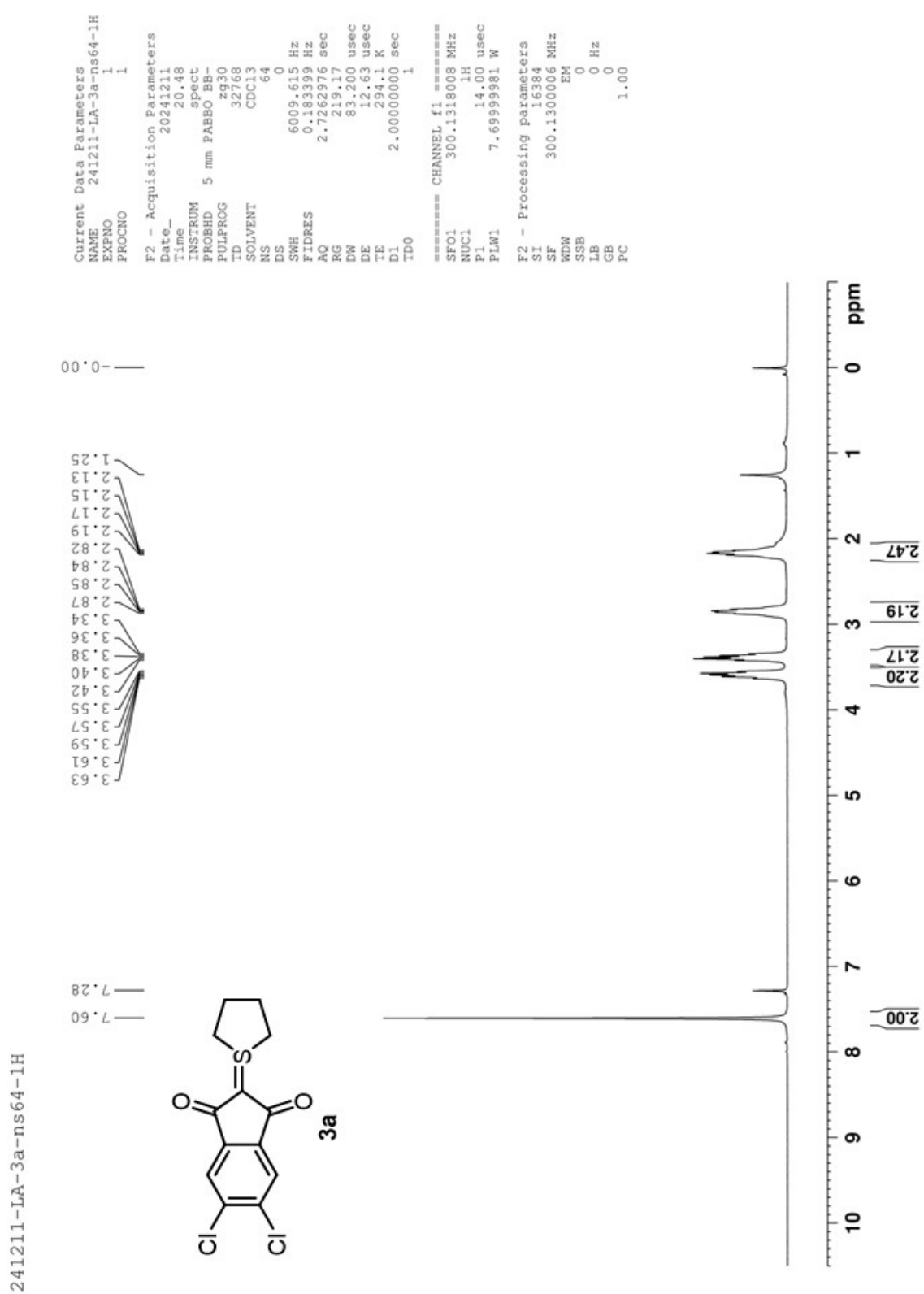
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for d24851. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	55(2)	58(2)	30(2)	15(2)	16(2)	9(2)
C(2)	54(3)	81(4)	40(2)	-17(2)	-3(2)	14(2)
C(3)	42(2)	88(4)	85(4)	-44(3)	25(3)	-25(2)
C(4)	33(2)	41(2)	46(2)	3(2)	17(2)	7(2)
C(5)	28(2)	24(1)	30(2)	2(1)	9(1)	-1(1)
C(6)	27(2)	26(2)	34(2)	-2(1)	11(1)	-2(1)
C(7)	21(1)	25(1)	28(1)	-2(1)	8(1)	-4(1)
C(8)	22(2)	31(2)	29(2)	-5(1)	6(1)	-2(1)
C(9)	18(2)	38(2)	22(1)	-1(1)	5(1)	0(1)
C(10)	28(2)	23(1)	26(2)	1(1)	11(1)	3(1)
C(11)	29(2)	27(2)	25(1)	-4(1)	7(1)	0(1)
C(12)	25(2)	24(1)	26(1)	-1(1)	10(1)	-3(1)
C(13)	28(2)	26(2)	25(1)	0(1)	10(1)	1(1)
Cl(1)	33(1)	42(1)	30(1)	-1(1)	-2(1)	6(1)
Cl(2)	44(1)	27(1)	30(1)	1(1)	4(1)	10(1)
O(1)	43(2)	24(1)	47(2)	-9(1)	6(1)	-6(1)
O(2)	39(1)	28(1)	32(1)	-5(1)	-2(1)	0(1)
S(1)	30(1)	21(1)	33(1)	1(1)	6(1)	0(1)

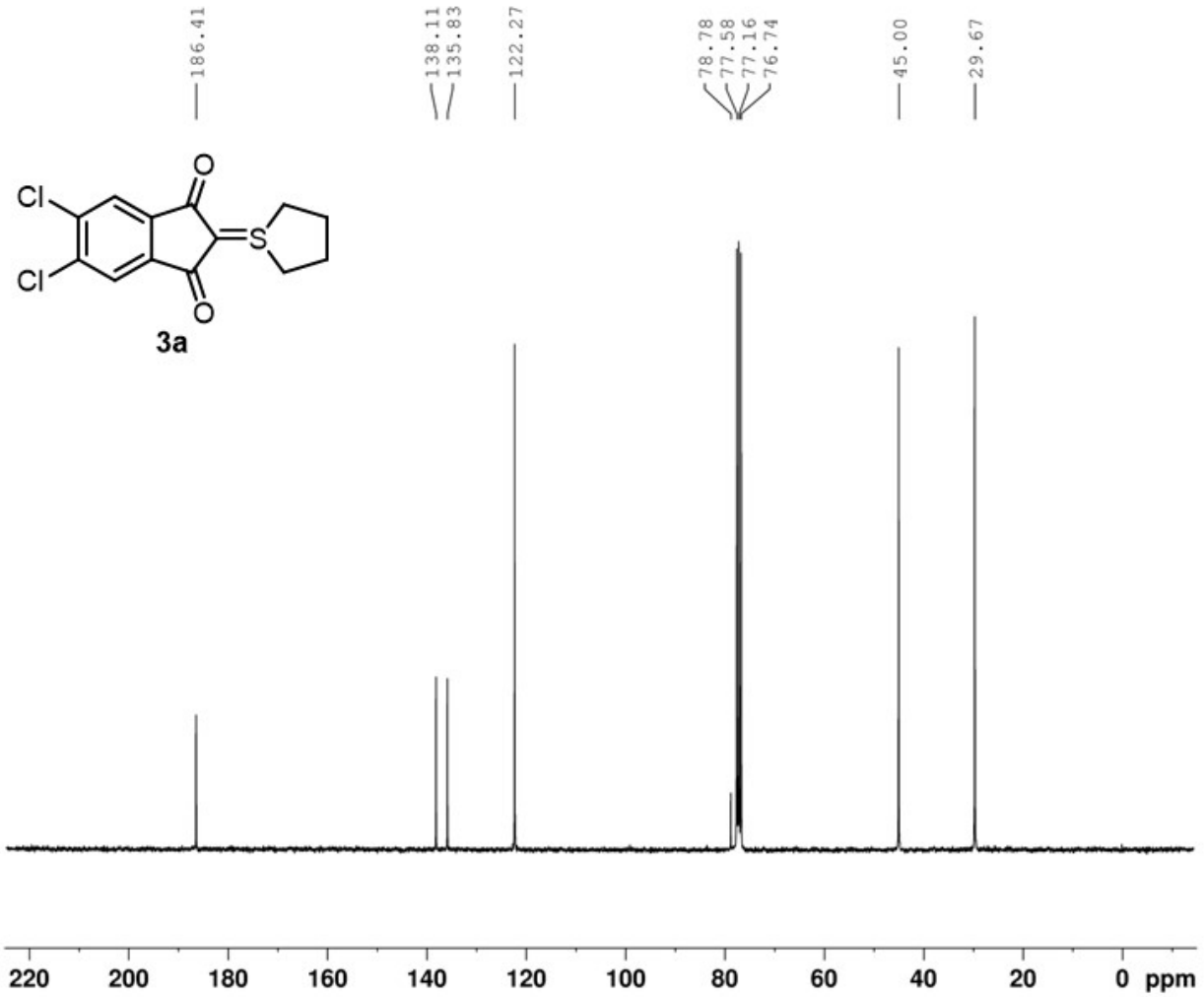
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for d24851.

	x	y	z	U(eq)
H(1A)	6772	3981	9444	58
H(1B)	7218	2974	9808	58
H(2A)	9082	4204	10804	79
H(2B)	9459	3247	10383	79
H(3A)	8922	4745	8362	86
H(3B)	10198	4070	8827	86
H(4A)	8922	3129	6874	48
H(4B)	8223	4024	5952	48
H(8)	2071	4628	1420	34
H(11)	4459	6740	5616	34

4. NMR spectra



240804-RICE-PC-OVERNIGHT-13C



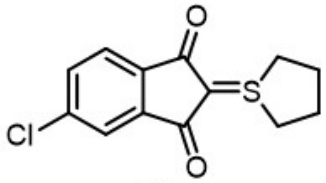

```
Current Data Parameters
NAME      240804-RICE-PC-OVERNIGHT
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240805
Time               3.23
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD              32768
SOLVENT          CDCl3
NS               6144
DS                  0
SWH          18028.846 Hz
FIDRES        0.550197 Hz
AQ            0.9087659 sec
RG              219.17
DW             27.733 usec
DE              6.50 usec
TE             297.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1        75.4756726 MHz
NUC1              13C
P1              10.00 usec
PLW1       28.29999924 W

======== CHANNEL f2 ========
SFO2       300.1312005 MHz
NUC2              1H
CPDPRG[2 bi_waltz65_256
PCPD2           90.00 usec
PLW2        8.30000019 W
PLW12       0.20084000 W
PLW13       0.16268000 W

F2 - Processing parameters
SI              32768
SF         75.4677412 MHz
WDW               EM
SSB                 0
LB               2.00 Hz
GB                  0
PC               1.00
```

250826-RICE-00473_PROTON-1-2.jdf

7.52 7.49 7.48 7.44 7.44 7.43 7.42 7.28

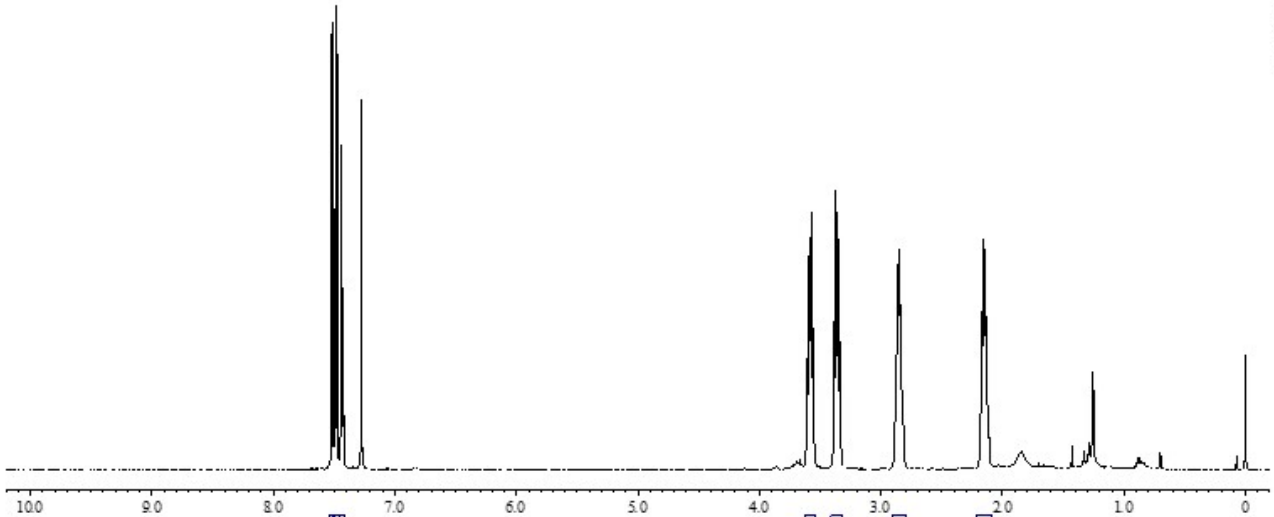
3.61 3.59 3.58 3.57 3.56 3.38 3.37 3.36 3.35 3.34 2.88 2.87 2.85 2.85 2.84 2.82 2.18 2.17 2.16 2.15 2.14 2.13 2.12 1.85 1.25

0.00

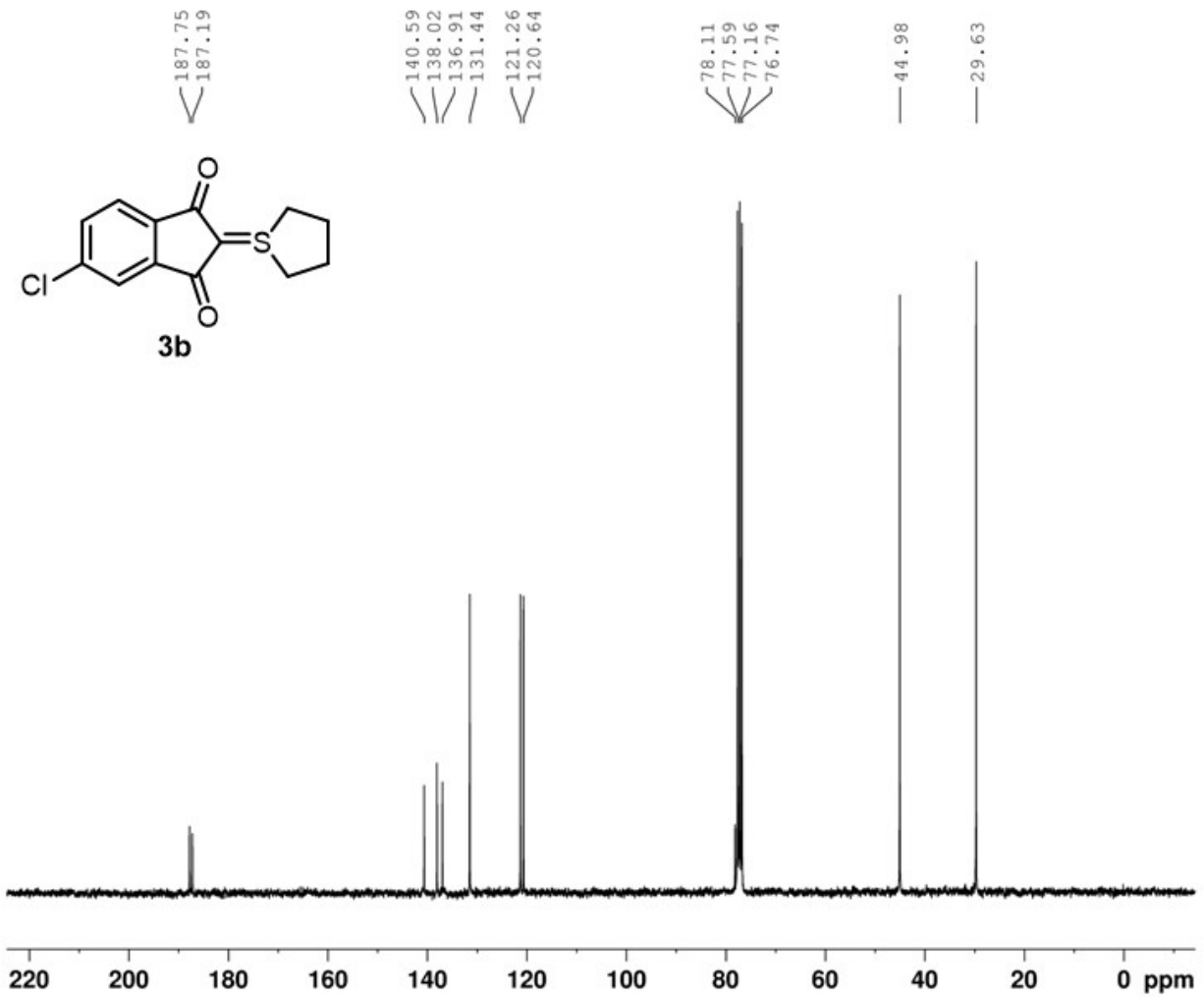


3b

```
---- PROCESSING PARAMETERS ----
sexp( 0.24406[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%],
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.02904[ppm], 0[pp
thresh( 11.47929[%], 0.11383[%

Sample_Id          = 250826-RIC
Actual_Start_Time  = 26-AUG-202
Spectrometer       = JNM-ECZL50
Probe_Id           = 2806
Experiment         = single_puls
X_Data_Points      = 65536
Solvent            = CHLOROFORM-
Scans              = 32
X_Prescans         = 0
X_Sweep_Input      = 20[ppm]
X_Resolution       = 0.48812173
X_Acq_Time         = 2.04866928
Recvr_Gain         = 52
Temp_Get           = 21.7[dC]
Relaxation_Delay   = 2[s]
X_Freq             = 500.159915
X_Domain           = Proton
X_Pulse            = 2.33333333
X_Atn              = 7.4[dB]
```

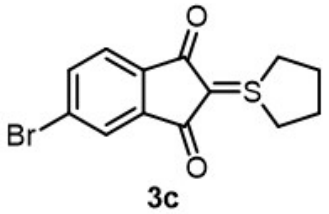


240908-RICE-00473-13C

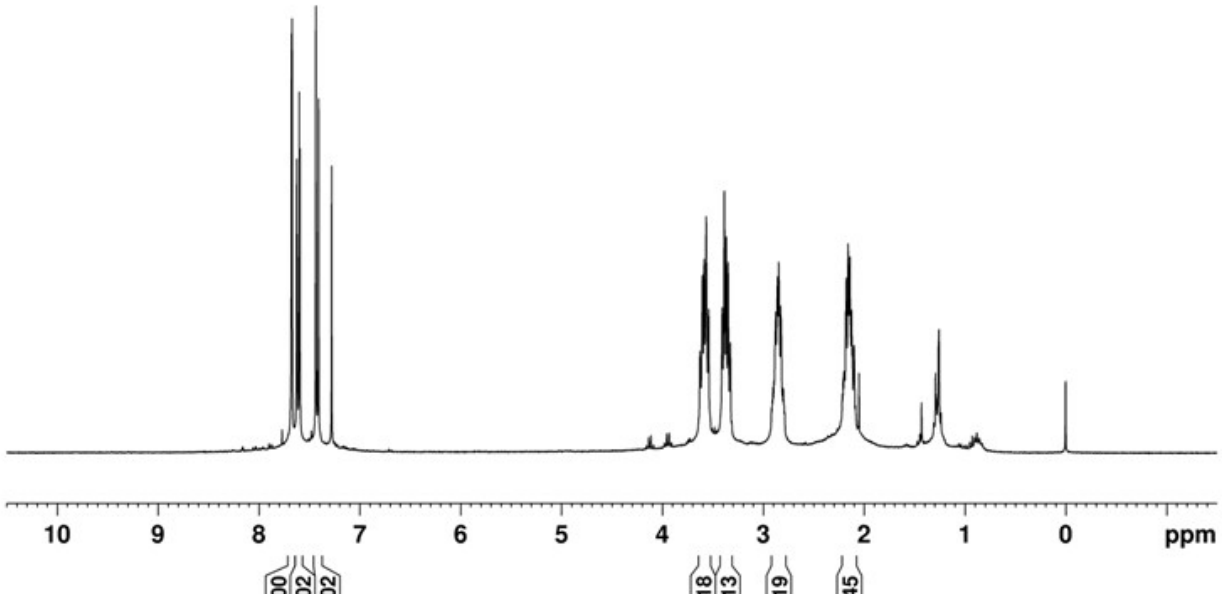



```
Current Data Parameters
NAME      240908-RICE-00473
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240908
Time                 20.05
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    2048
DS                       0
SWH              18028.846 Hz
FIDRES           0.550197 Hz
AQ               0.9087659 sec
RG                  219.17
DW                  27.733 usec
DE                    6.50 usec
TE                  298.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                   13C
P1                   10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                   32768
SF              75.4677417 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

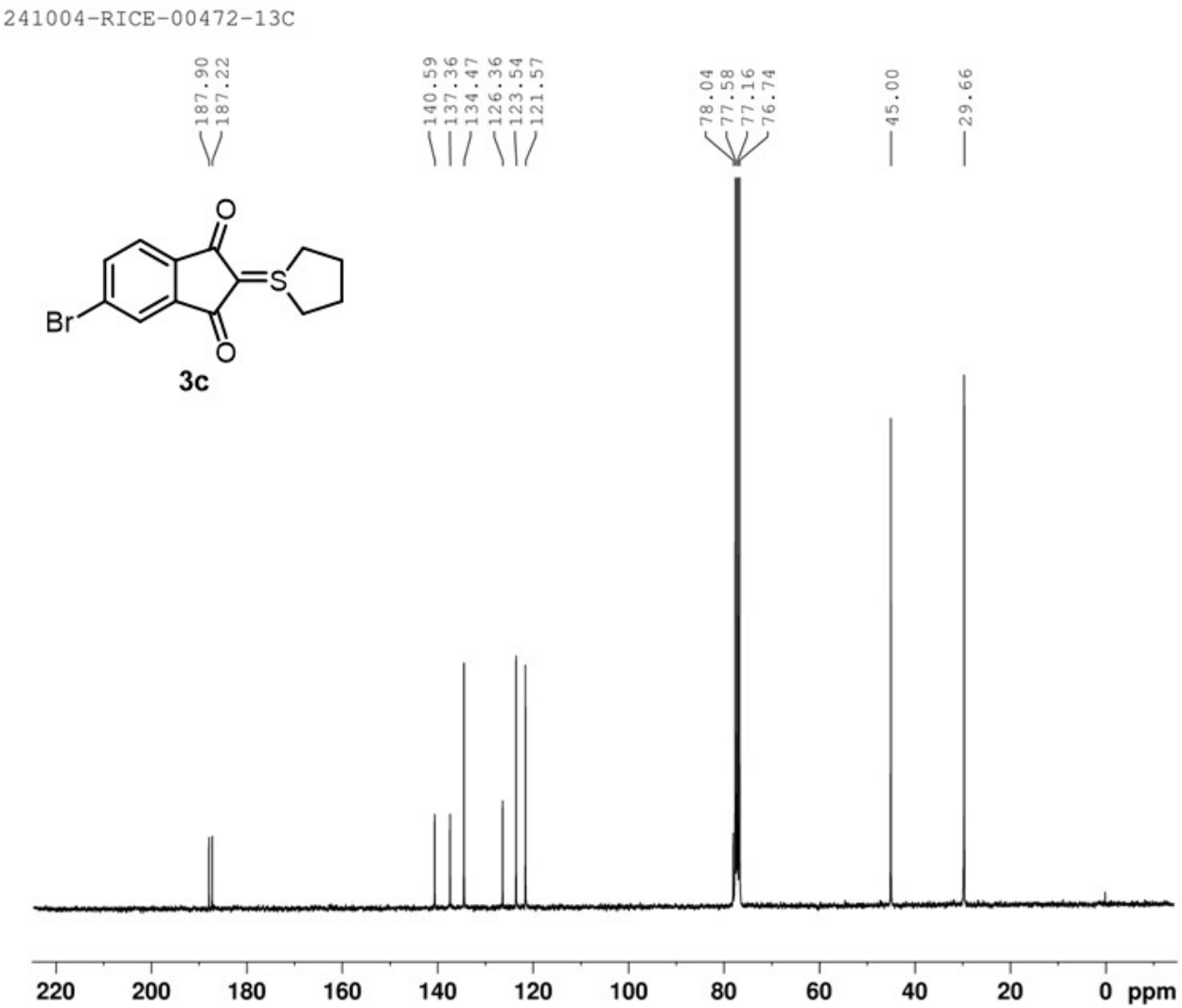
250126-RICE-03513



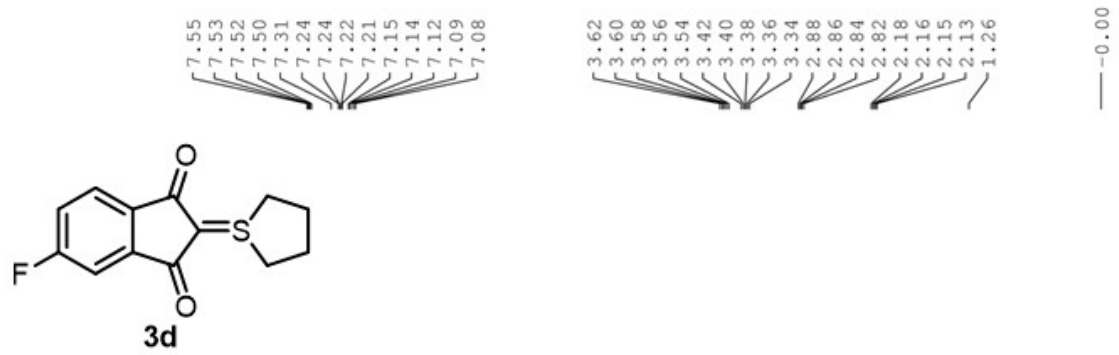
3c

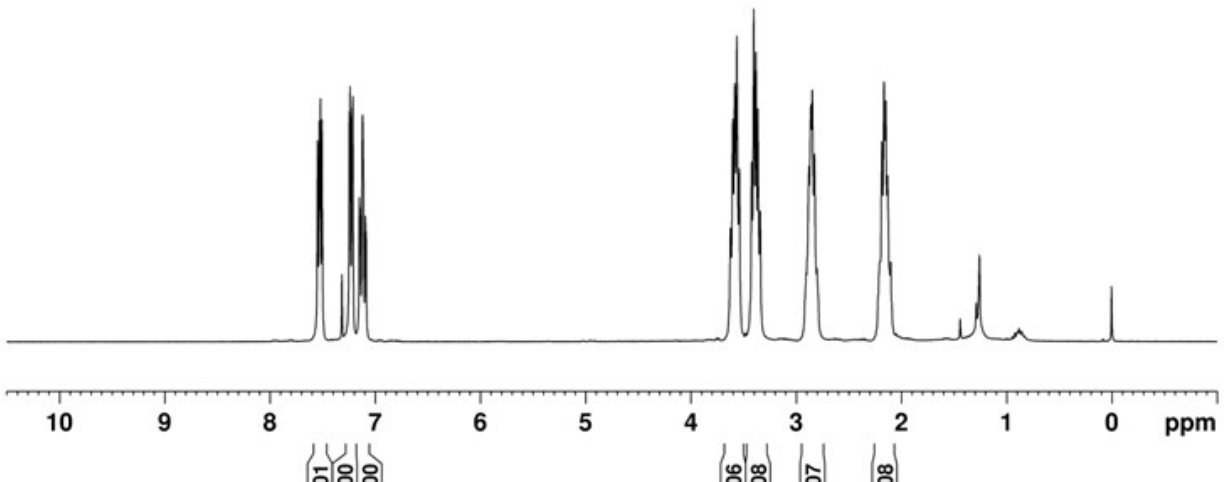



```
Current Data Parameters
NAME      250126-RICE-03513
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20250126
Time                 17.52
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ               2.7262976 sec
RG                  219.17
DW                  83.200 usec
DE                  12.63 usec
TE                  295.0 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300016 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

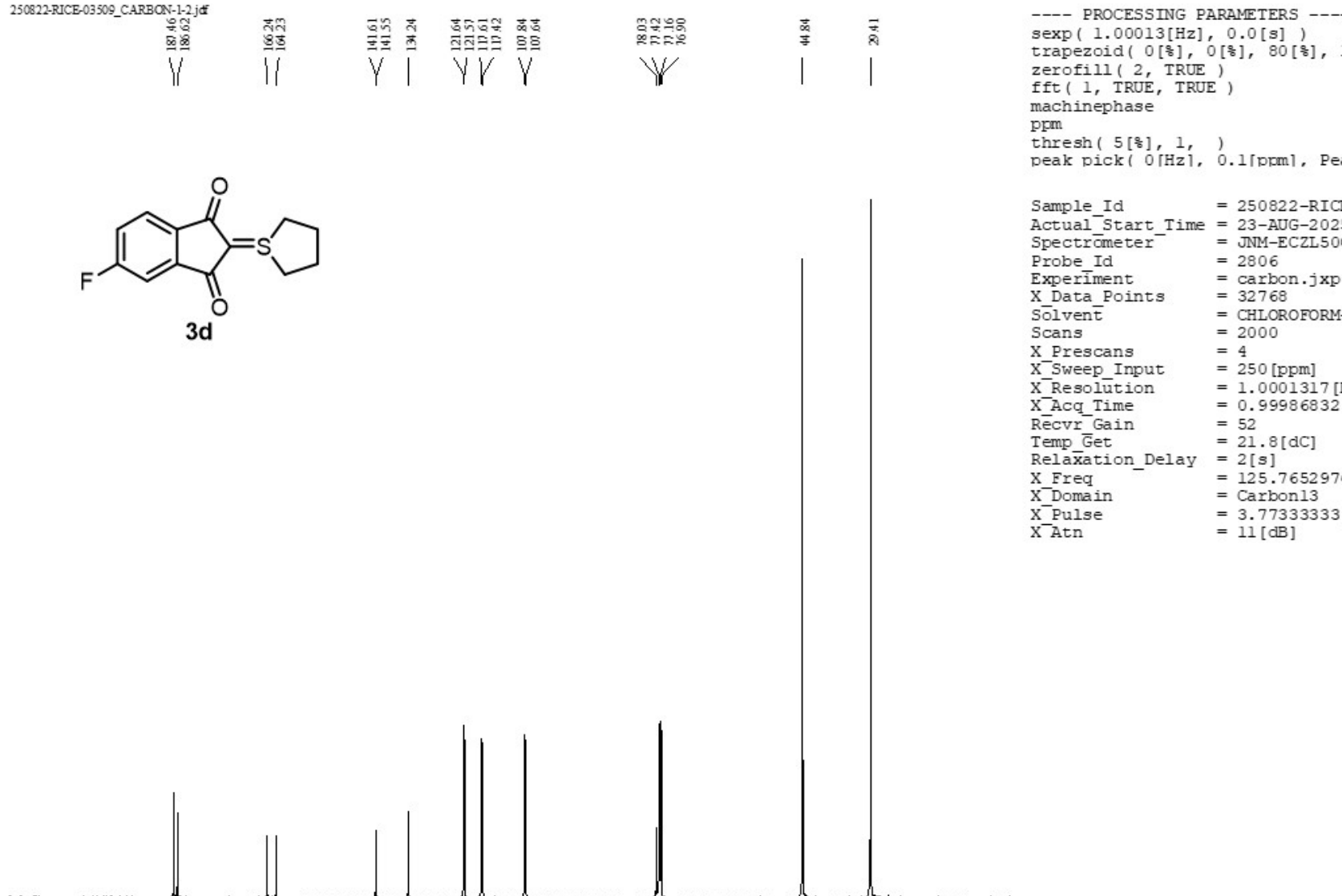

241004-RICE-00472-13C
187.90
187.22
140.59
137.36
134.47
126.36
123.54
121.57
78.04
77.58
77.16
76.74
45.00
29.66
Br
O
O
S
3c
220
200
180
160
140
120
100
80
60
40
20
0 ppm
Current Data Parameters
NAME 241004-RICE-00472
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20241005
Time 4.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 8192
DS 0
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 219.17
DW 27.733 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4756726 MHz
NUC1 13C
P1 10.00 usec
PLW1 28.29999924 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 90.00 usec
PLW2 8.30000019 W
PLW12 0.20084000 W
PLW13 0.16268000 W
F2 - Processing parameters
SI 32768
SF 75.4677407 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

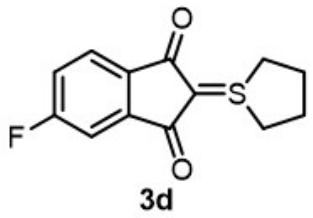
250219-RICE-03509-NS64






```
Current Data Parameters
NAME      250219-RICE-03509-NS64
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20250219
Time                   20.11
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDC13
NS                       64
DS                        0
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                   148.08
DW                   83.200 usec
DE                    12.63 usec
TE                    293.6 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                     1H
P1                    14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                    16384
SF            300.1299906 MHz
WDW                      EM
SSB                       0
LB                        0 Hz
GB                        0
PC                     1.00
```

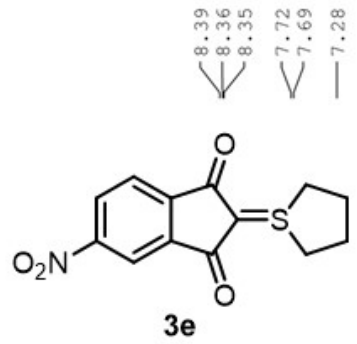

250822-RICE-03509_CARBON-1-2.jdf
187.46
186.62
166.24
164.23
141.61
141.55
134.24
121.64
121.57
121.61
117.42
103.84
103.64
78.03
77.42
77.16
76.90
44.84
29.41
O
S
F
O
3d
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250822-RIC
Actual_Start_Time = 23-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 21.8[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]



3d

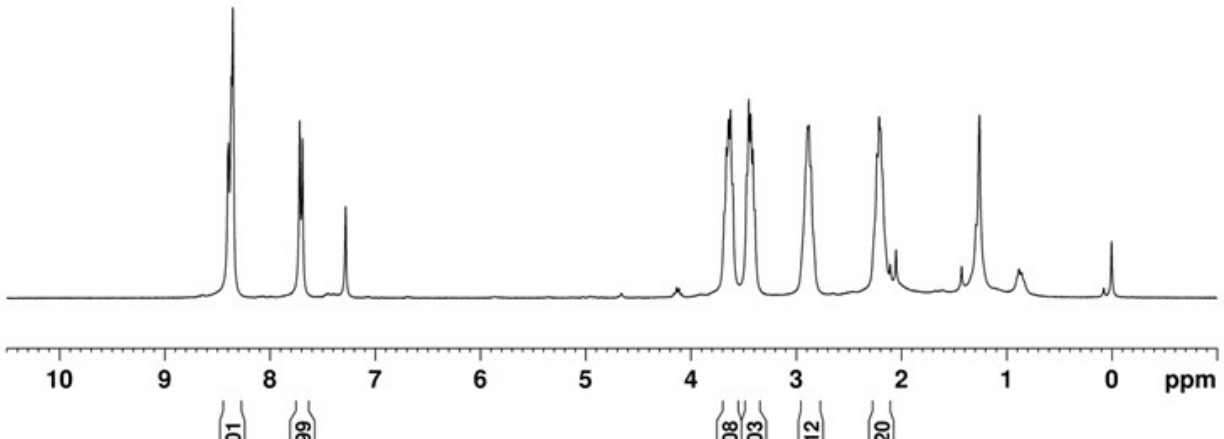

```
Current Data Parameters
NAME                  3d_19F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250226
Time                  11.48
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgig30
TD                   131072
SOLVENT                CDCl3
NS                        56
DS                         0
SWH                66964.289 Hz
FIDRES             0.510897 Hz
AQ                 0.9786710 sec
RG                    219.17
DW                     7.467 usec
DE                      6.50 usec
TE                     293.4 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            282.3874119 MHz
NUC1                   19F
P1                    15.50 usec
PLW1            6.09999990 W

======== CHANNEL f2 ========
SFO2            300.1312005 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2            8.30000019 W
PLW12           0.20084000 W

F2 - Processing parameters
SI                     65536
SF              282.4043552 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

250114-RICE-03507

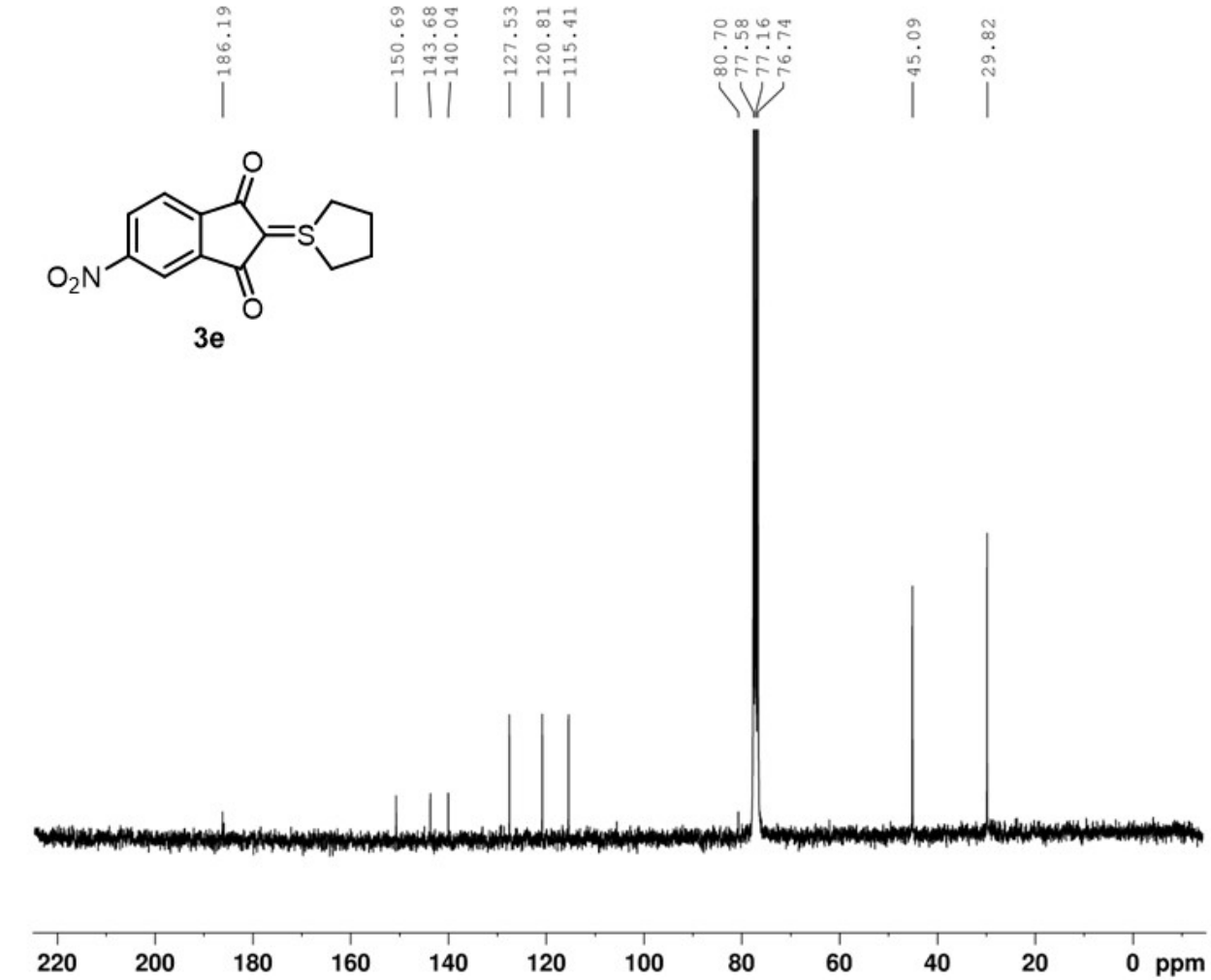


3e

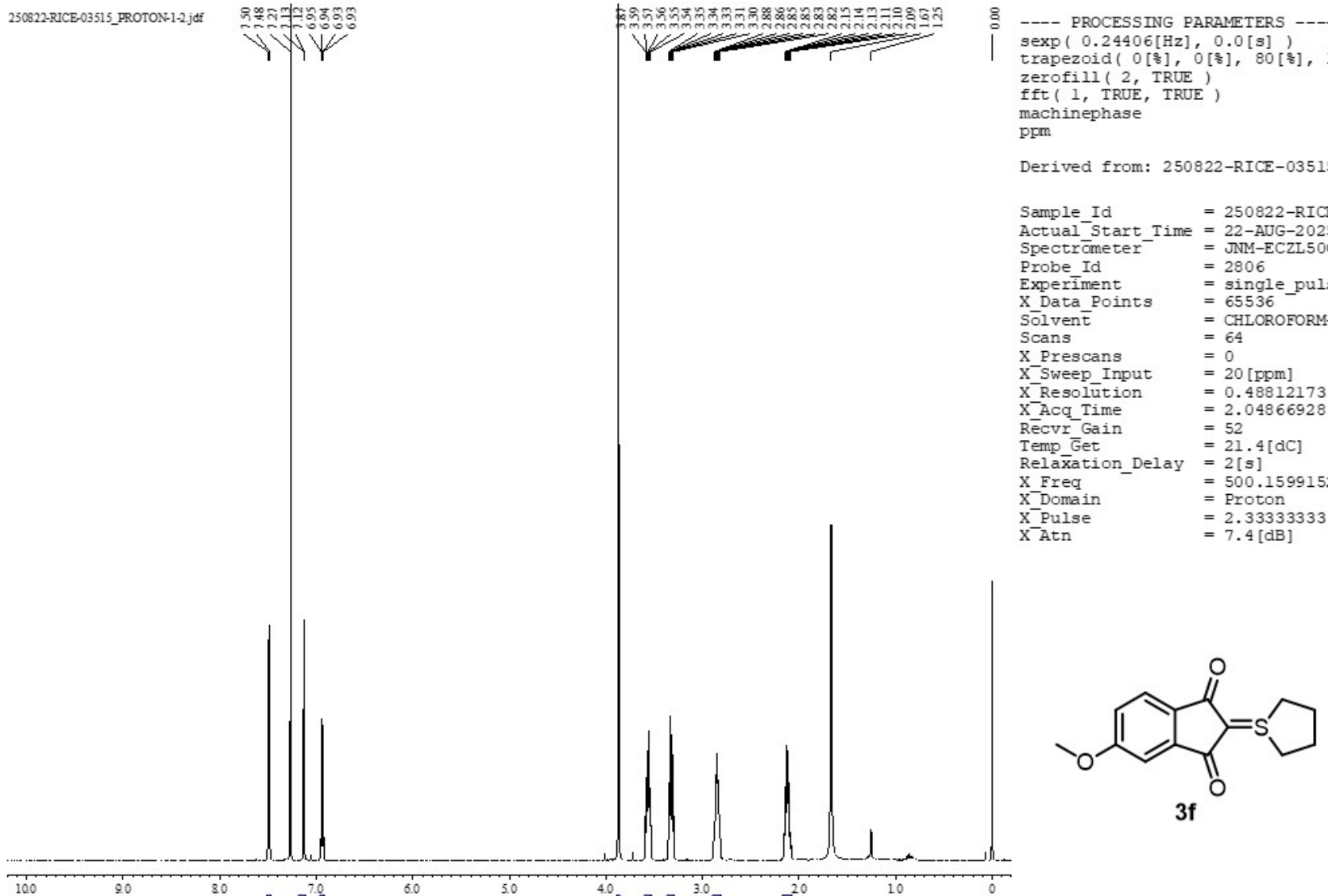

```
Current Data Parameters
NAME      250114-RICE-03507
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20250114
Time                 21.14
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                     108
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ               2.7262976 sec
RG                   219.17
DW                   83.200 usec
DE                   12.63 usec
TE                   294.4 K
D1             2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                   14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                   16384
SF            300.1300014 MHz
WDW                    EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```



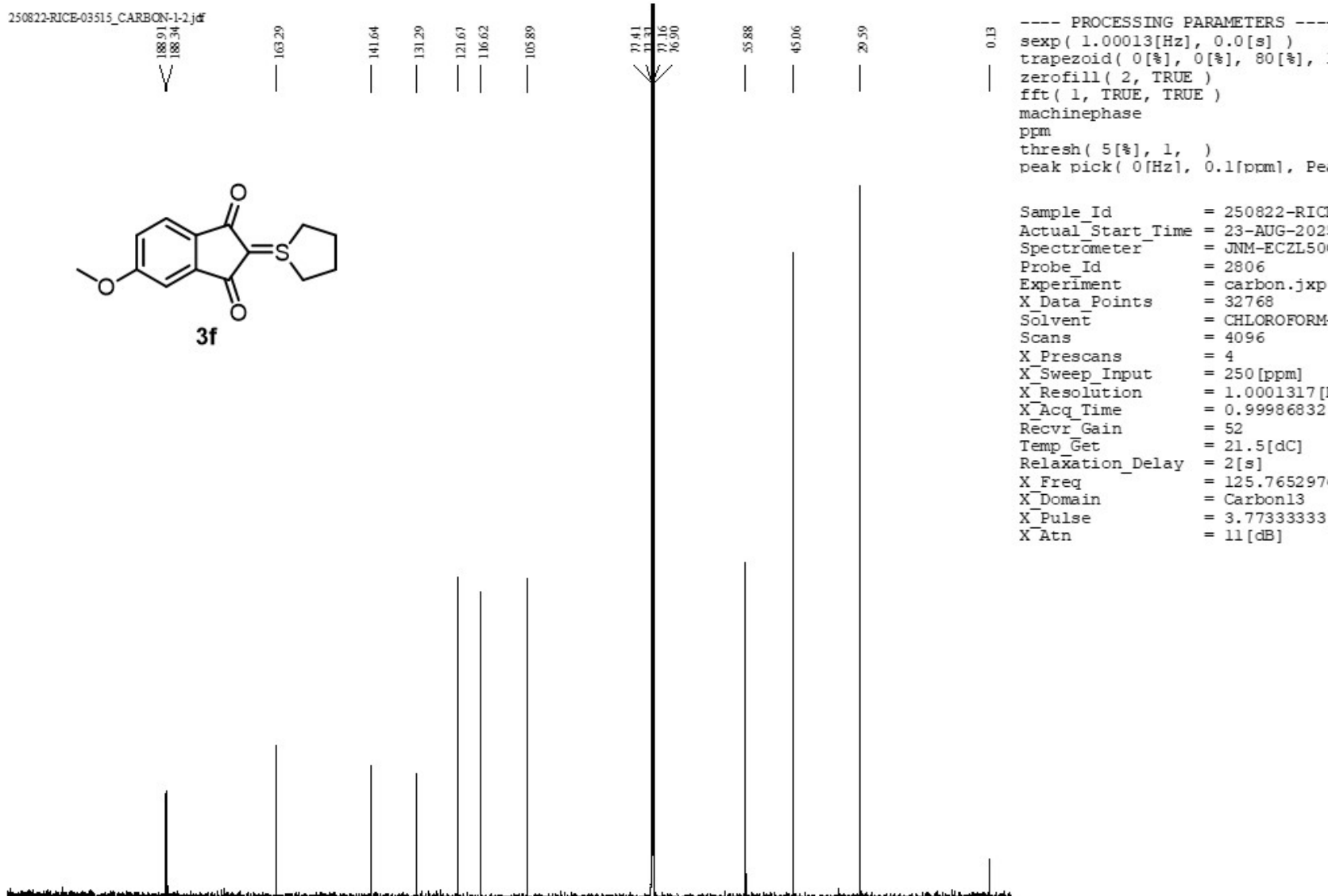
240901-RICE-00482-NO2-13C



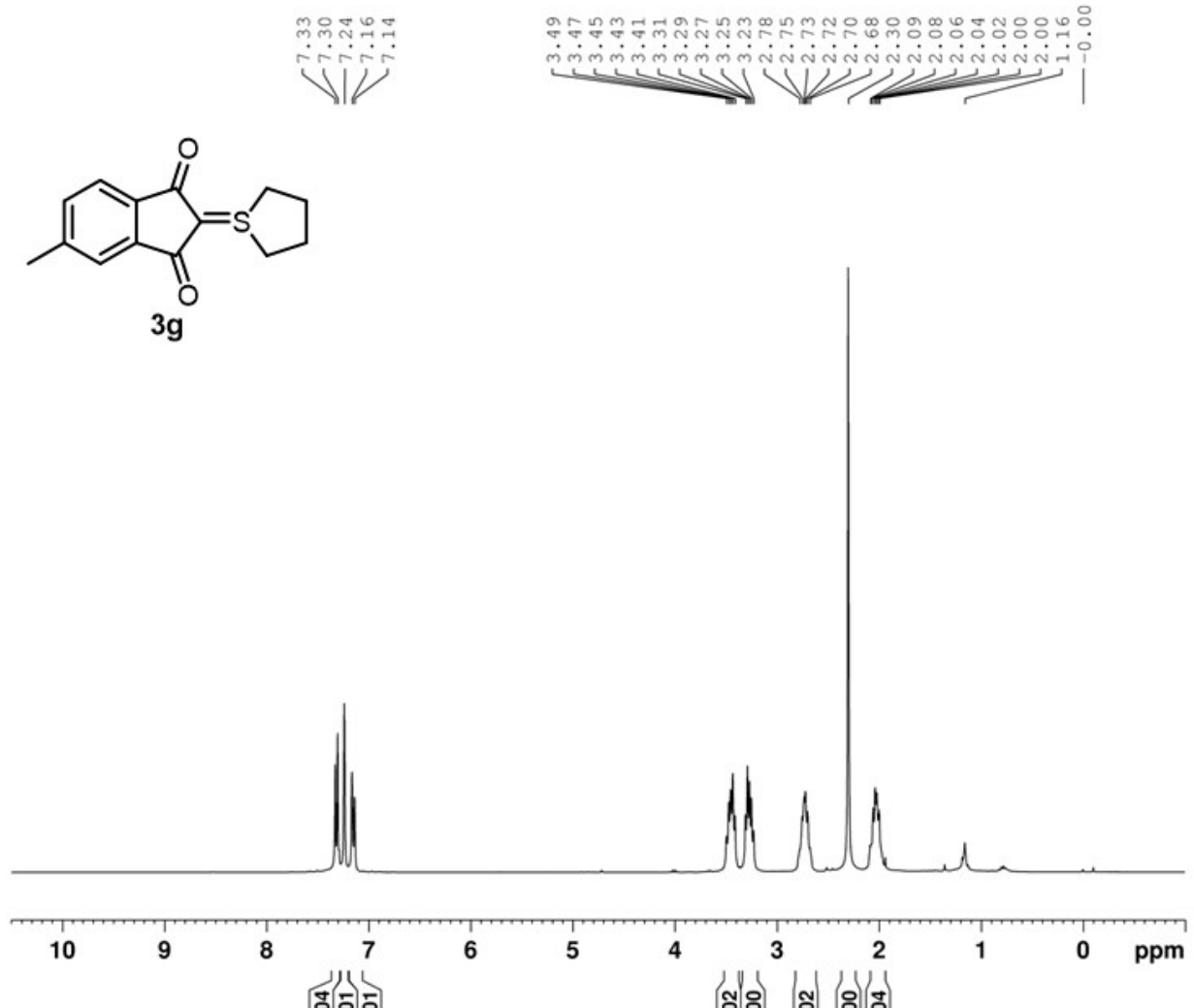

```
Current Data Parameters
NAME          240901-RICE-00482-NO2-13C
EXPNO                                1
PROCNO                               1

F2 - Acquisition Parameters
Date_                         20240902
Time                              5.46
INSTRUM                          spect
PROBHD    5 mm PABBO BB-
PULPROG                       zgpg30
TD                               32768
SOLVENT                        CDCl3
NS                               10240
DS                                   0
SWH                       18028.846 Hz
FIDRES                     0.550197 Hz
AQ                         0.9087659 sec
RG                               219.17
DW                           27.733 usec
DE                            6.50 usec
TE                              294.8 K
D1                        2.00000000 sec
D11                       0.03000000 sec
TD0                                  1

======== CHANNEL f1 ========
SFO1                   75.4756726 MHz
NUC1                           13C
P1                           10.00 usec
PLW1                  28.29999924 W

======== CHANNEL f2 ========
SFO2                  300.1312005 MHz
NUC2                           1H
CPDPRG[2 bi_waltz65_256
PCPD2                        90.00 usec
PLW2                   8.30000019 W
PLW12                  0.20084000 W
PLW13                  0.16268000 W

F2 - Processing parameters
SI                               32768
SF                    75.4677387 MHz
WDW                             EM
SSB                              0
LB                            2.00 Hz
GB                               0
PC                            1.00
```


250822-RICE-03515_PROTON-1-2.jdf
7.50
7.48
7.27
7.13
7.12
6.95
6.94
6.93
6.93
3.87
3.59
3.57
3.56
3.55
3.54
3.35
3.34
3.33
3.31
3.30
2.88
2.86
2.85
2.85
2.83
2.82
2.15
2.14
2.13
2.11
2.10
2.09
1.67
1.25
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250822-RICE-0351
Sample_Id = 250822-RIC
Actual_Start_Time = 22-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 64
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 21.4[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
O
S
O

3f


250822-RICE-03515_CARBON-1-2.jdf
188.91
188.34
163.29
141.64
131.29
121.67
116.62
105.89
77.41
77.16
76.90
55.88
45.06
29.59
0.13
3f
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250822-RIC
Actual_Start_Time = 23-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 4096
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 21.5[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]

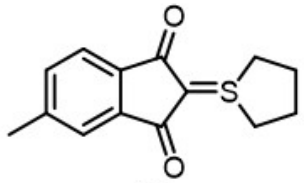
250114-RICE-03508



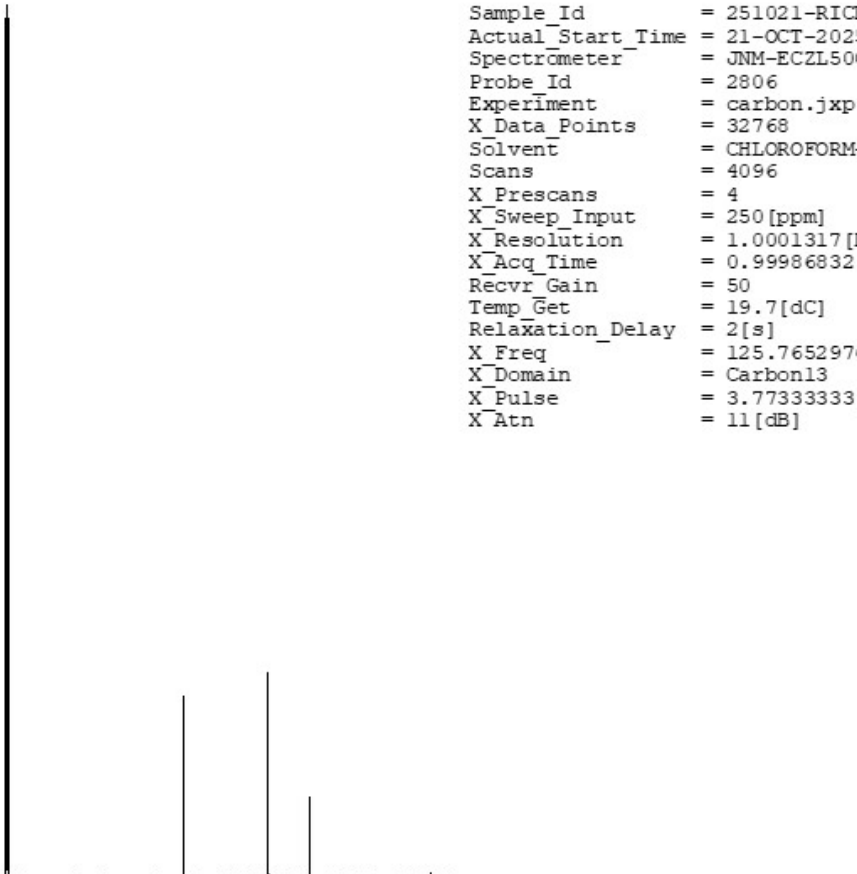

```
Current Data Parameters
NAME      250114-RICE-03508
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20250114
Time                 21.25
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      64
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                    36.7
DW                  83.200 usec
DE                  12.63 usec
TE                  294.4 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318008 MHz
NUC1                   1H
P1                  14.00 usec
PLW1            7.69999981 W

F2 - Processing parameters
SI                   16384
SF             300.1300000 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

251021-RICE-03508_Carbon-1-2.jdf

189.16
189.15
142.49
139.31
136.39
132.13
120.90
120.02
77.41
77.21
77.15
76.90
44.98
29.60
21.98

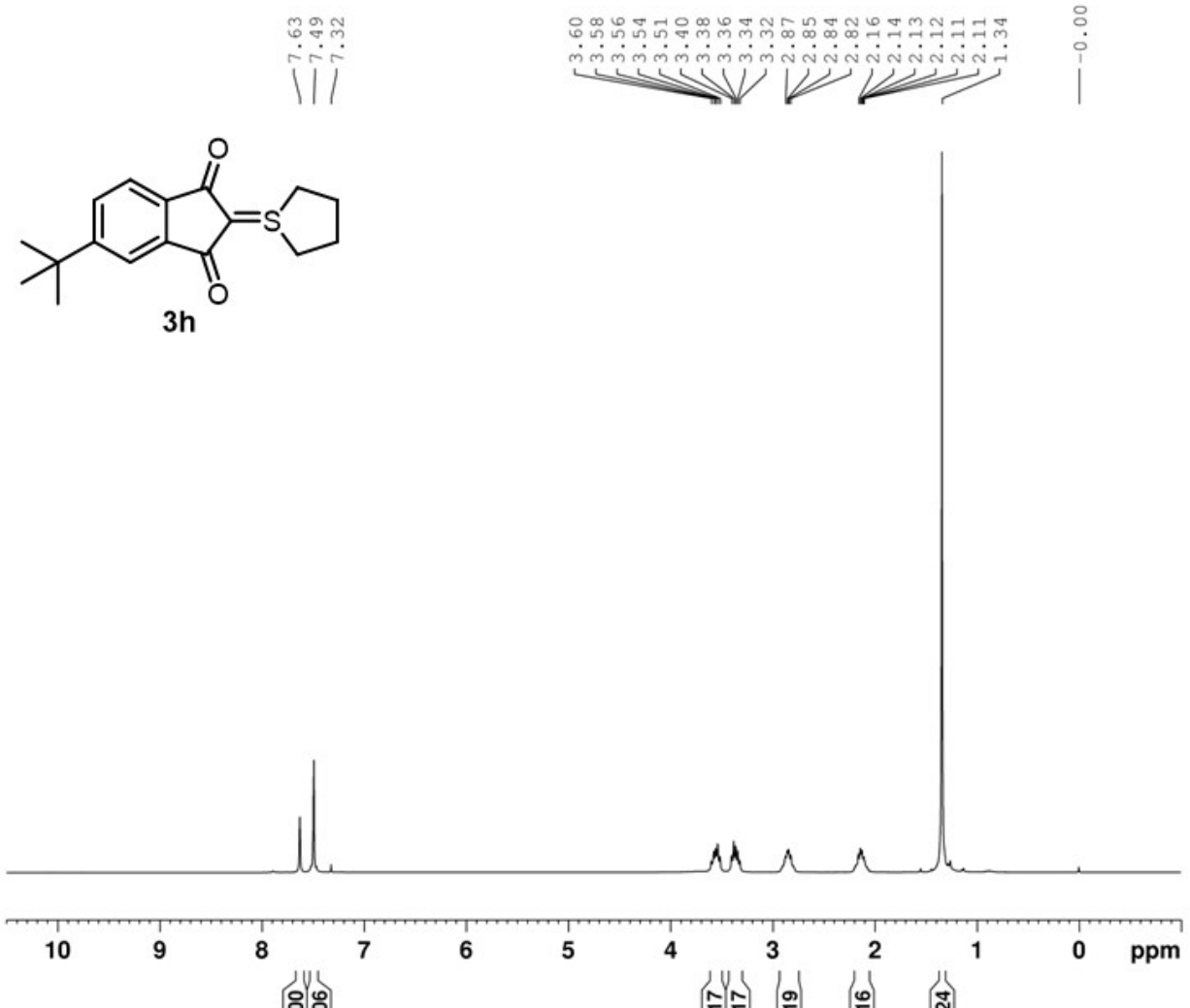


3g

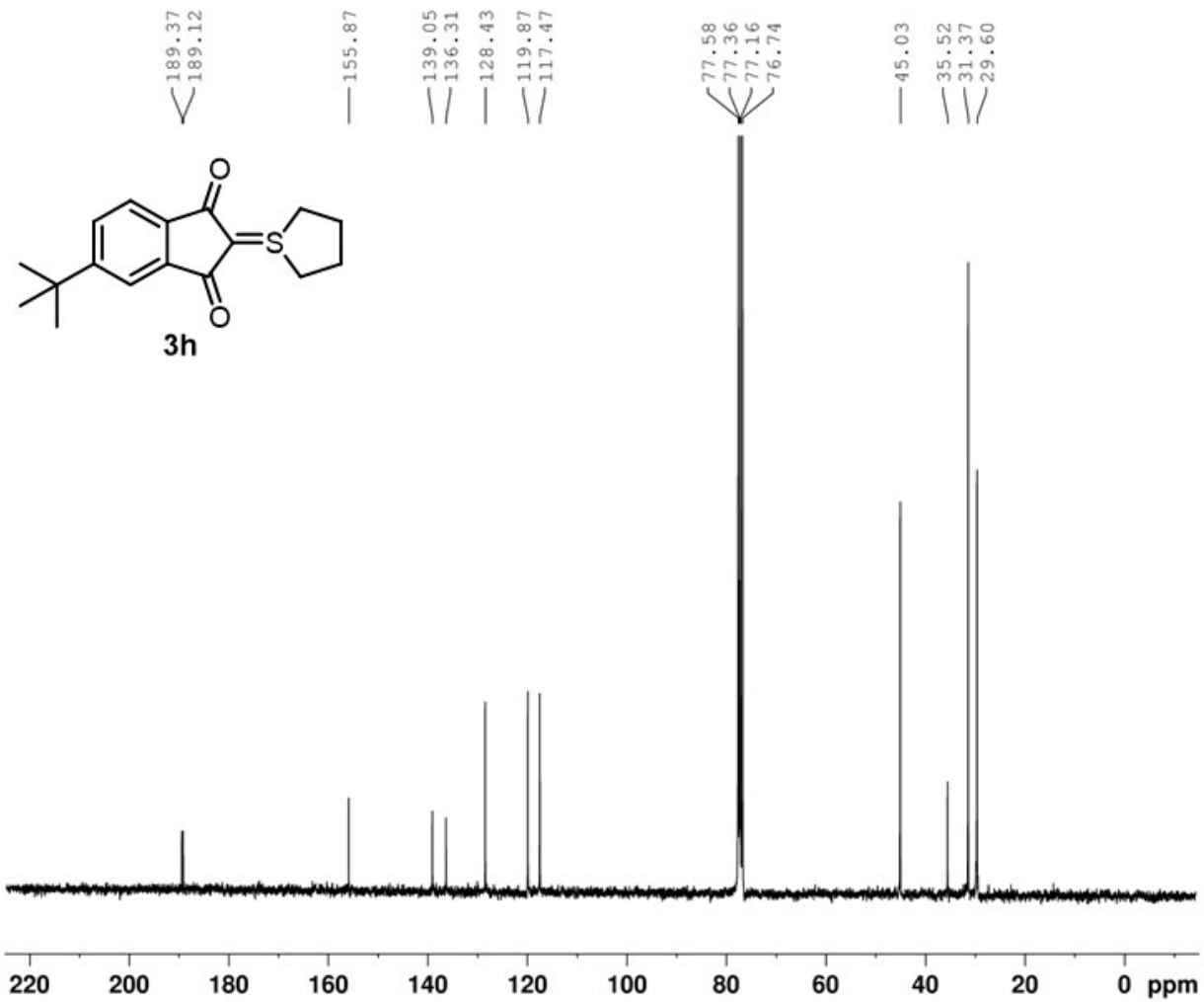


```
---- PROCESSING PARAMETERS ----
sexp( 1.00013[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%],
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.11517[ppm], 77.1
thresh( 1.7074[%], 1,  )

Sample_Id          = 251021-RIC
Actual_Start_Time  = 21-OCT-202
Spectrometer       = JNM-ECZL50
Probe_Id           = 2806
Experiment         = carbon.jxp
X_Data_Points      = 32768
Solvent            = CHLOROFORM
Scans              = 4096
X_Prescans         = 4
X_Sweep_Input      = 250[ppm]
X_Resolution       = 1.0001317[
X_Acq_Time         = 0.99986832
Recvr_Gain         = 50
Temp_Get           = 19.7[dC]
Relaxation_Delay   = 2[s]
X_Freq             = 125.765297
X_Domain           = Carbon13
X_Pulse            = 3.77333333
X_Atn              = 11[dB]
```

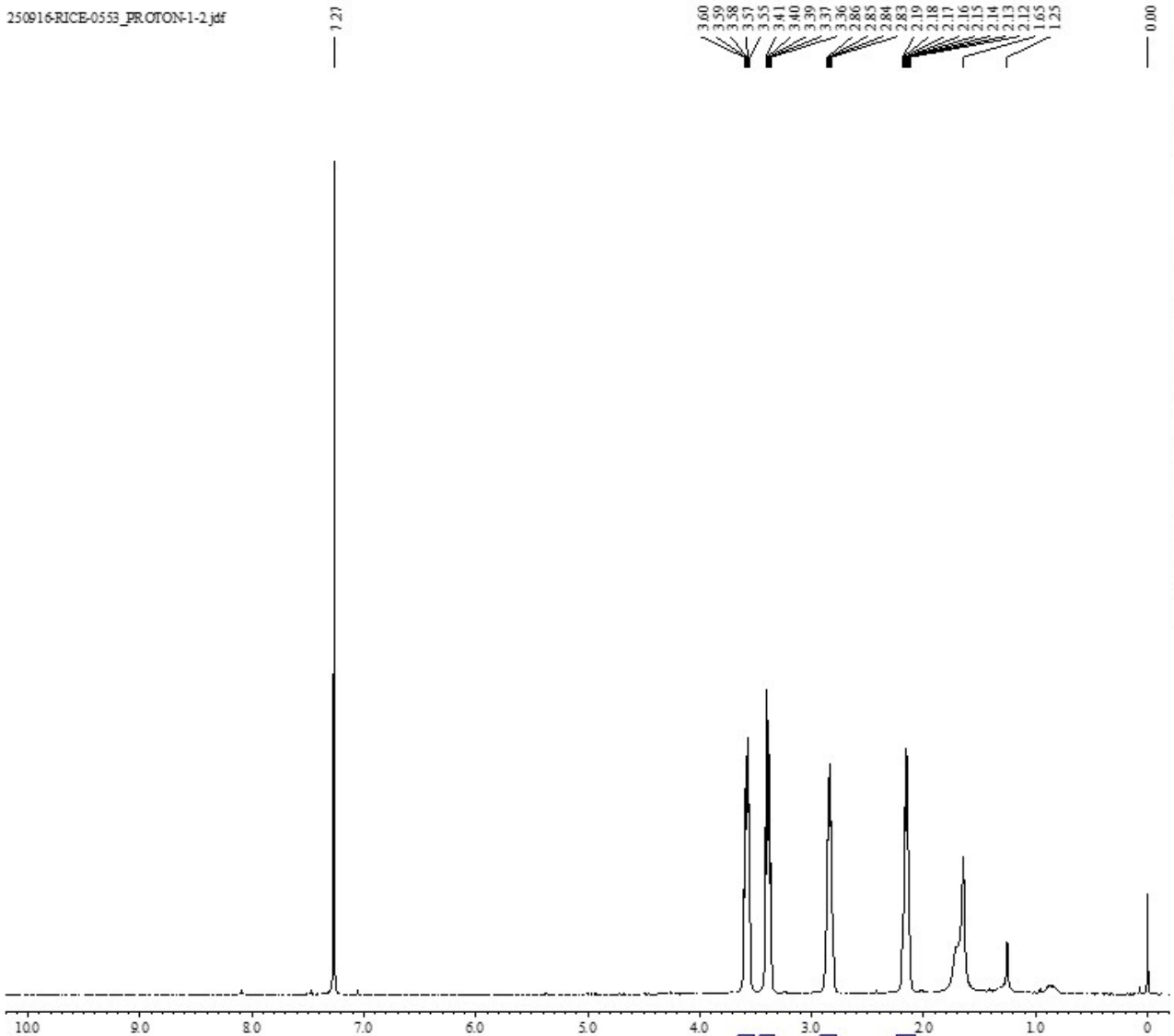
250219-RICE-03510-NS64

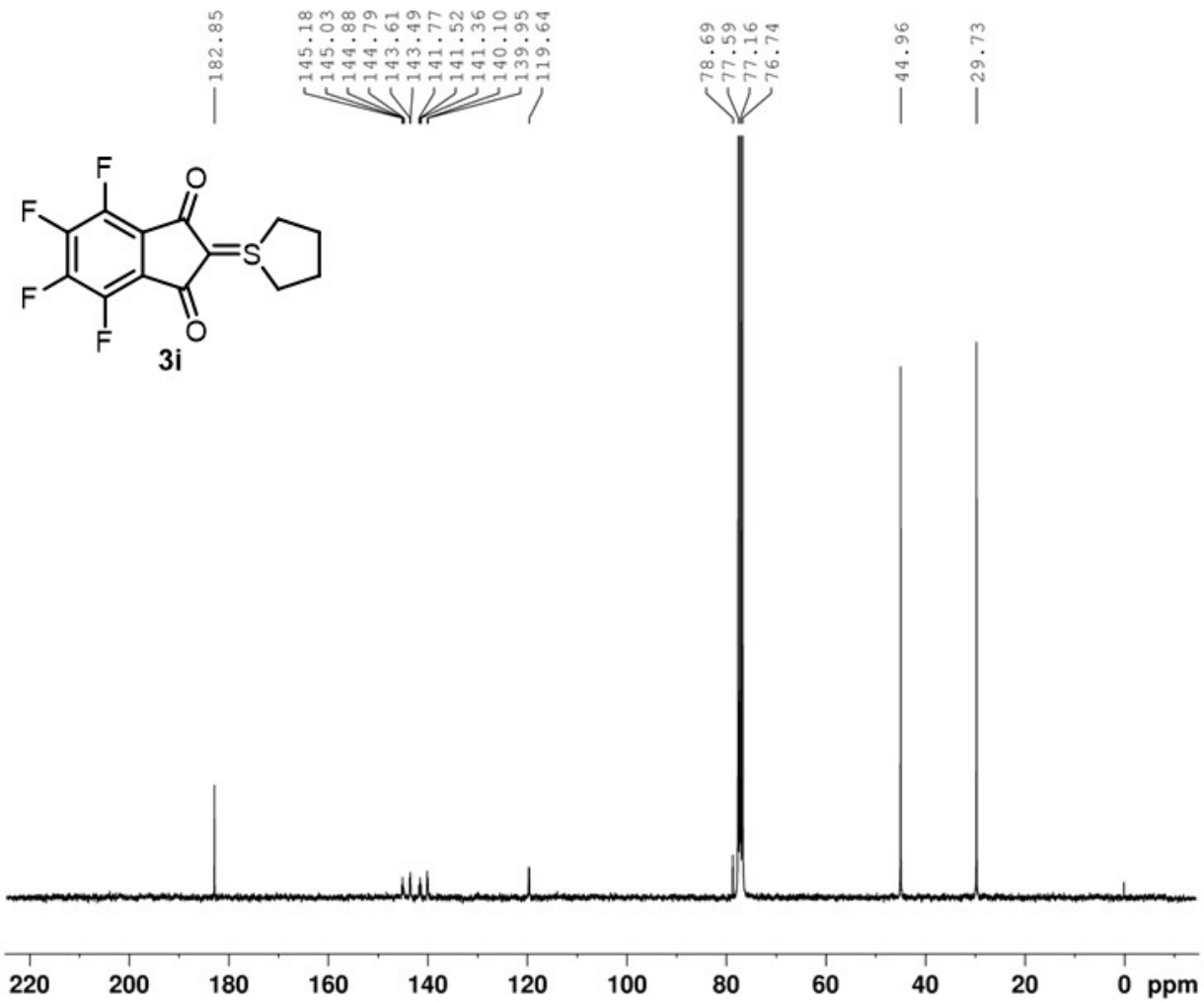



```
Current Data Parameters
NAME      250219-RICE-03510-NS64
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20250219
Time                       20.18
INSTRUM                    spect
PROBHD   5 mm PABBO BB-
PULPROG                     zg30
TD                         32768
SOLVENT                    CDC13
NS                            64
DS                             0
SWH                     6009.615 Hz
FIDRES                  0.183399 Hz
AQ                     2.7262976 sec
RG                         85.67
DW                         83.200 usec
DE                         12.63 usec
TE                         293.6 K
D1                    2.00000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                300.1318008 MHz
NUC1                        1H
P1                         14.00 usec
PLW1                7.69999981 W

F2 - Processing parameters
SI                         16384
SF                  300.1299884 MHz
WDW                           EM
SSB                            0
LB                             0 Hz
GB                             0
PC                          1.00
```

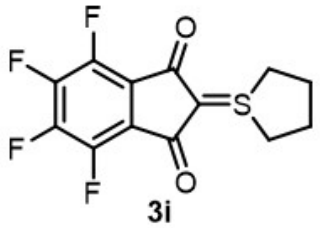



```
Current Data Parameters
NAME                  3h_13C
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20241211
Time                  16.32
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    1712
DS                       0
SWH              18028.846 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                   27.733 usec
DE                    6.50 usec
TE                   294.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                   13C
P1                   10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                   32768
SF              75.4677412 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

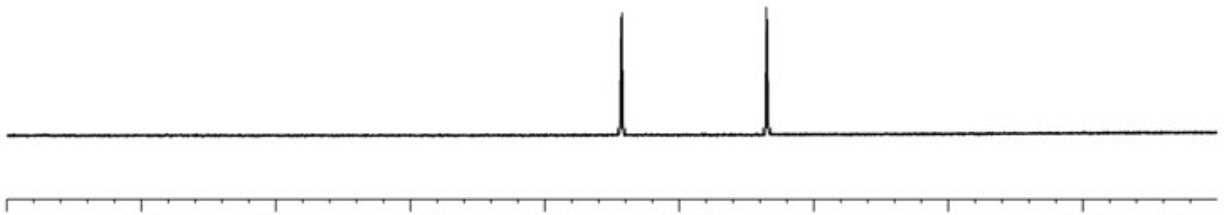

250916-RICE-0553_PROTON-1-2.jdf
7.27
3.60
3.59
3.58
3.57
3.55
3.41
3.40
3.39
3.37
3.36
2.86
2.85
2.84
2.83
2.19
2.18
2.17
2.16
2.15
2.14
2.13
2.12
1.65
1.25
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250916-RICE-0553
Sample_Id = 250916-RIC
Actual_Start_Time = 16-SEP-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 64
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 21.6[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
F
F
F
F
O
O
S
3i




```
Current Data Parameters
NAME                  3i_13C
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20241111
Time                   6.09
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zgpg30
TD                     32768
SOLVENT                CDCl3
NS                     10240
DS                         0
SWH               18028.846 Hz
FIDRES             0.550197 Hz
AQ                 0.9087659 sec
RG                    219.17
DW                    27.733 usec
DE                     6.50 usec
TE                    296.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                 90.00 usec
PLW2            8.30000019 W
PLW12           0.20084000 W
PLW13           0.16268000 W

F2 - Processing parameters
SI                     32768
SF              75.4677395 MHz
WDW                       EM
SSB                        0
LB                     2.00 Hz
GB                         0
PC                      1.00
```

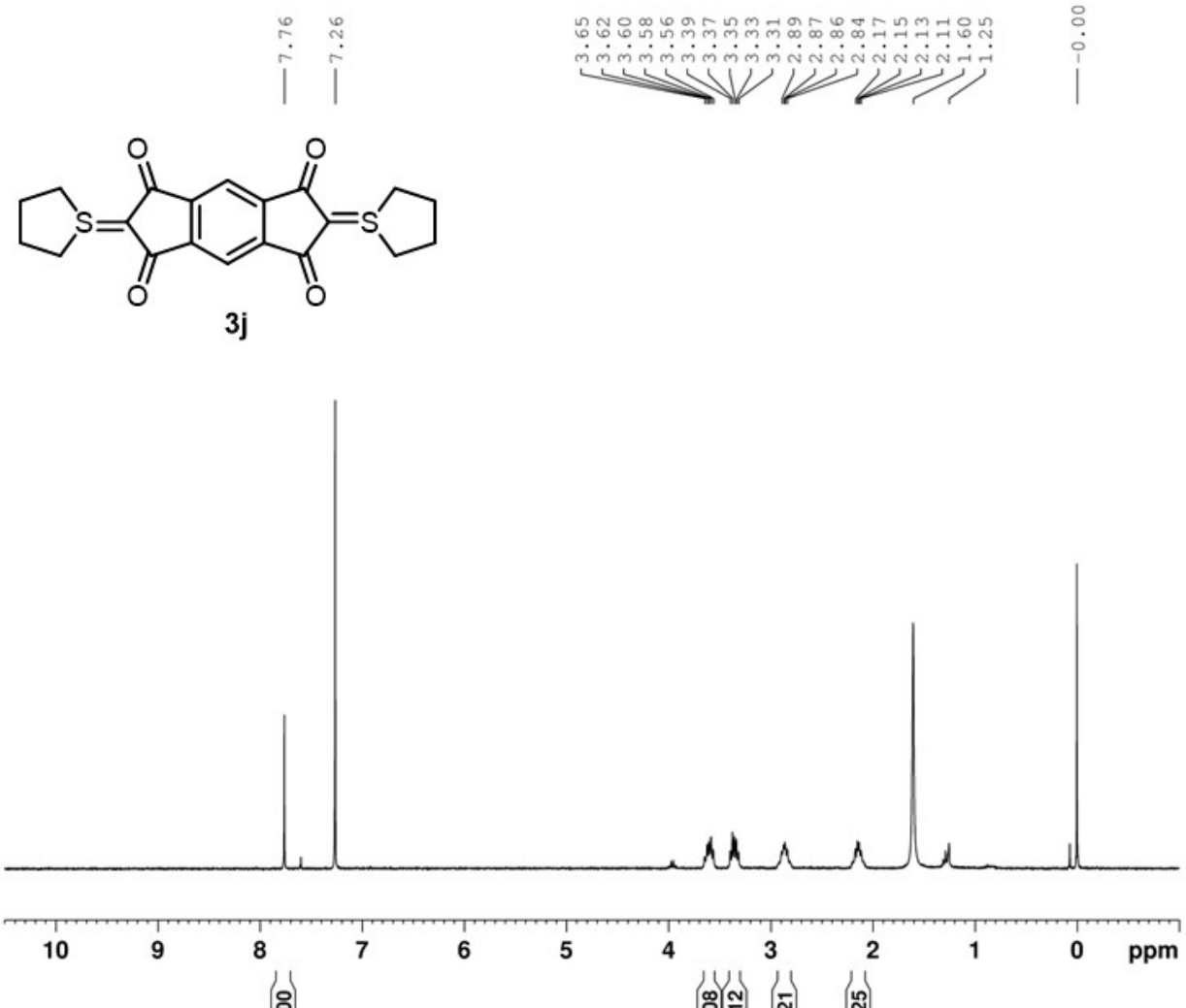


3i



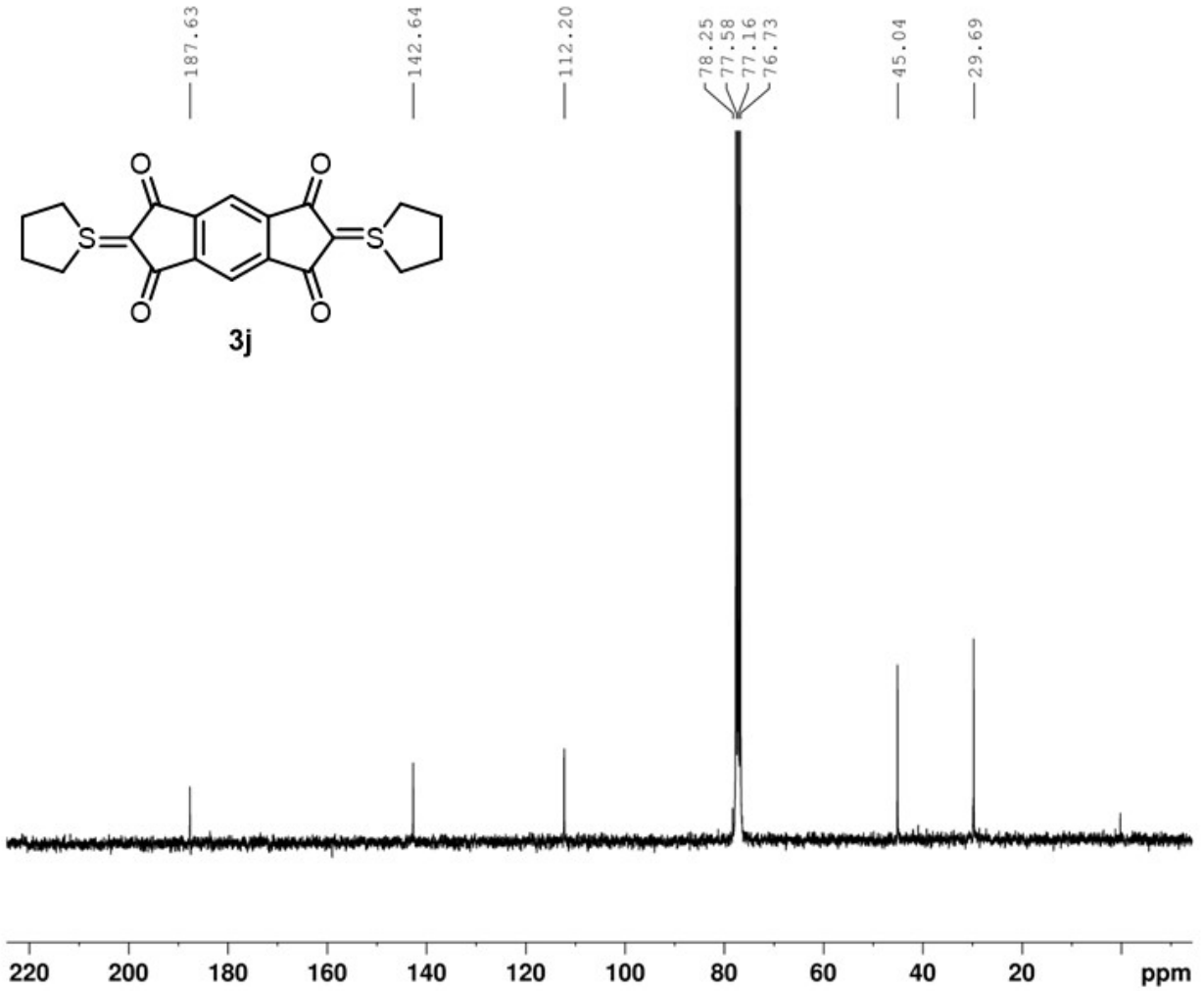

```
Current Data Parameters
NAME                  3i_19F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250226
Time                  11.54
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG               zgig30
TD                    131072
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                66964.289 Hz
FIDRES             0.510897 Hz
AQ                 0.9786710 sec
RG                    219.17
DW                     7.467 usec
DE                     6.50 usec
TE                     293.4 K
D1               1.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             282.3874119 MHz
NUC1                    19F
P1                    15.50 usec
PLW1             6.09999990 W

======== CHANNEL f2 ========
SFO2             300.1312005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             8.30000019 W
PLW12            0.20084000 W

F2 - Processing parameters
SI                     65536
SF               282.4043552 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

250212-RICE-03514

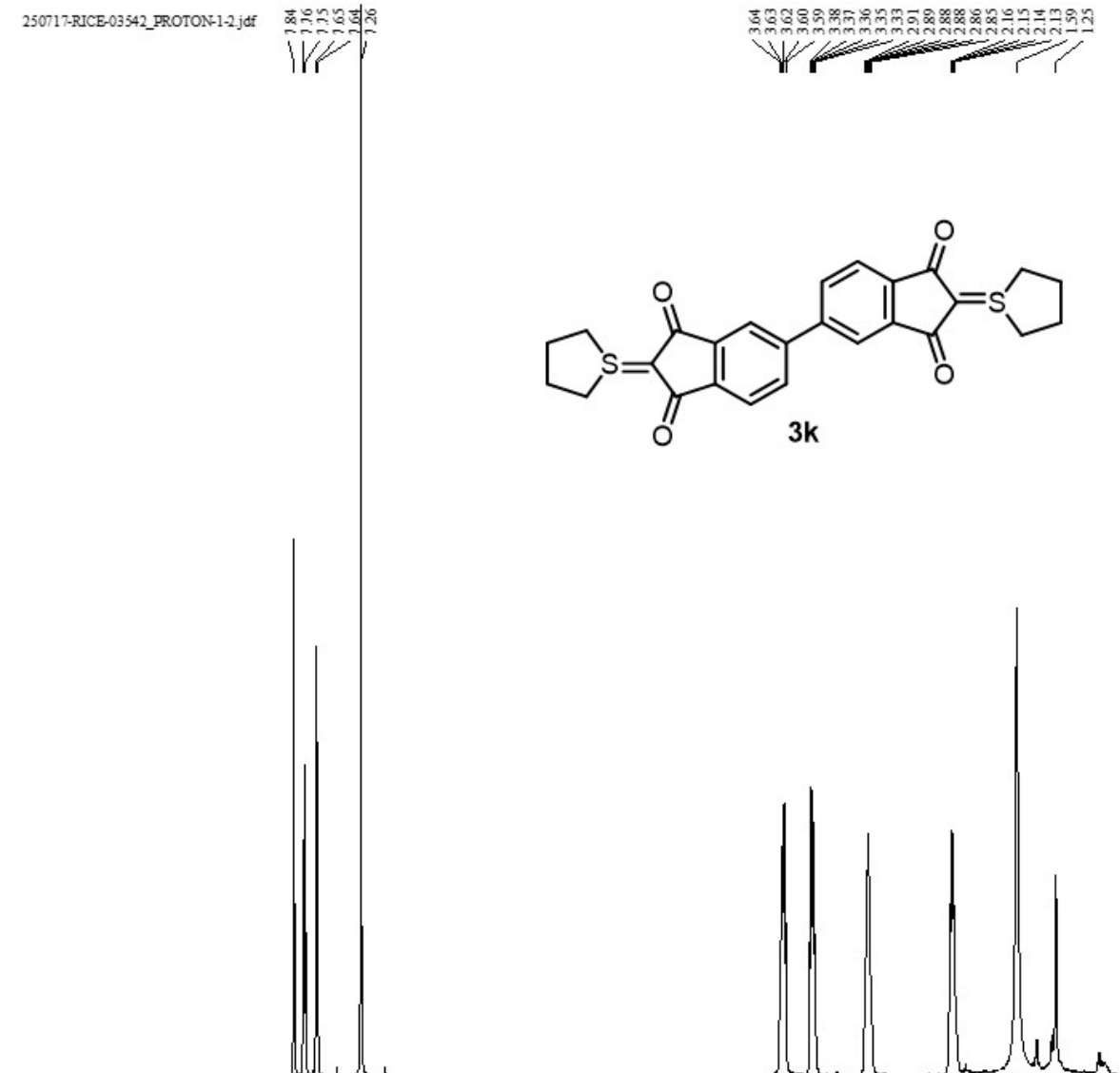


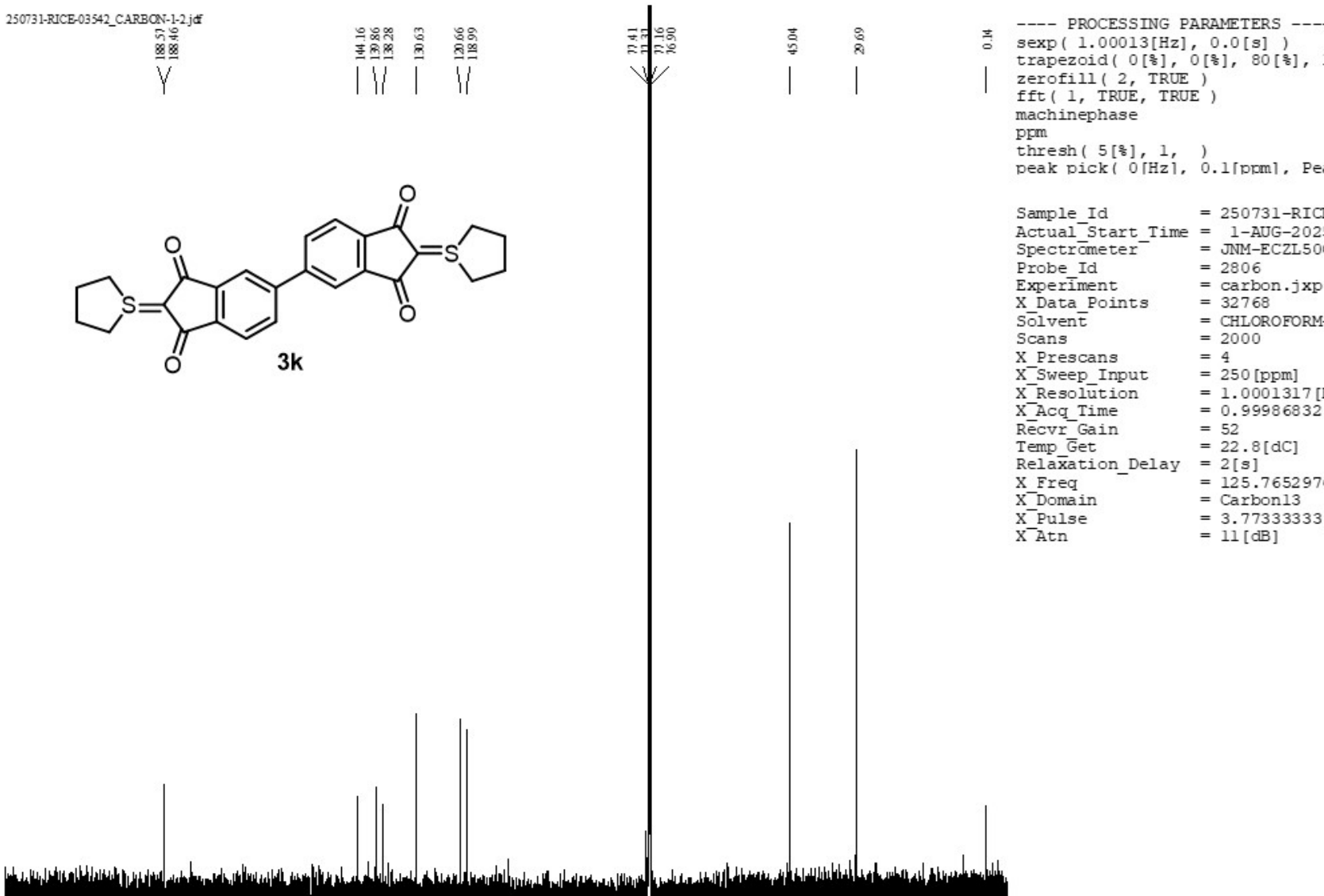

```
Current Data Parameters
NAME      250212-RICE-03514
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20250212
Time                 21.20
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      64
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                  219.17
DW                  83.200 usec
DE                  12.63 usec
TE                  294.3 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318008 MHz
NUC1                    1H
P1                   14.00 usec
PLW1            7.69999981 W

F2 - Processing parameters
SI                   16384
SF             300.1300060 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```

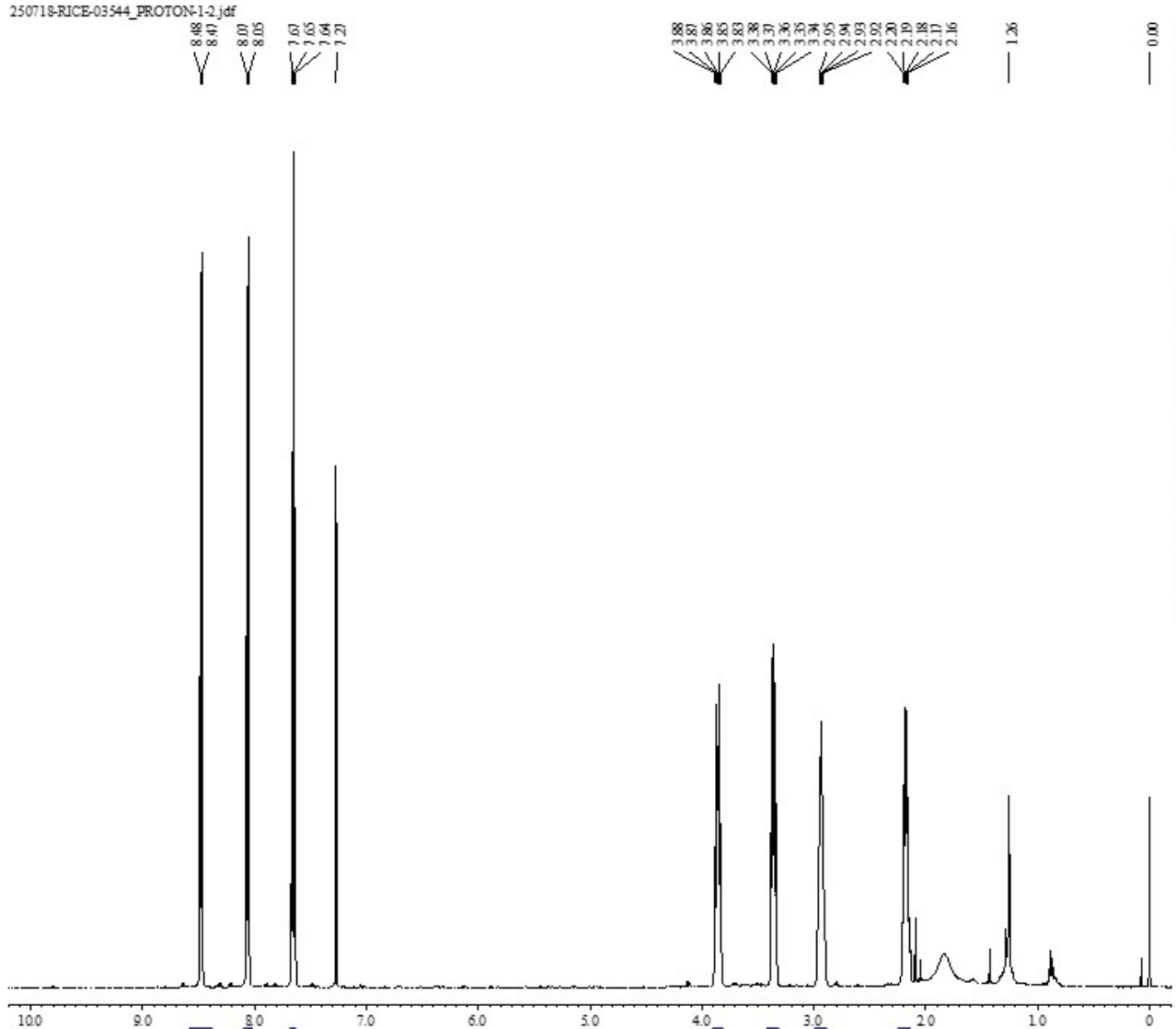
241027-RICE-00497-LONGTIME-13C



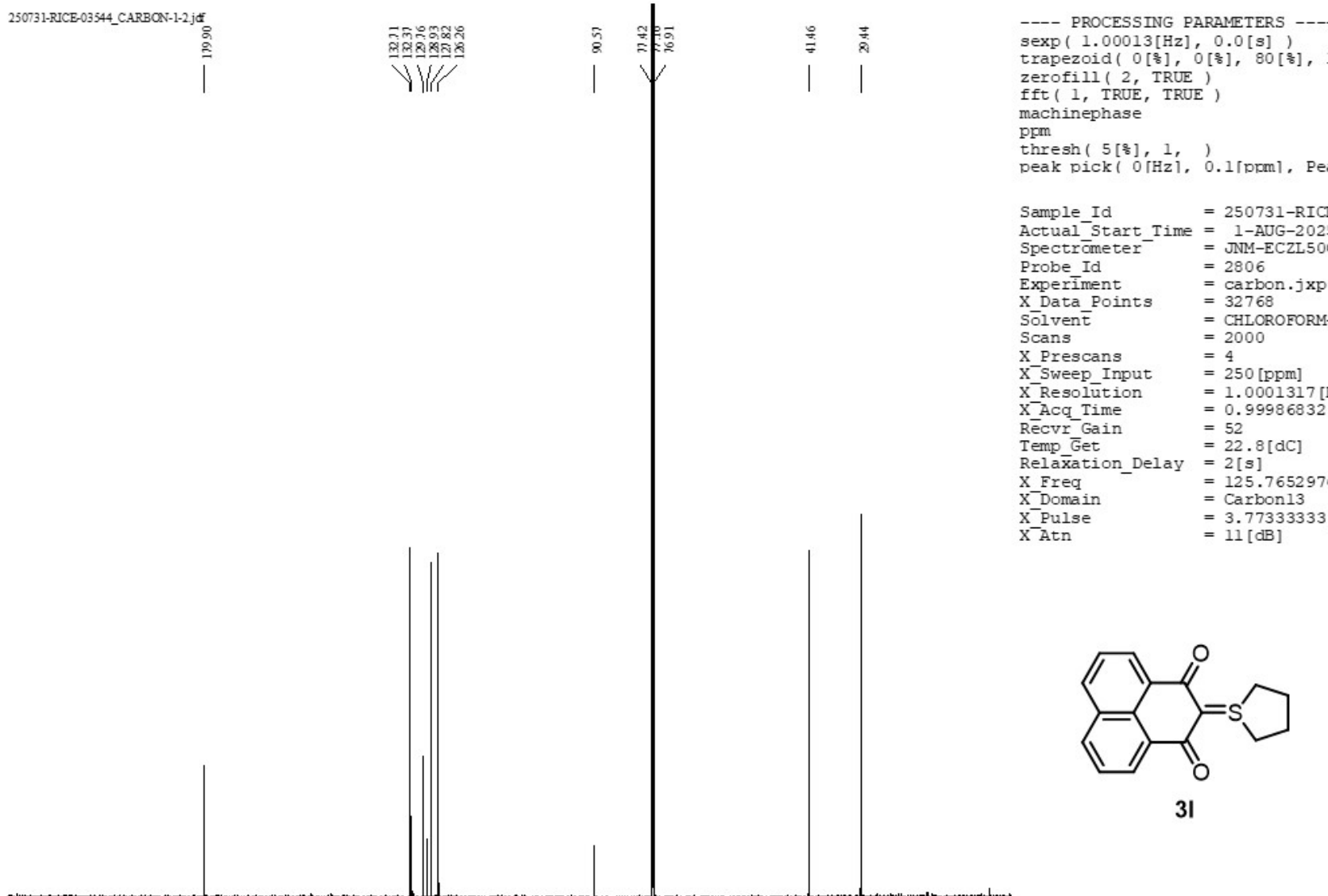

```
Current Data Parameters
NAME          241027-RICE-00497-LONGTIME
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20241028
Time                   5.38
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   8192
DS                      0
SWH             18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677390 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

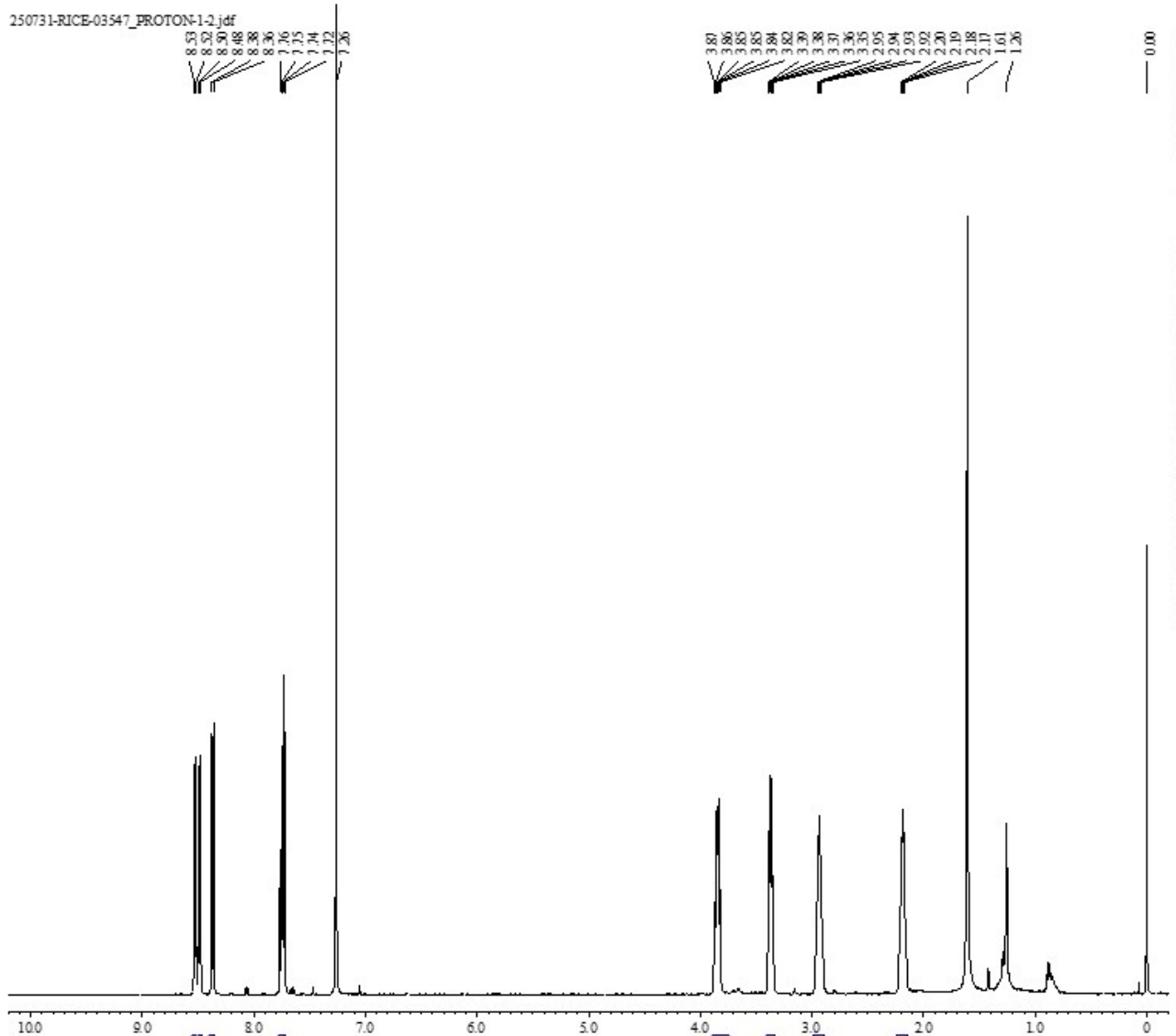

250717-RICE-03542_PROTON-1-2.jdf
7.84
7.76
7.75
7.65
7.64
7.26
3.64
3.63
3.62
3.60
3.59
3.38
3.37
3.36
3.35
3.33
2.91
2.89
2.88
2.88
2.86
2.85
2.16
2.15
2.14
2.13
1.59
1.25
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.01529[ppm], 0[pp
thresh(2.60008[%], 0.28377[%]
Sample_Id = 250717-RIC
Actual_Start_Time = 17-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 62
Temp_Get = 23.5[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
3k

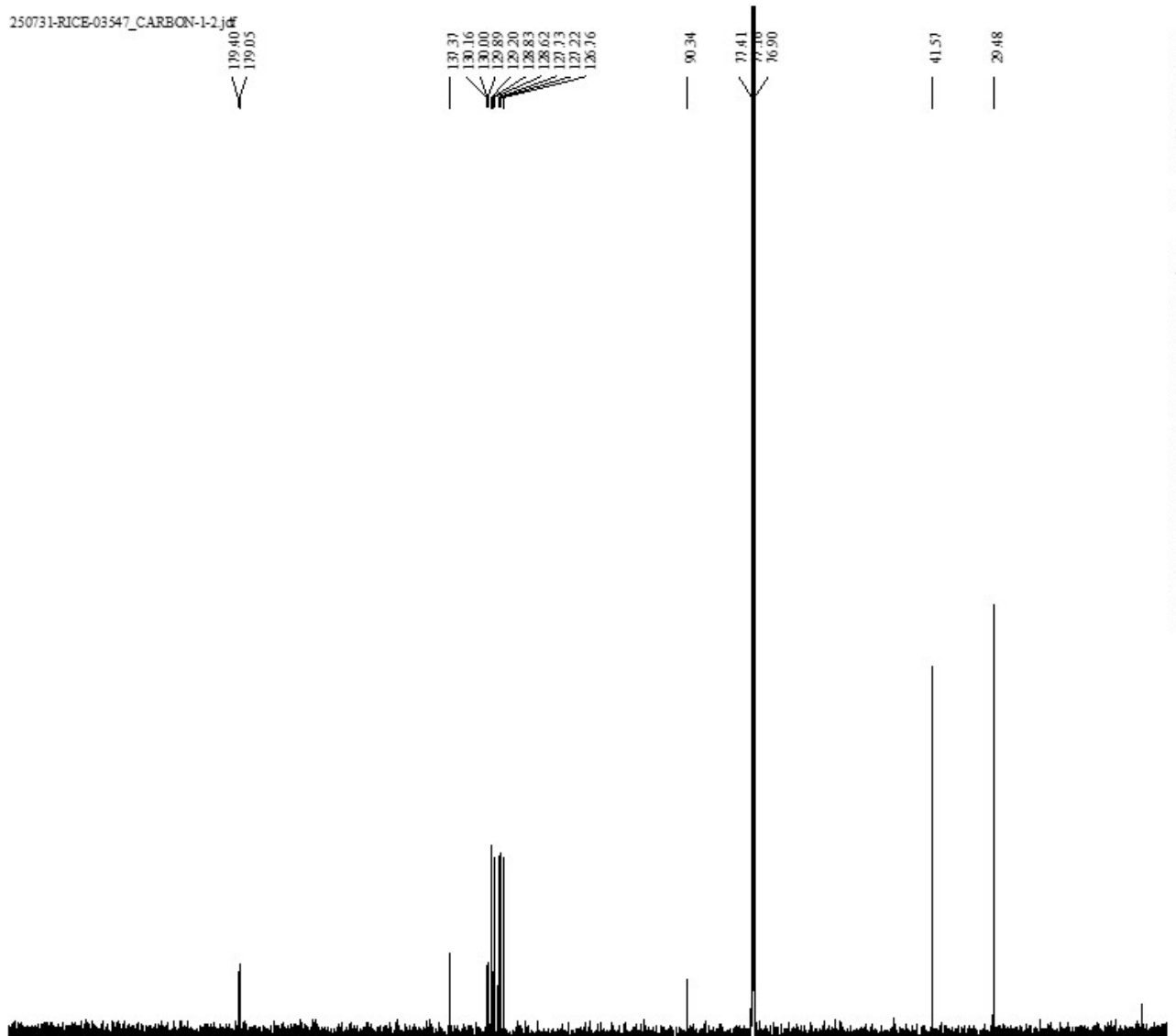

250731-RICE-03542_CARBON-1-2.jdf
188.57
188.46
144.16
139.86
138.28
130.63
120.66
118.99
77.41
77.33
77.16
76.90
45.04
29.69
0.14
3k
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250731-RIC
Actual_Start_Time = 1-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 22.8[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]

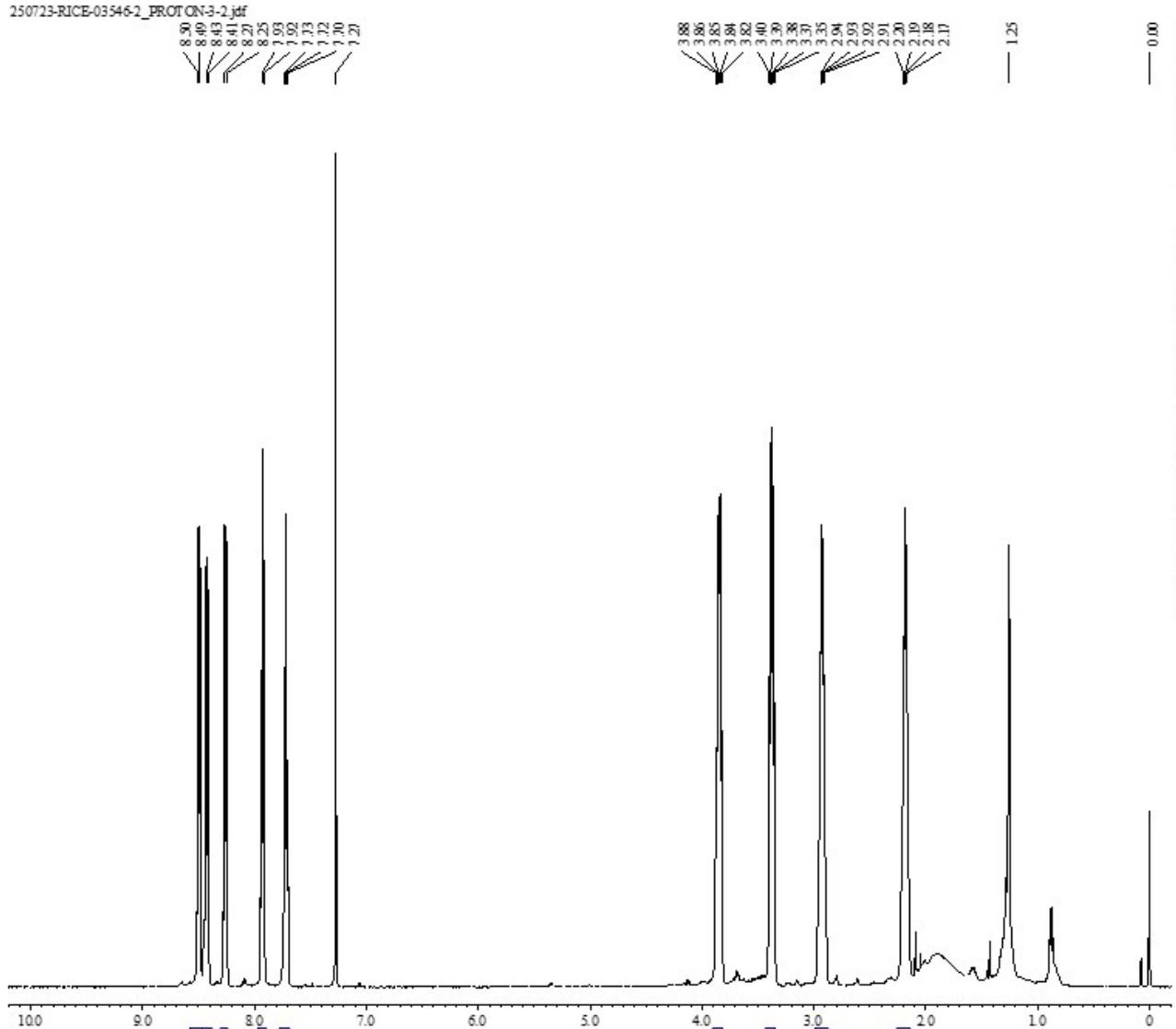

250718-RICE-03544_PROTON-1-2.jdf
8.48
8.47
8.01
8.05
7.61
7.65
7.64
7.27
3.88
3.87
3.86
3.85
3.83
3.38
3.37
3.36
3.35
3.34
2.95
2.94
2.93
2.92
2.20
2.19
2.18
2.17
2.16
1.26
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250718-RICE-0354
Sample_Id = 250718-RIC
Actual_Start_Time = 18-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 23.3[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
O
O
S

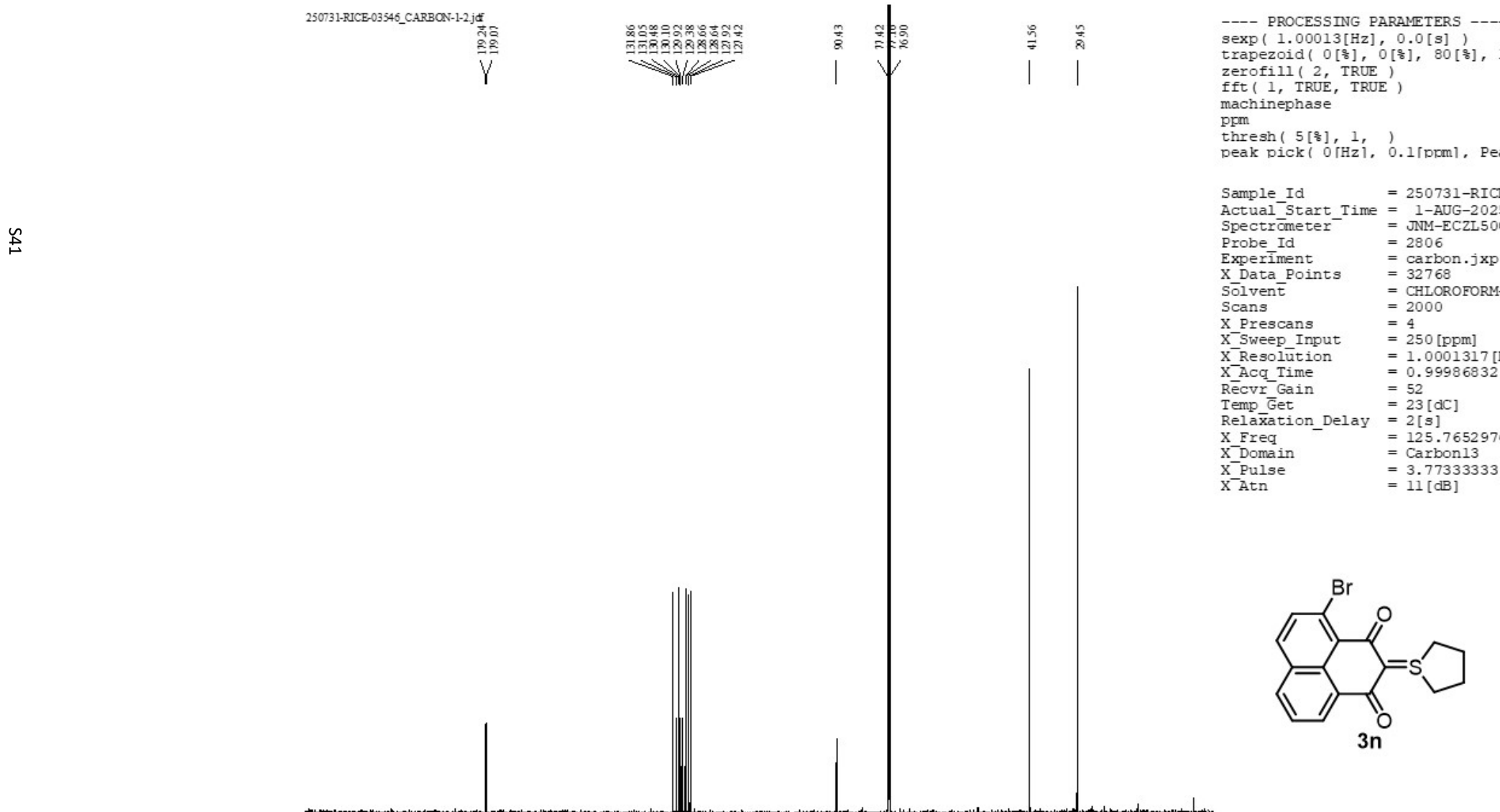
3l

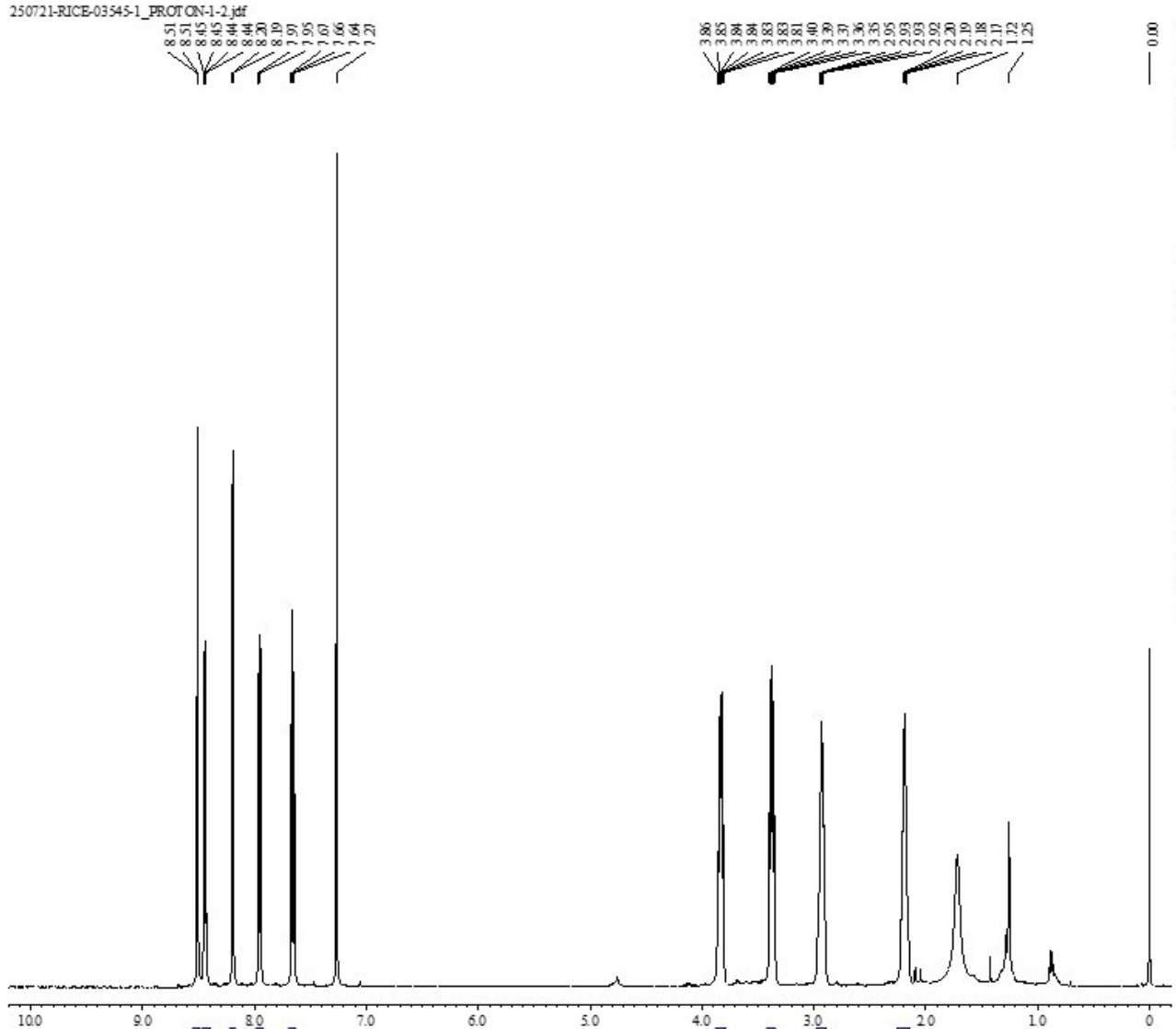

250731-RICE-03544_CARBON-1-2.jdf
179.90
132.11
132.37
129.16
128.93
127.82
126.26
90.57
77.42
77.16
76.91
41.46
29.44
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250731-RIC
Actual_Start_Time = 1-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 22.8[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
O
S
O
3l

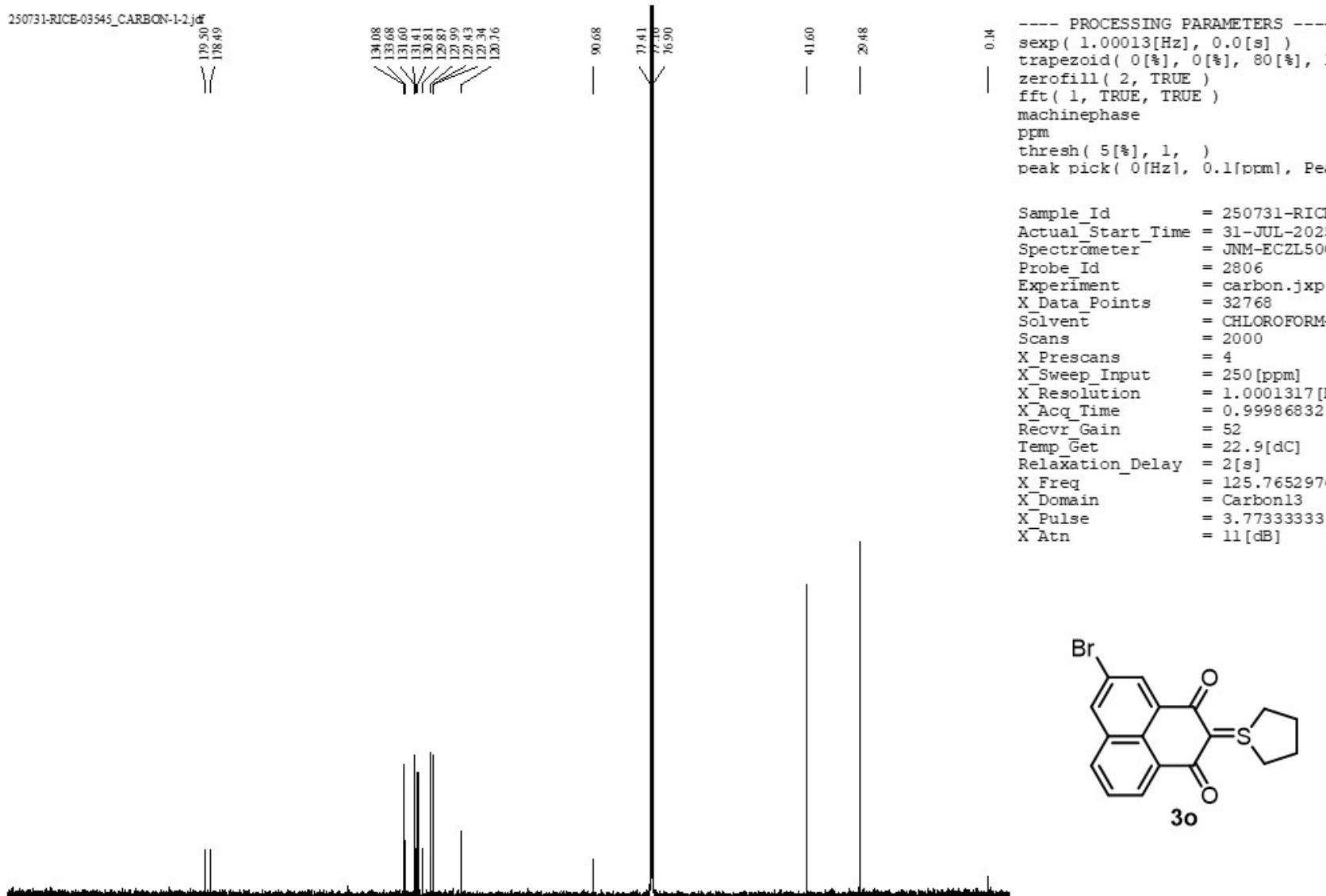

250731-RICE-03547_PROTON-1-2.jdf
8.53
8.52
8.50
8.48
8.38
8.36
7.76
7.75
7.74
7.72
7.26
3.87
3.86
3.85
3.83
3.84
3.82
3.39
3.38
3.37
3.36
3.35
2.95
2.94
2.93
2.92
2.20
2.19
2.18
2.17
1.61
1.26
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250731-RICE-0354
Sample_Id = 250731-RIC
Actual_Start_Time = 31-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 62
Temp_Get = 23.2[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
Cl
O
O
S
3m

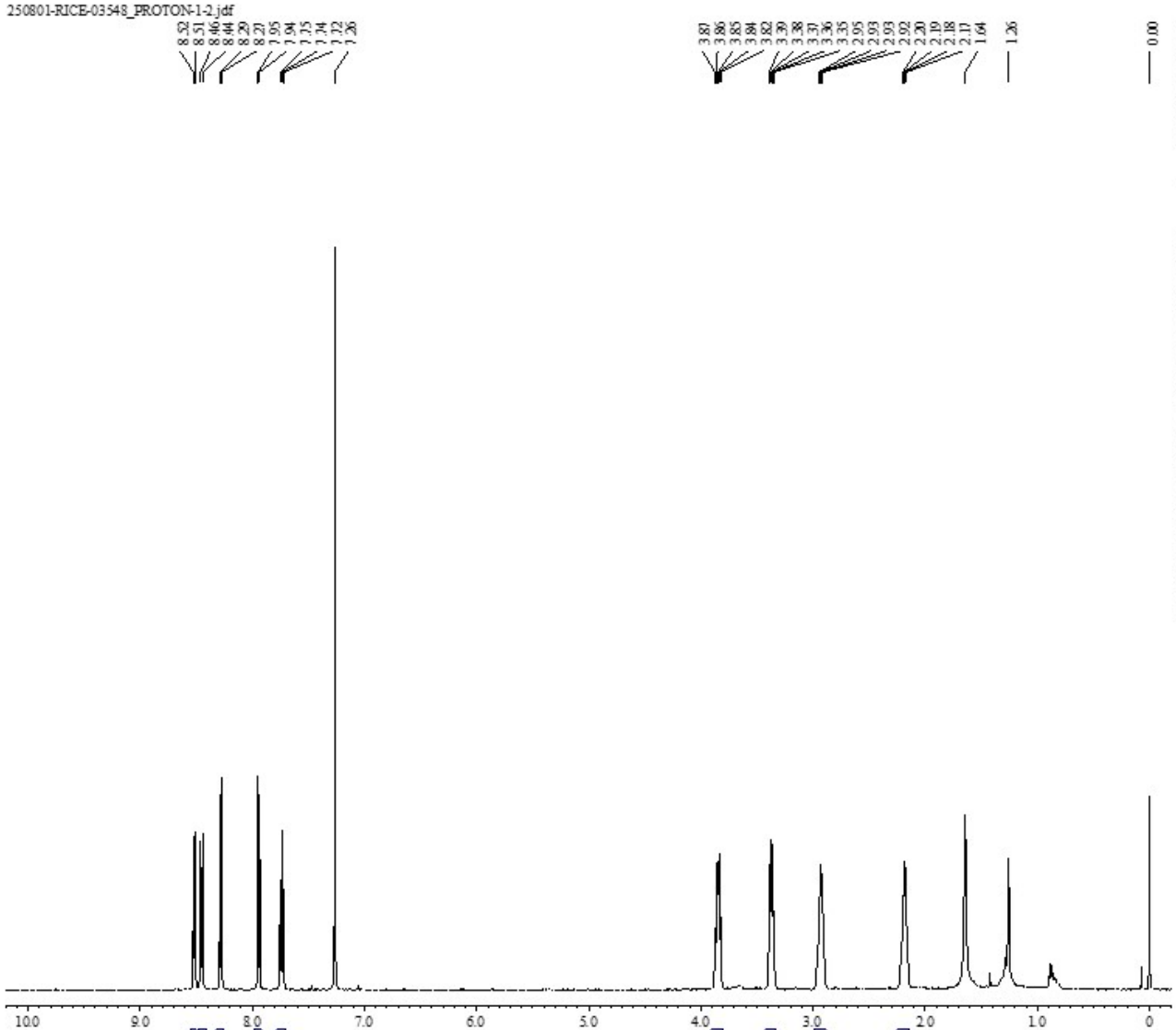

250731-RICE-03547_CARBON-1-2.jdf
179.40
179.05
137.37
130.16
130.00
129.89
129.20
128.83
128.62
127.73
127.22
126.76
90.34
77.41
77.16
76.90
41.57
29.48
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250731-RIC
Actual_Start_Time = 31-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 23.2[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
Cl
O
O
S
3m

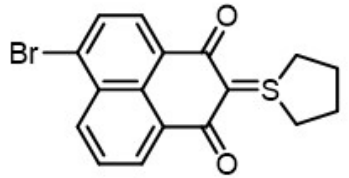

250723-RICE-03546-2_PROTON-3-2.jdf
8.50
8.49
8.43
8.41
8.27
8.25
7.93
7.92
7.73
7.72
7.70
7.27
3.88
3.86
3.85
3.84
3.82
3.40
3.39
3.38
3.37
3.35
2.94
2.93
2.92
2.91
2.20
2.19
2.18
2.17
1.25
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250723-RICE-0354
Sample_Id = 250723-RIC
Actual_Start_Time = 23-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 22.8[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
Br
O
O
S
3n
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0


250731-RICE-03546_CARBON-1-2.jdf
179.24
179.07
131.86
131.05
130.48
130.10
129.92
129.38
128.66
128.64
127.92
127.42
90.43
77.42
77.10
76.90
41.56
29.45
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250731-RIC
Actual_Start_Time = 1-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 23[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
Br
O
O
S
3n

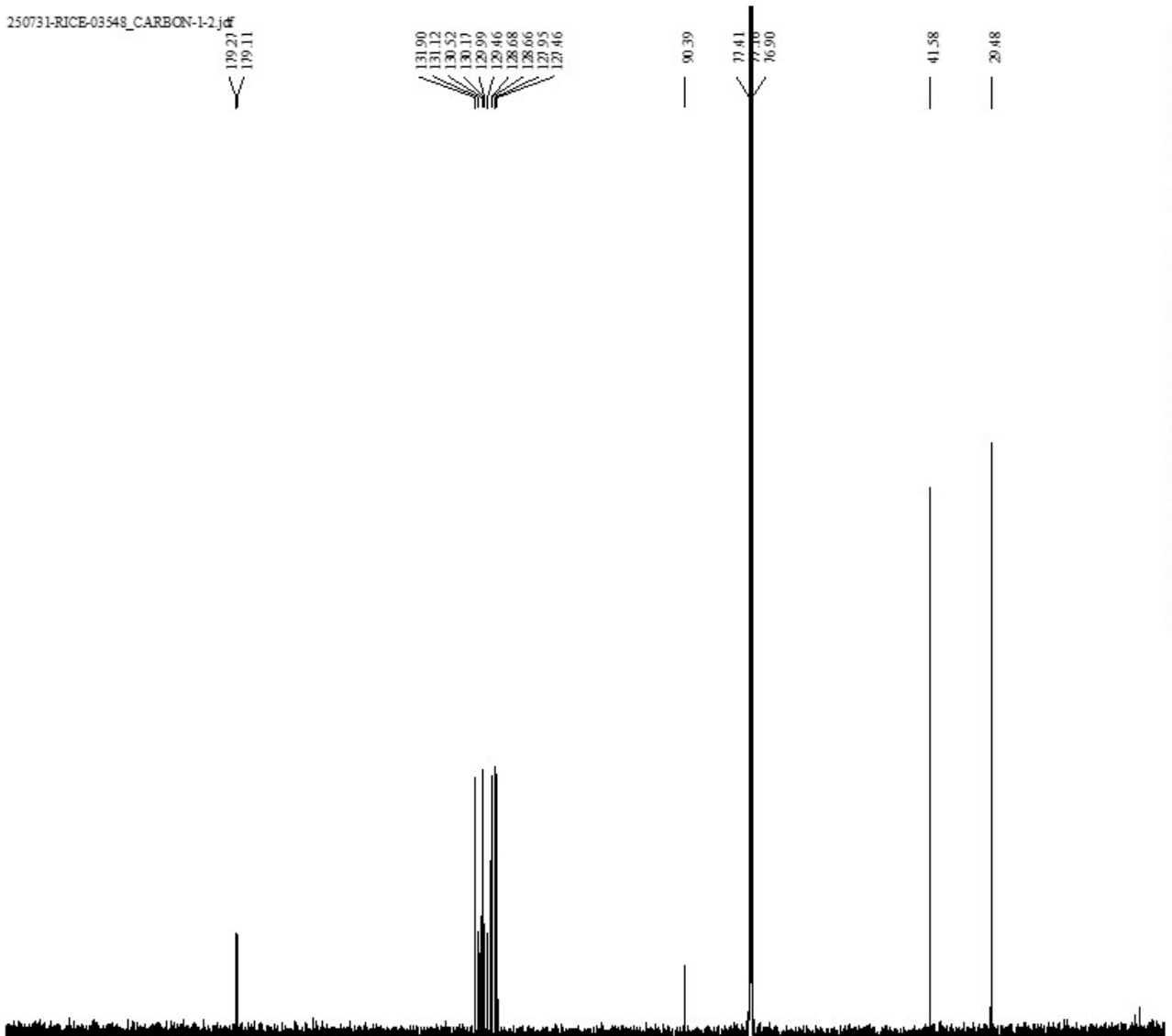

250721-RICE-03545-1_PROTON-1-2.jdf
8.51
8.51
8.45
8.45
8.44
8.44
8.20
8.19
7.93
7.95
7.67
7.66
7.64
7.27
3.86
3.85
3.84
3.84
3.83
3.83
3.81
3.40
3.39
3.37
3.36
3.35
2.95
2.93
2.93
2.92
2.20
2.19
2.18
2.17
1.72
1.25
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250721-RICE-0354
Sample_Id = 250721-RIC
Actual_Start_Time = 21-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 22.2[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Br
O
O
S
3o


250731-RICE-03545_CARBON-1-2.jdf
179.50
178.49
134.08
133.68
131.60
131.41
130.81
129.83
127.99
127.43
127.34
120.76
90.68
77.41
77.10
76.90
41.60
29.48
0.14
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250731-RIC
Actual_Start_Time = 31-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 22.9[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
Br
O
O
S
3o

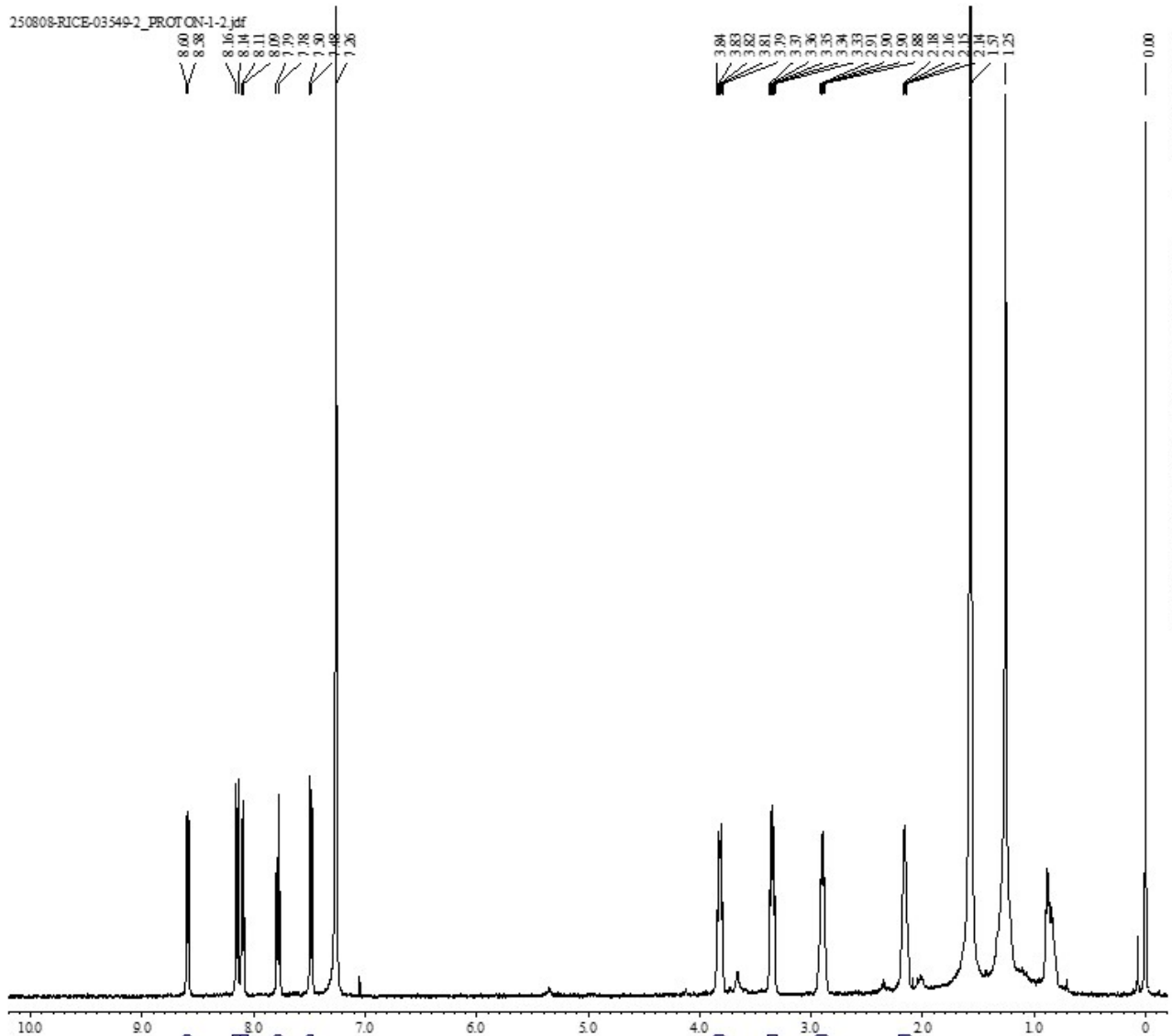

250801-RICE-03548_PROTON-1-2.jdf
8.52
8.51
8.46
8.44
8.29
8.27
7.95
7.94
7.75
7.74
7.72
7.26
3.87
3.86
3.85
3.84
3.82
3.39
3.38
3.37
3.36
3.35
2.95
2.93
2.93
2.92
2.20
2.19
2.18
2.17
1.64
1.26
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250801-RICE-0354
Sample_Id = 250801-RIC
Actual_Start_Time = 1-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 62
Temp_Get = 23.5[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

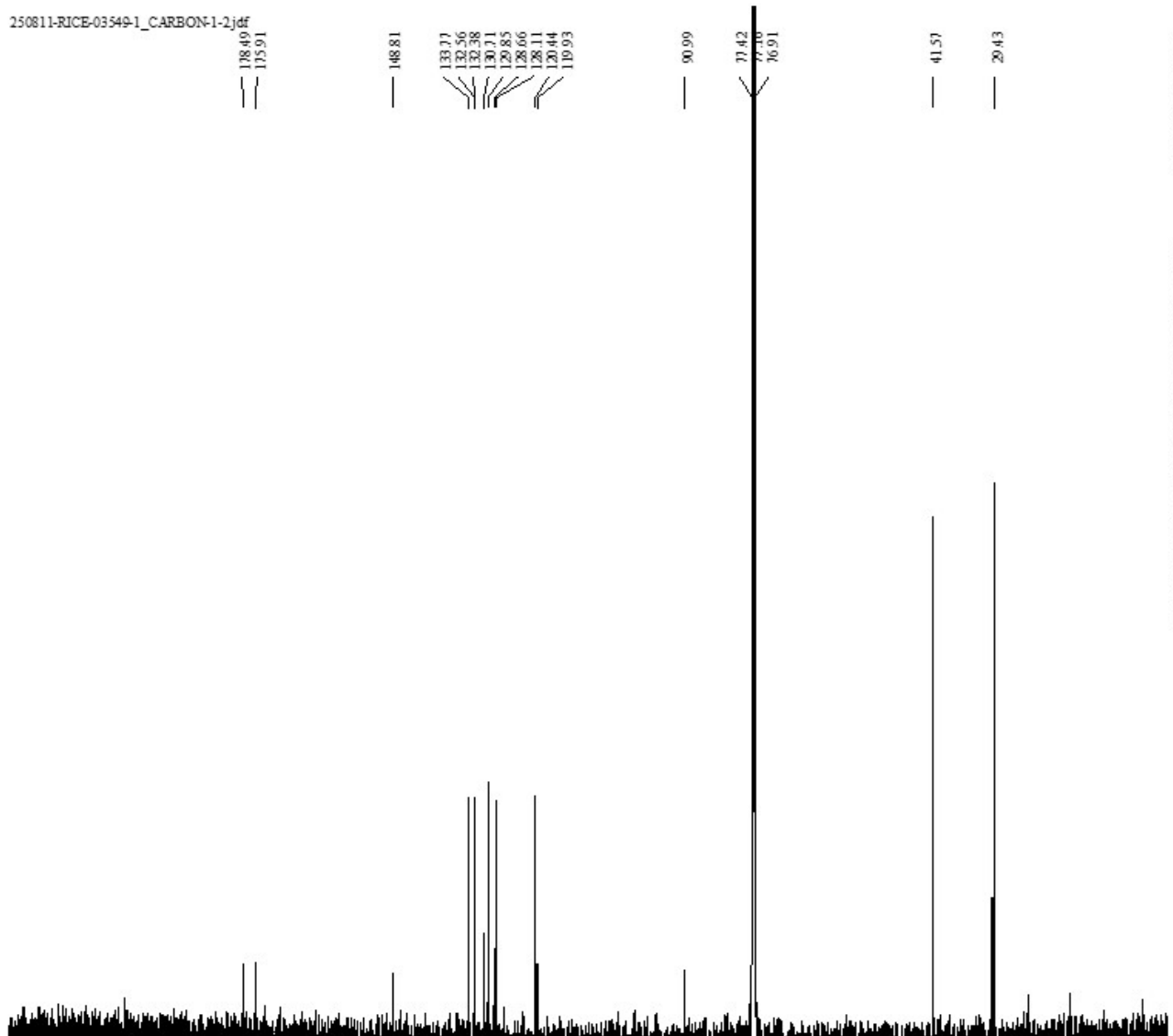

Br
O
S
O

3p

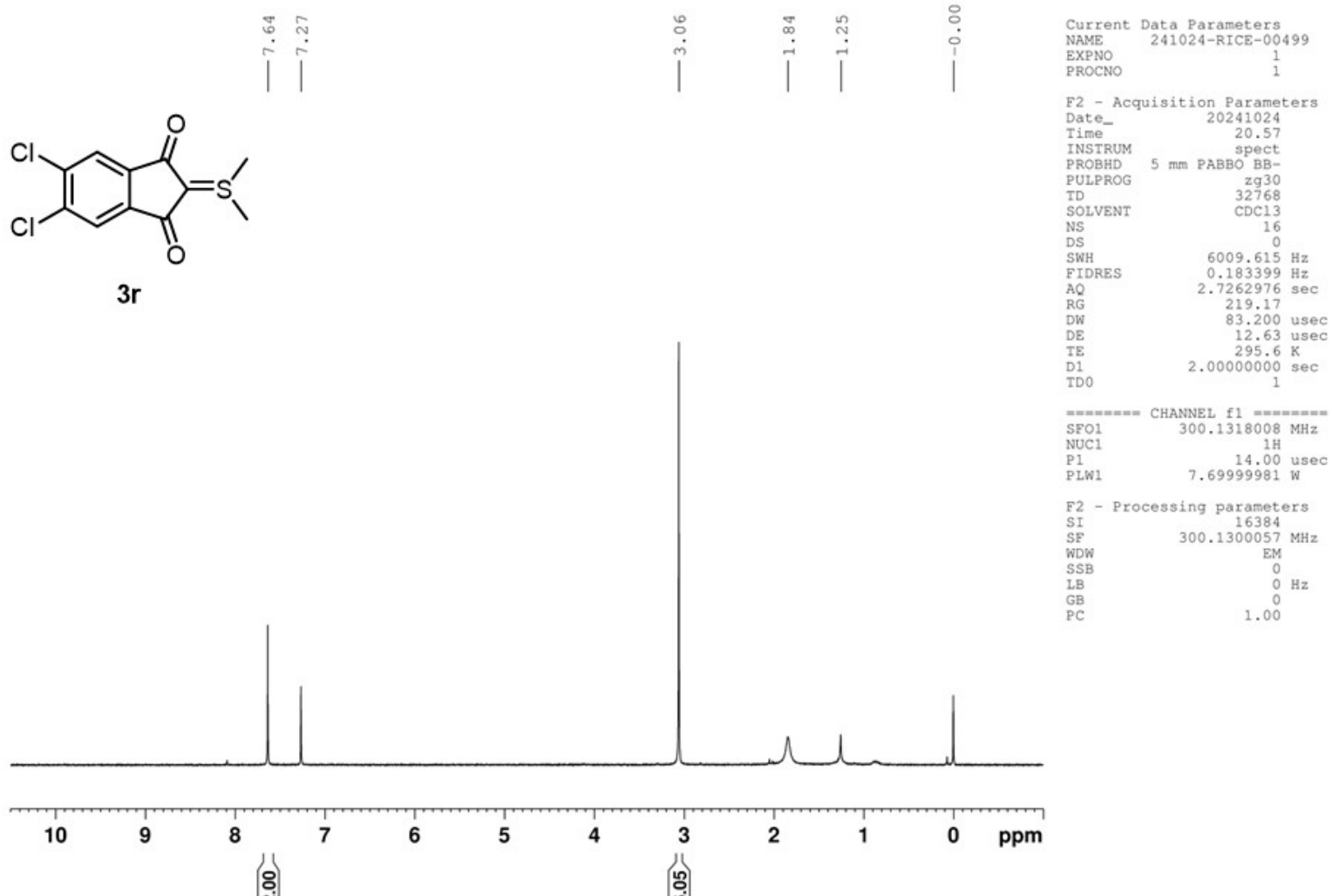

250731-RICE-03548_CARBON-1-2.jdf
179.27
179.11
131.90
131.12
130.52
130.17
129.99
129.46
128.68
128.66
127.95
127.46
90.39
77.41
77.10
76.90
41.58
29.48
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250731-RIC
Actual_Start_Time = 31-JUL-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 23[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
Br
O
S
O

3p


250808-RICE-03549-2_PROTON-1-2.jdf
8.60
8.58
8.16
8.14
8.11
8.09
7.79
7.78
7.50
7.48
7.26
3.84
3.83
3.82
3.81
3.39
3.37
3.36
3.35
3.34
3.33
2.91
2.90
2.90
2.88
2.18
2.16
2.15
2.14
1.57
1.25
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250808-RICE-0354
Sample_Id = 250808-RIC
Actual_Start_Time = 8-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 62
Temp_Get = 22.9[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
NO2
O
O
S
3q

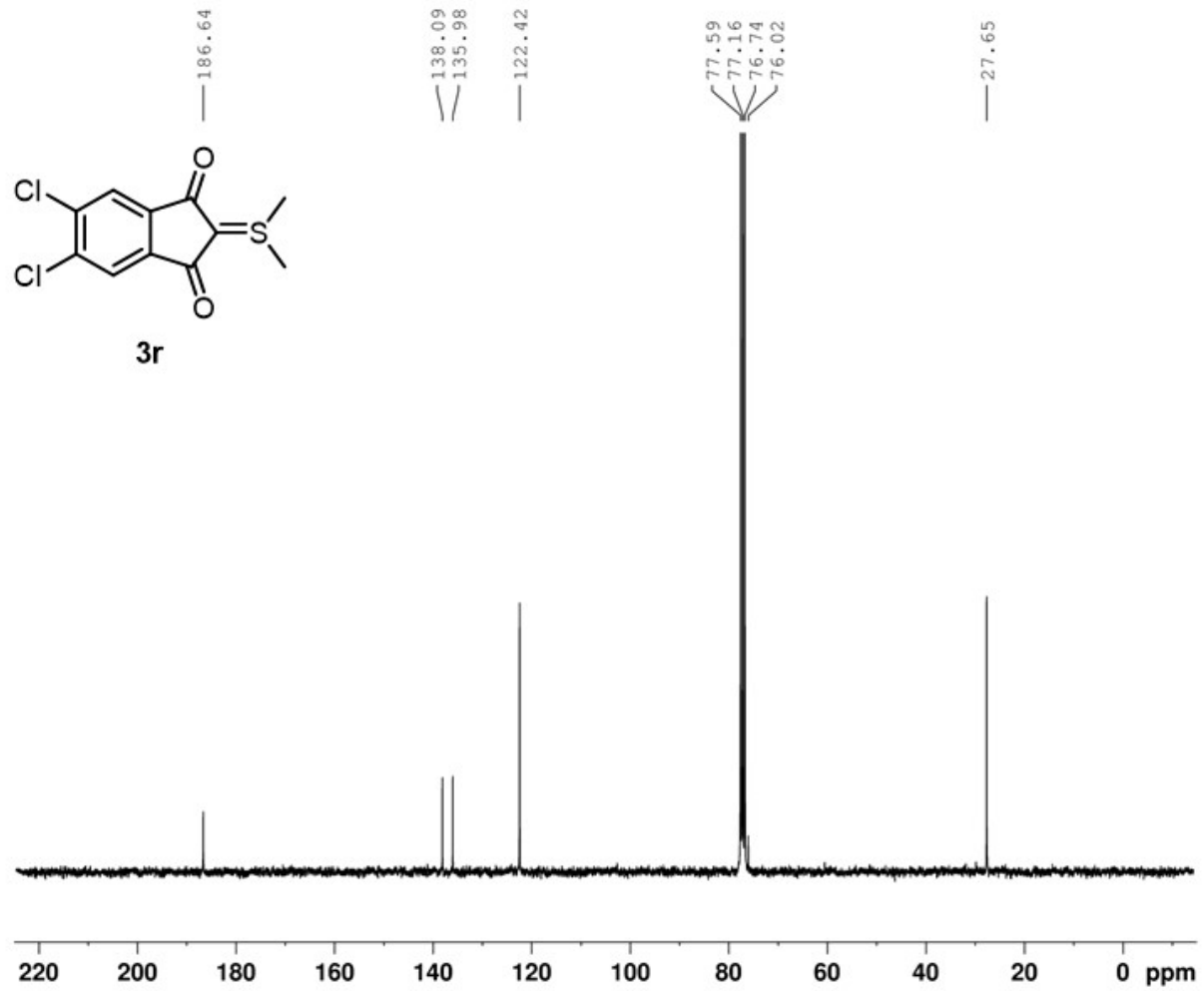

250811-RICE-03549-1_CARBON-1-2.jdf
178.49
175.91
148.81
133.77
132.56
132.38
130.71
129.85
128.66
128.11
120.44
119.93
90.99
77.42
77.00
76.91
41.57
29.43
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(0.57115[%], 0.46102[%]
Sample_Id = 250811-RIC
Actual_Start_Time = 11-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2000
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 23.5[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
NO2
O
O
S
3q

241024-RICE-00499

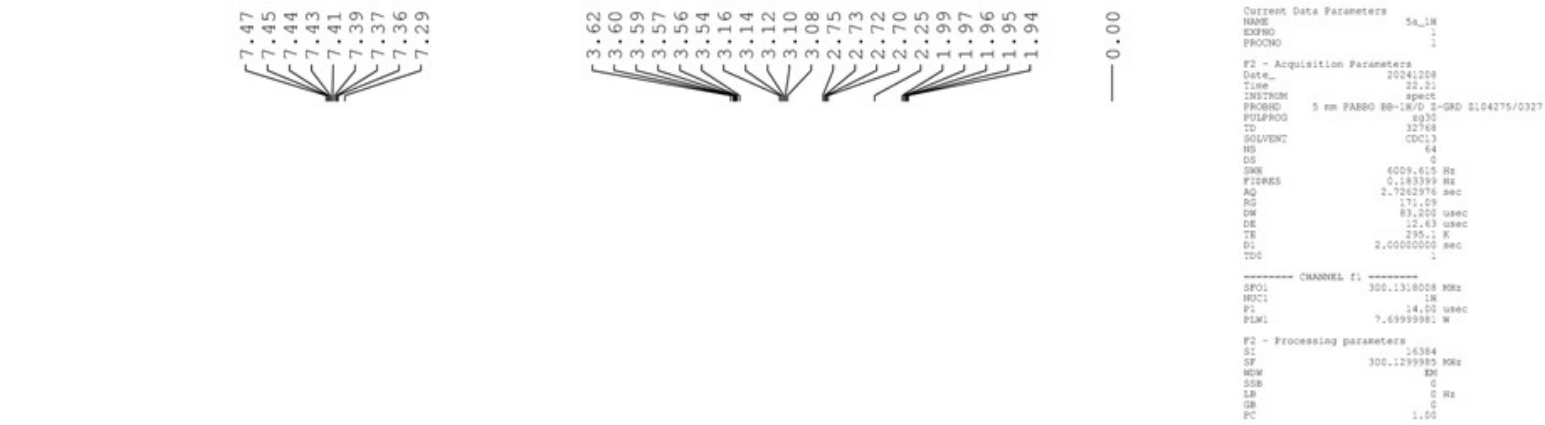



```
Current Data Parameters
NAME      241024-RICE-00499
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20241024
Time                 20.57
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       0
SWH                6009.615 Hz
FIDRES             0.183399 Hz
AQ                 2.7262976 sec
RG                   219.17
DW                   83.200 usec
DE                   12.63 usec
TE                   295.6 K
D1                 2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            300.1318008 MHz
NUC1                    1H
P1                   14.00 usec
PLW1            7.69999981 W

F2 - Processing parameters
SI                   16384
SF              300.1300057 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```

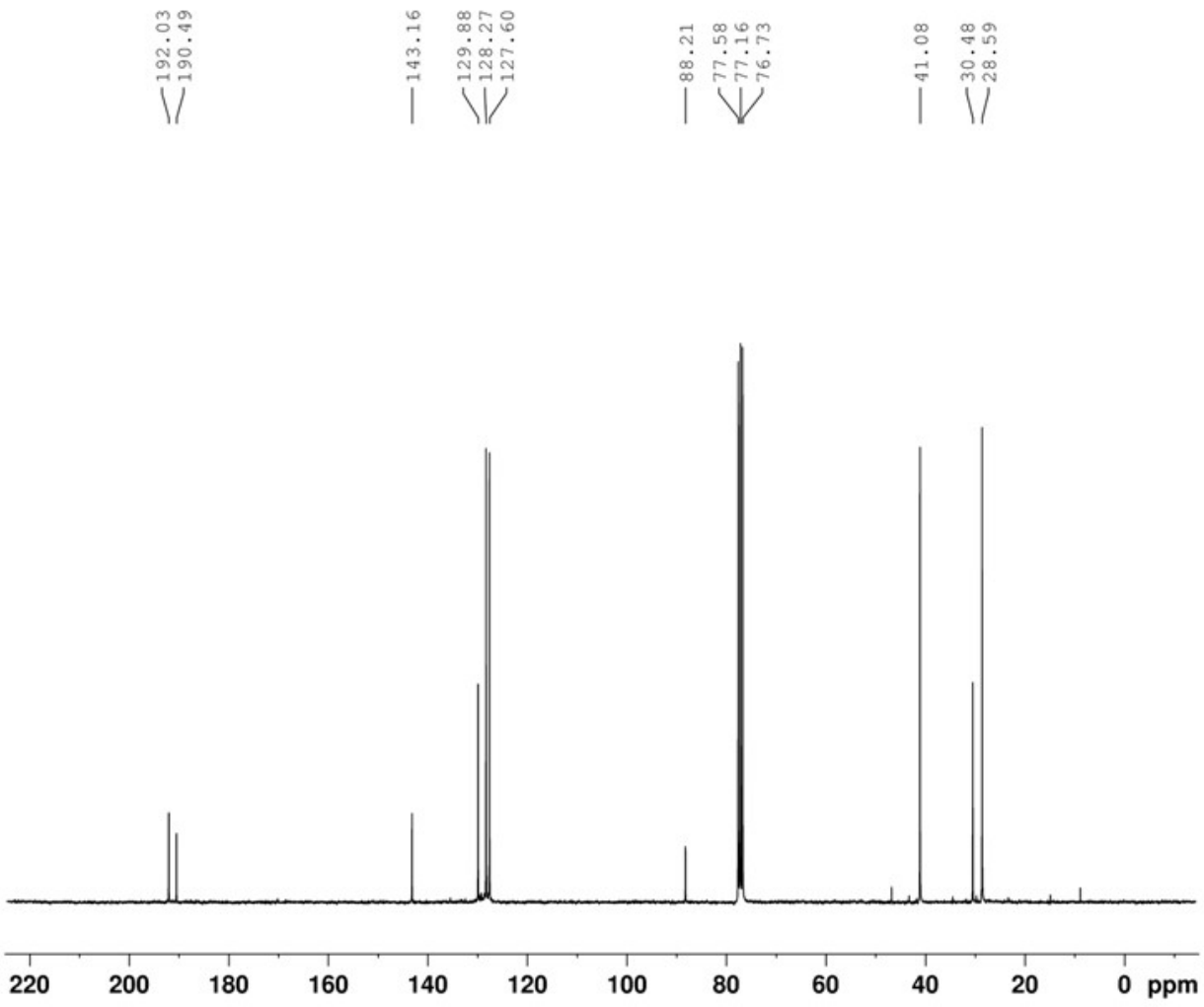
240828-LA-01071-13C



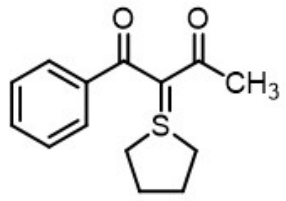

```
Current Data Parameters
NAME      240828-LA-01071-13C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20240828
Time                  17.08
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    1975
DS                       0
SWH              18028.846 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                   27.733 usec
DE                     6.50 usec
TE                   297.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                   13C
P1                   10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                   32768
SF              75.4677390 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```


7.47
7.45
7.44
7.43
7.41
7.39
7.37
7.36
7.29
3.62
3.60
3.59
3.57
3.56
3.54
3.16
3.14
3.12
3.10
3.08
2.75
2.73
2.72
2.70
2.25
1.99
1.97
1.96
1.95
1.94
0.00
Current Data Parameters
NAME 5a_1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20241208
Time 22.21
INSTRUM spect
PROBHD 5 mm PABBO BB-1H/D Z-GRD Z104275/0327
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 171.09
DW 83.200 usec
DE 12.63 usec
TE 295.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318008 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.69999981 W
F2 - Processing parameters
SI 16384
SF 300.1299985 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
3.00
2.02
2.10
2.03
1.05
1.18
O
O
CH3
S

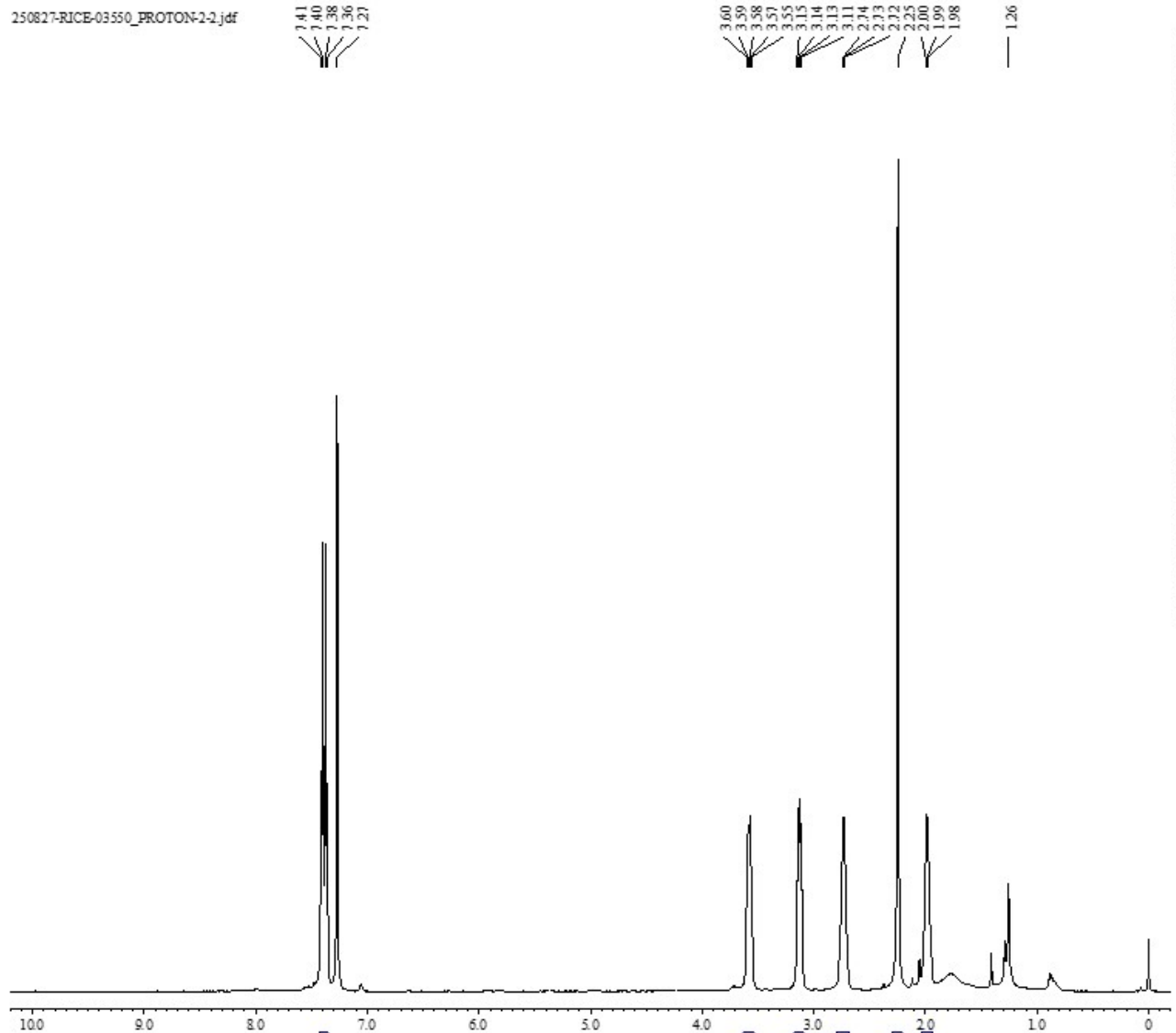
5a



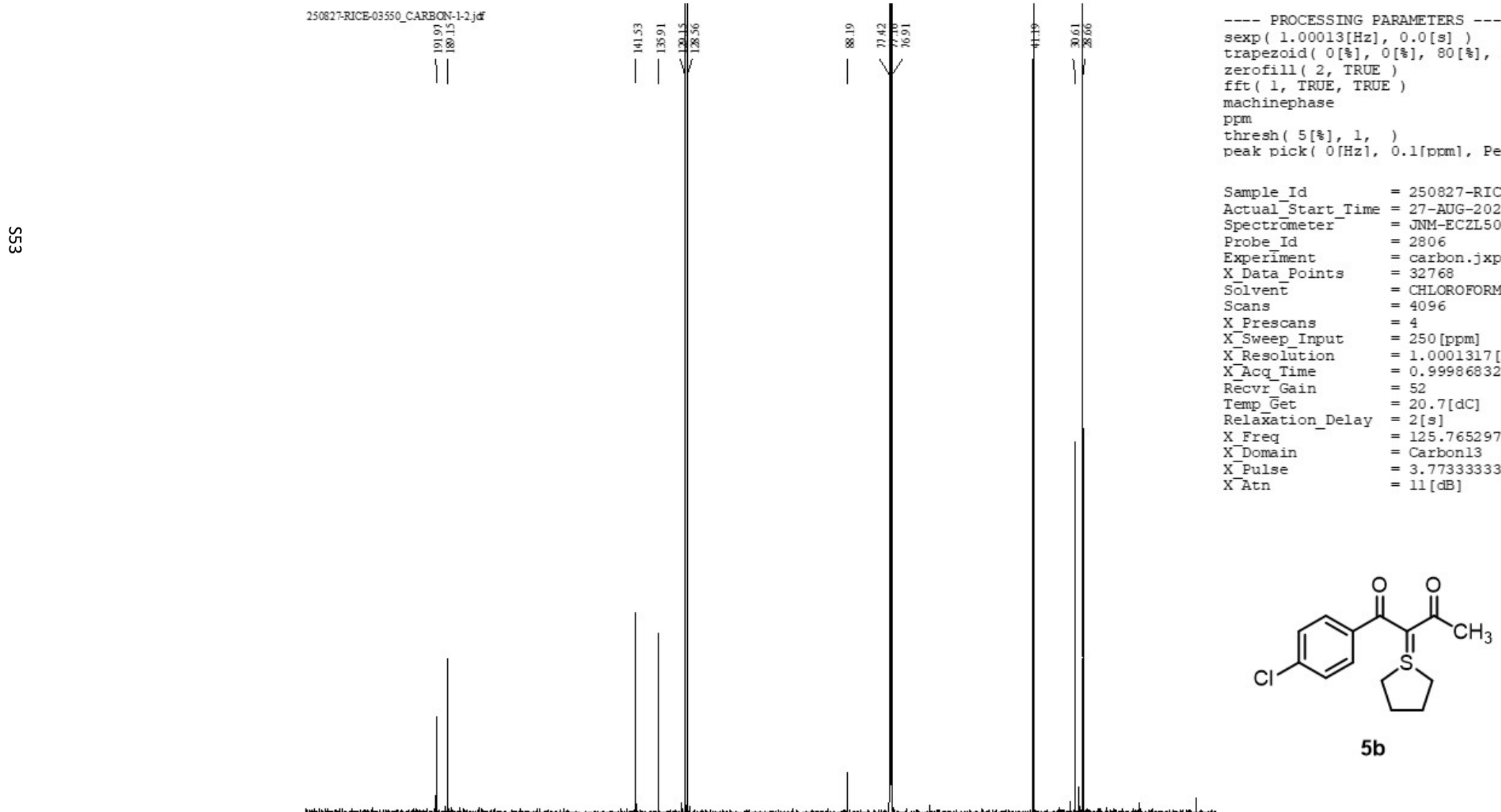

```
Current Data Parameters
NAME                  5a_13C
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20241209
Time                   3.31
INSTRUM                spect
PROBHD     5 mm PABBO BB-1H/D Z-GRD Z104275/0327
PULPROG             zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      6144
DS                         0
SWH                18028.846 Hz
FIDRES              0.550197 Hz
AQ                  0.9087659 sec
RG                     219.17
DW                     27.733 usec
DE                       6.50 usec
TE                      296.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1               75.4756726 MHz
NUC1                     13C
P1                     10.00 usec
PLW1               28.29999924 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2]      bi_waltz65_256
PCPD2                  90.00 usec
PLW2               8.30000019 W
PLW12              0.20084000 W
PLW13              0.16268000 W

F2 - Processing parameters
SI                      32768
SF                 75.4677440 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.00
```



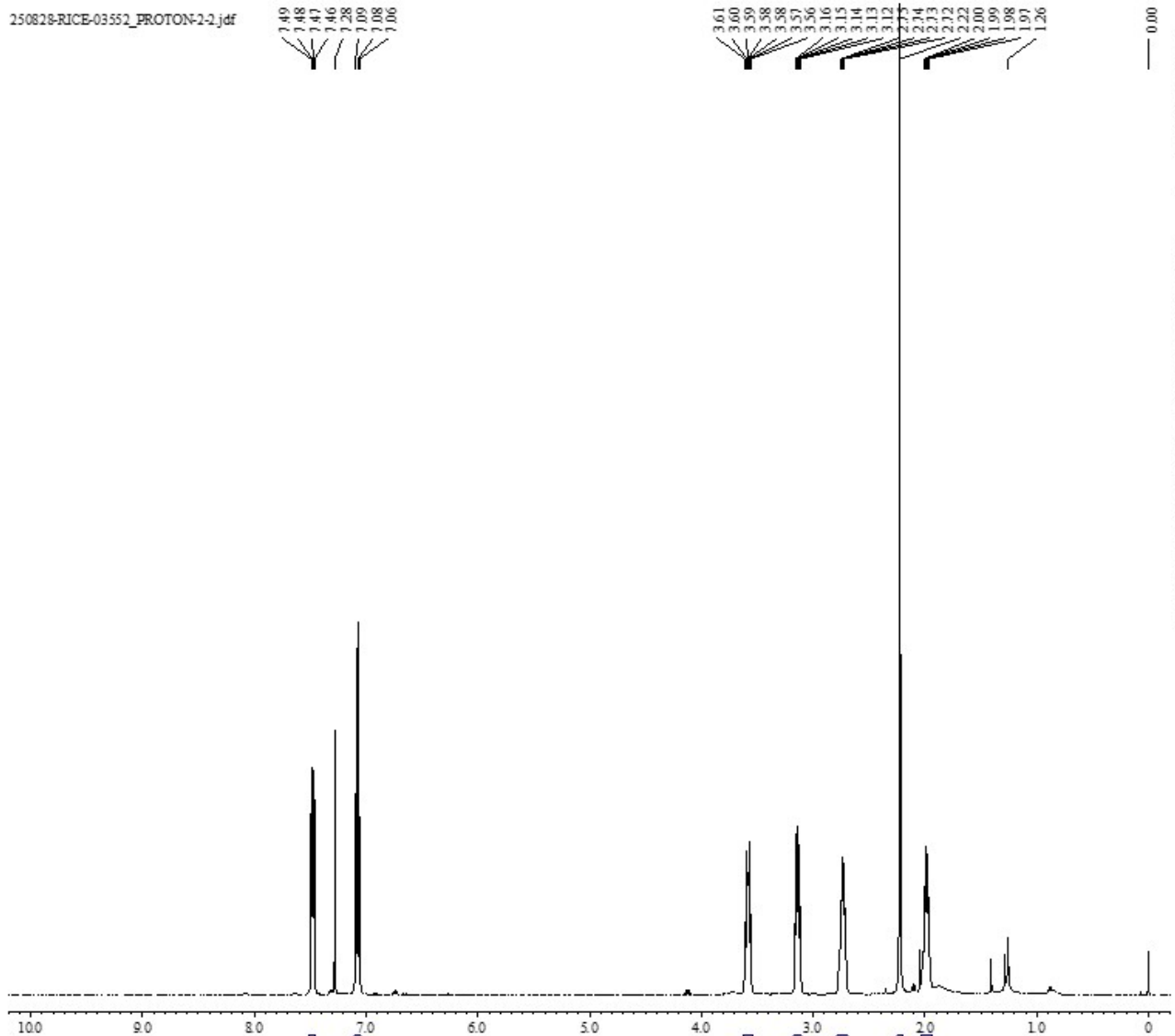
5a


250827-RICE-03550_PROTON-2-2.jdf
7.41
7.40
7.38
7.36
7.27
3.60
3.59
3.58
3.57
3.55
3.15
3.14
3.13
3.11
2.74
2.73
2.72
2.25
2.00
1.99
1.98
1.26
---- PROCESSING PARAMETERS ----
sexp(0.05[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(-0.02445[ppm], 0[pp
phase(0, 0, 43.83703[%])
Sample_Id = 250827-RIC
Actual_Start_Time = 27-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 32
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 20.8[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
O
O
CH3
S
Cl
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

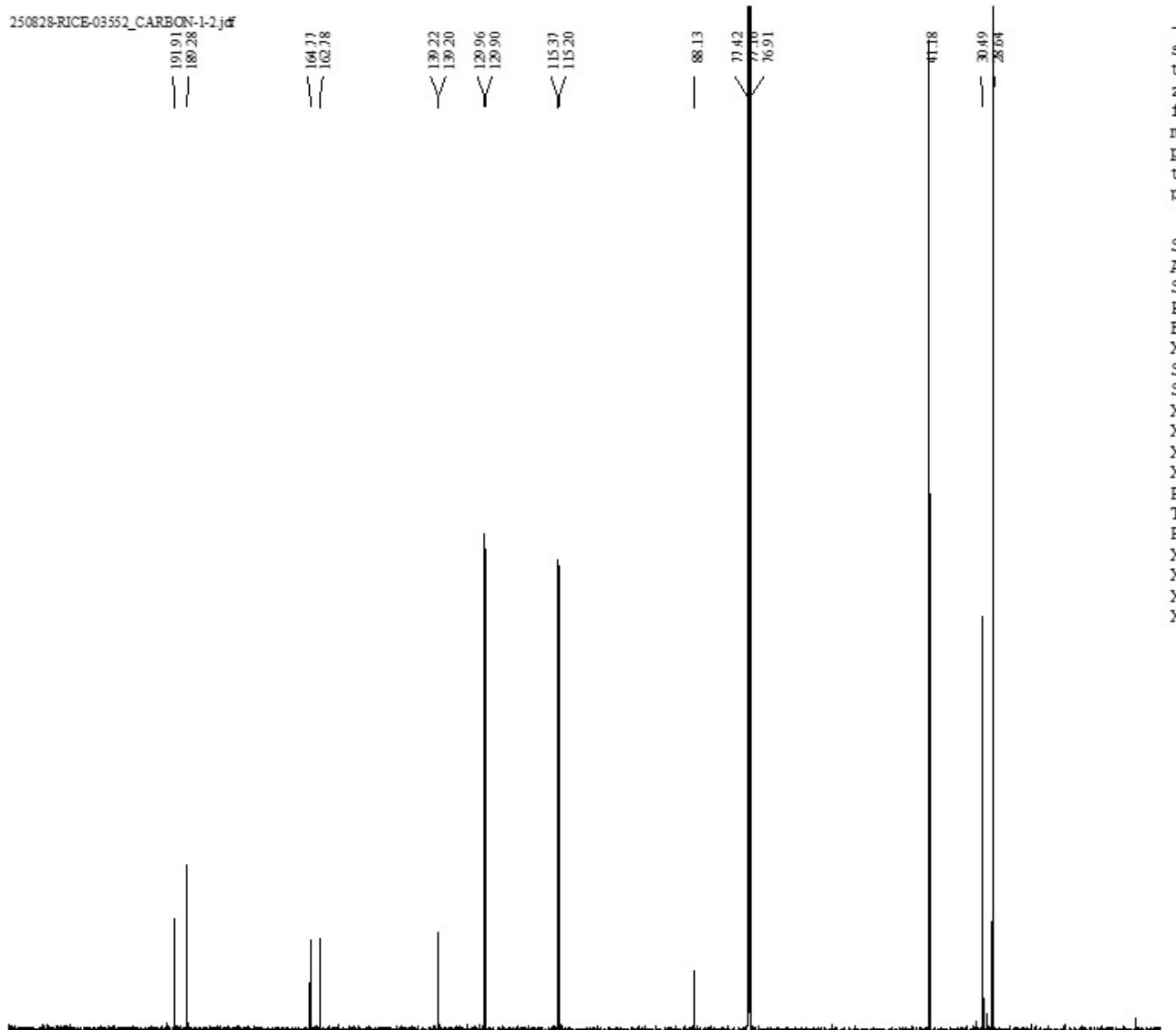
5b


250827-RICE-03550_CARBON-1-2.jdf
191.93
189.15
141.53
135.91
130.15
128.56
88.19
77.42
77.00
76.91
41.19
30.61
28.66
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250827-RIC
Actual_Start_Time = 27-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 4096
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 20.7[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
O
O
CH3
S
Cl

5b


250828-RICE-03552_PROTON-2-2.jdf
7.49
7.48
7.47
7.46
7.28
7.09
7.08
7.06
3.61
3.60
3.59
3.58
3.58
3.57
3.56
3.16
3.15
3.14
3.13
3.12
2.75
2.24
2.23
2.22
2.00
1.99
1.98
1.93
1.26
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250828-RICE-0355
Sample_Id = 250828-RIC
Actual_Start_Time = 28-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 64
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 20.6[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
O
O
CH3
S
F
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0

5c

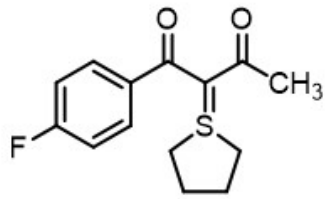

250828-RICE-03552_CARBON-1-2.jdf
191.91
189.28
164.77
162.78
130.22
130.20
129.96
129.90
115.33
115.20
88.13
77.42
77.00
76.91
41.18
30.49
28.04
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250828-RIC
Actual_Start_Time = 28-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 2048
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 20.6[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
O
O
CH3
S
F

5c

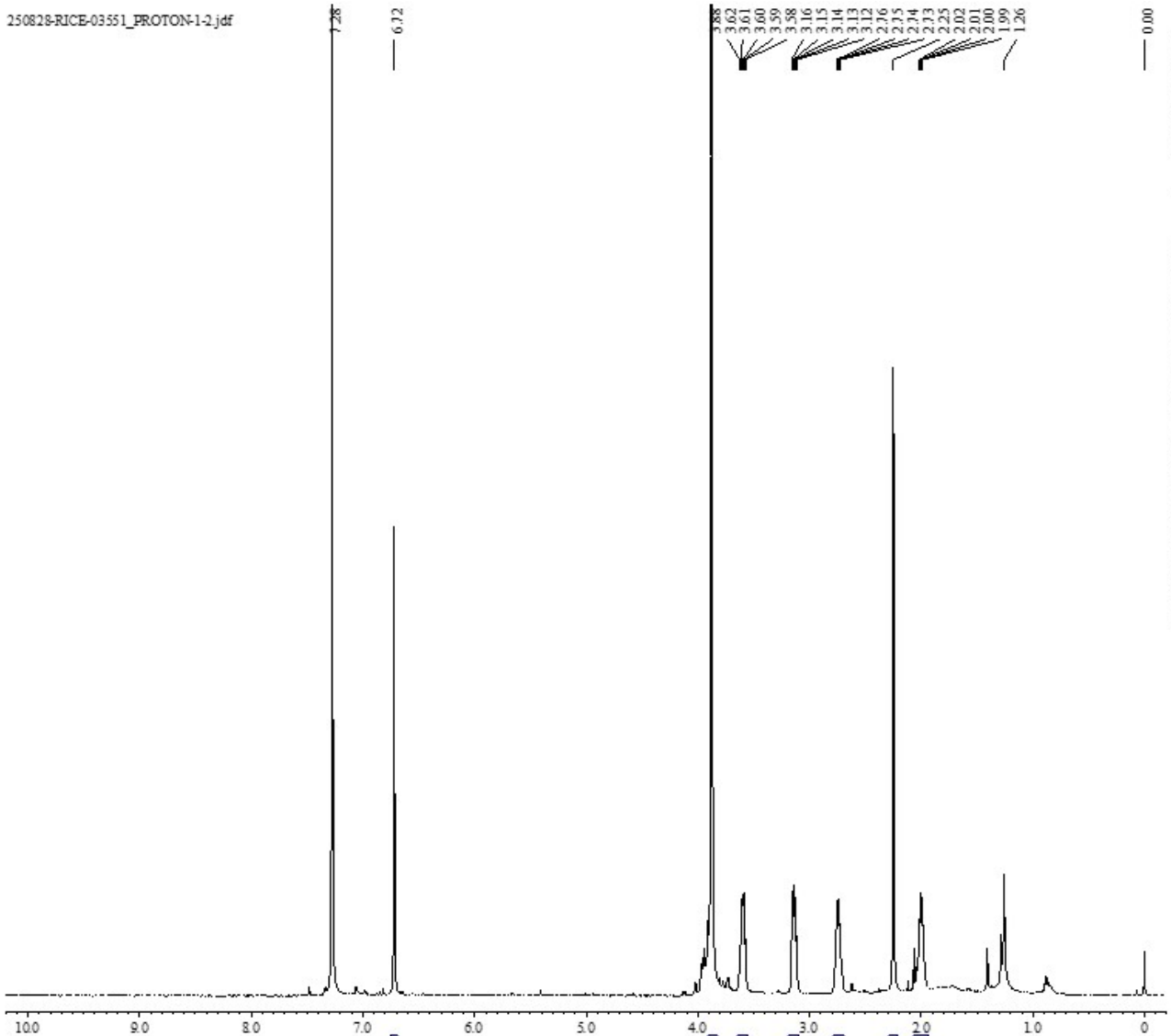
250829-rice-03552_Fluorine-1-2.jdf

-110.28

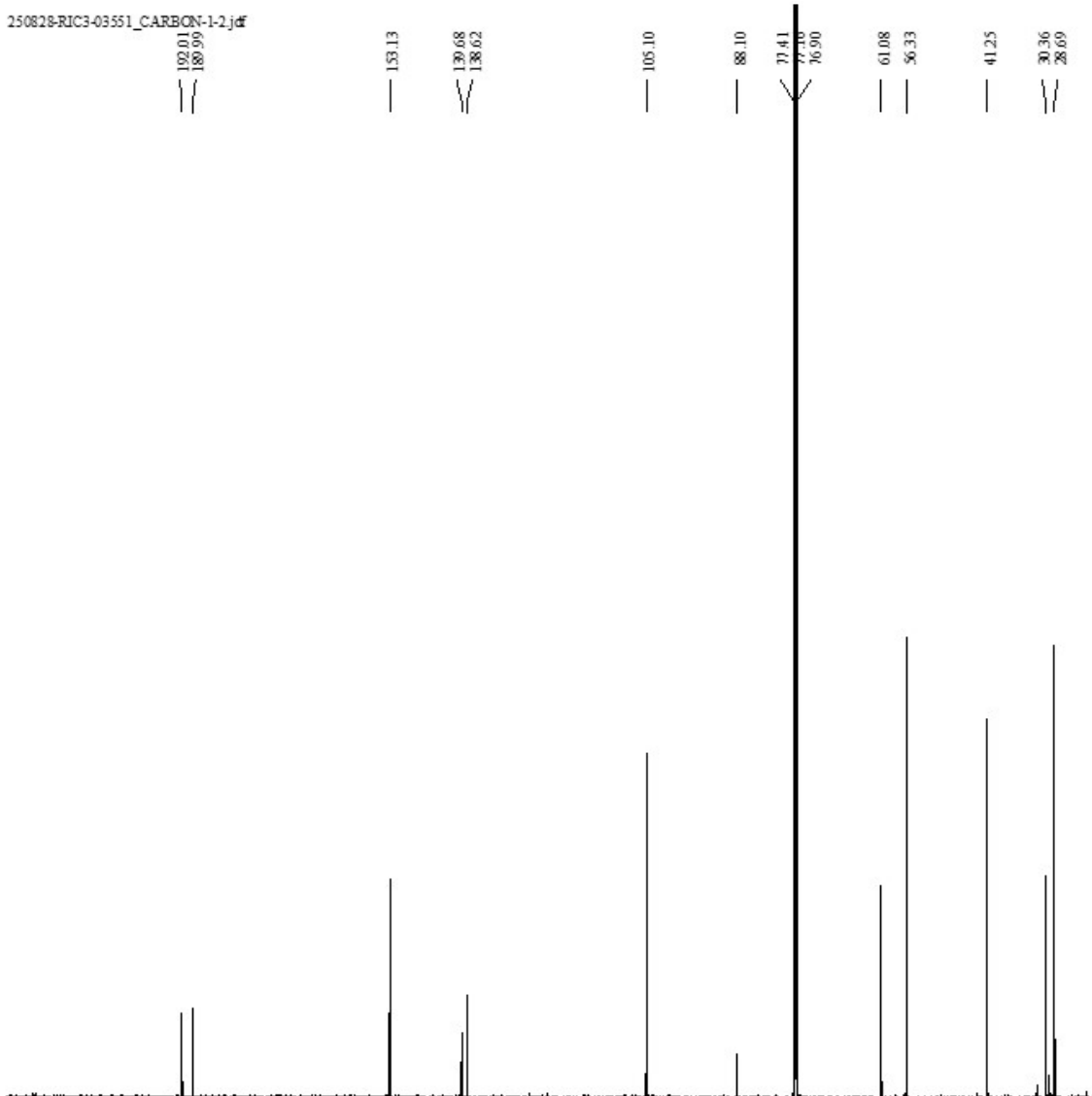
```
---- PROCESSING PARAMETERS ----
sexp( 0.48777[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%],
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 250829-rice-0355

Sample_Id          = 250829-ric
Actual_Start_Time  = 29-AUG-202
Spectrometer       = JNM-ECZL50
Probe_Id           = 2806
Experiment         = single_pul
X_Data_Points      = 65536
Solvent            = CHLOROFORM
Scans              = 64
X_Prescans         = 0
X_Sweep_Input      = 199[ppm]
X_Resolution       = 0.48776943
X_Acq_Time         = 2.050149[s
Recvr_Gain         = 52
Temp_Get           = 20.9[dC]
Relaxation_Delay   = 4[s]
X_Freq             = 470.620460
X_Domain           = Fluorine19
X_Pulse            = 3.89[us]
X_Atn              = 8.7[dB]
```



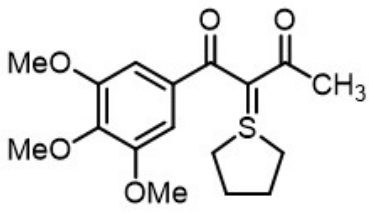
5c


250828-RICE-03551_PROTON-1-2.jdf
7.28
6.72
3.63
3.62
3.61
3.60
3.59
3.58
3.16
3.15
3.14
3.13
3.12
2.76
2.75
2.74
2.73
2.25
2.02
2.01
2.00
1.99
1.26
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250828-RICE-0355
Sample_Id = 250828-RIC
Actual_Start_Time = 28-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 16
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 20.9[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
MeO
MeO
OMe
O
O
CH3
S

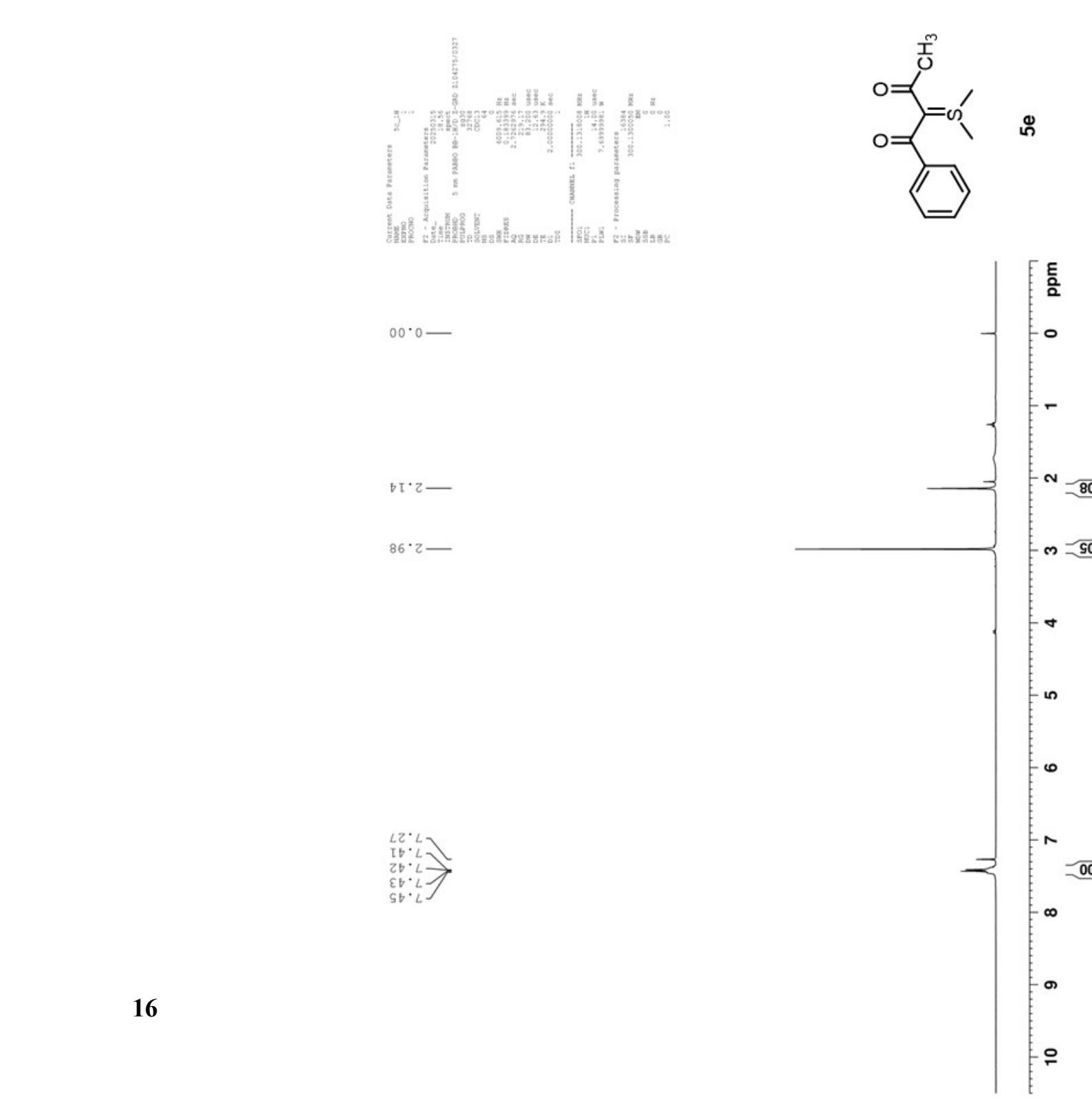
5d



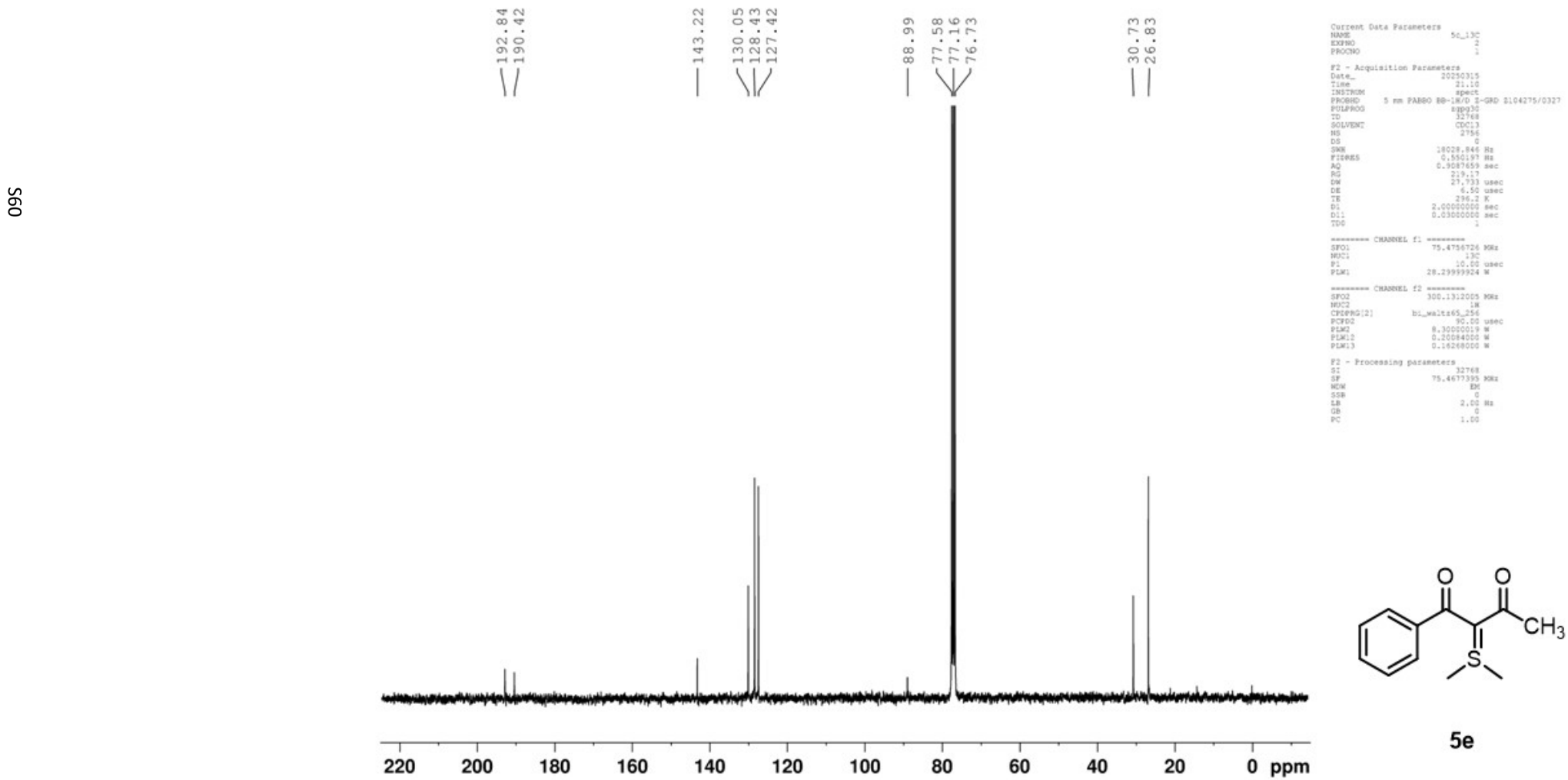

```
---- PROCESSING PARAMETERS ----
sexp( 1.00013[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%],
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1,  )
peak pick( 0[Hz], 0.1[ppm], Pe

Sample_Id          = 250828-RIC
Actual_Start_Time  = 28-AUG-202
Spectrometer       = JNM-ECZL50
Probe_Id           = 2806
Experiment         = carbon.jxp
X_Data_Points      = 32768
Solvent            = CHLOROFORM
Scans              = 4096
X_Prescans         = 4
X_Sweep_Input      = 250[ppm]
X_Resolution       = 1.0001317[
X_Acq_Time         = 0.99986832
Recvr_Gain         = 52
Temp_Get           = 20.8[dC]
Relaxation_Delay   = 2[s]
X_Freq             = 125.765297
X_Domain           = Carbon13
X_Pulse            = 3.77333333
X_Atn              = 11[dB]
```



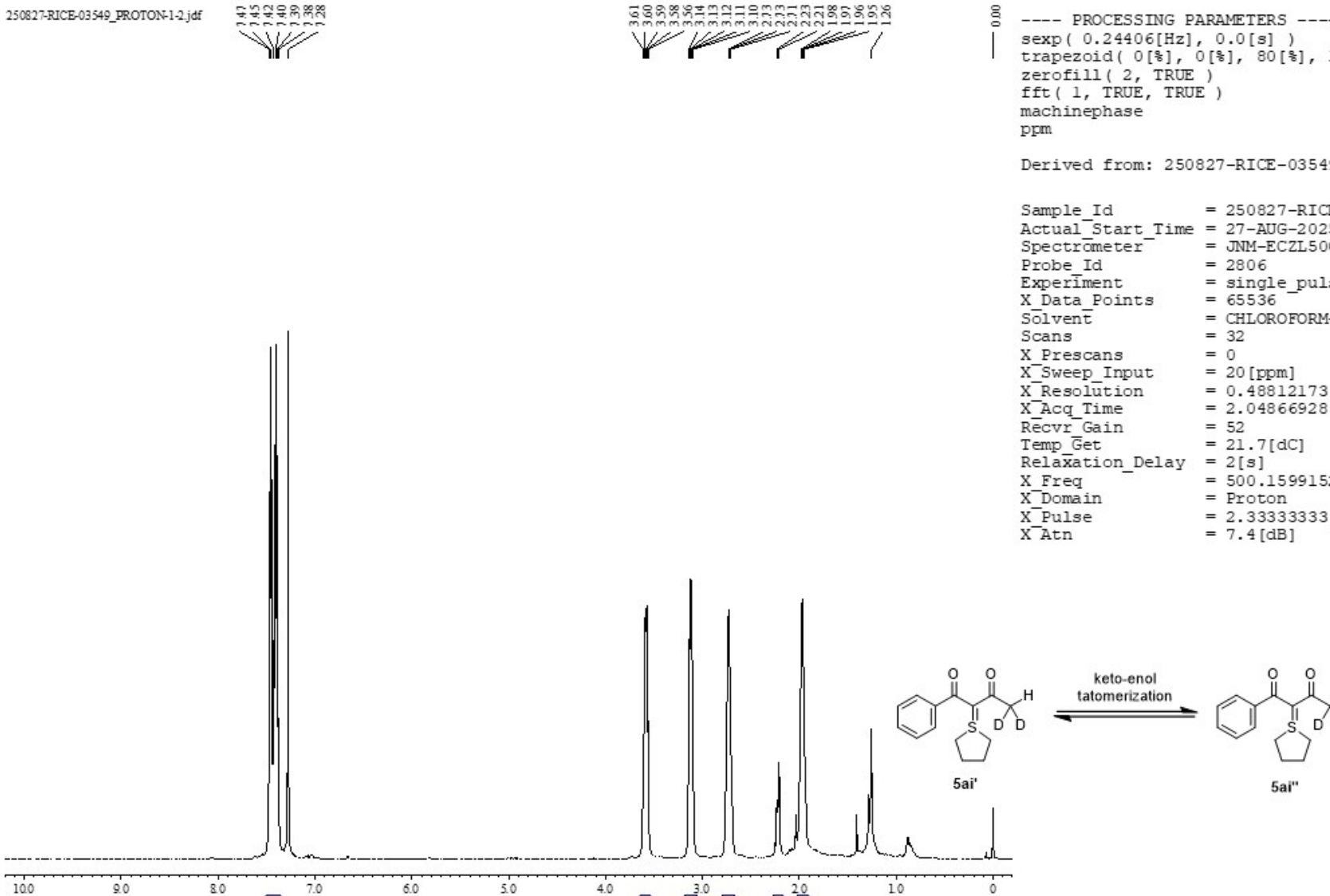
5d

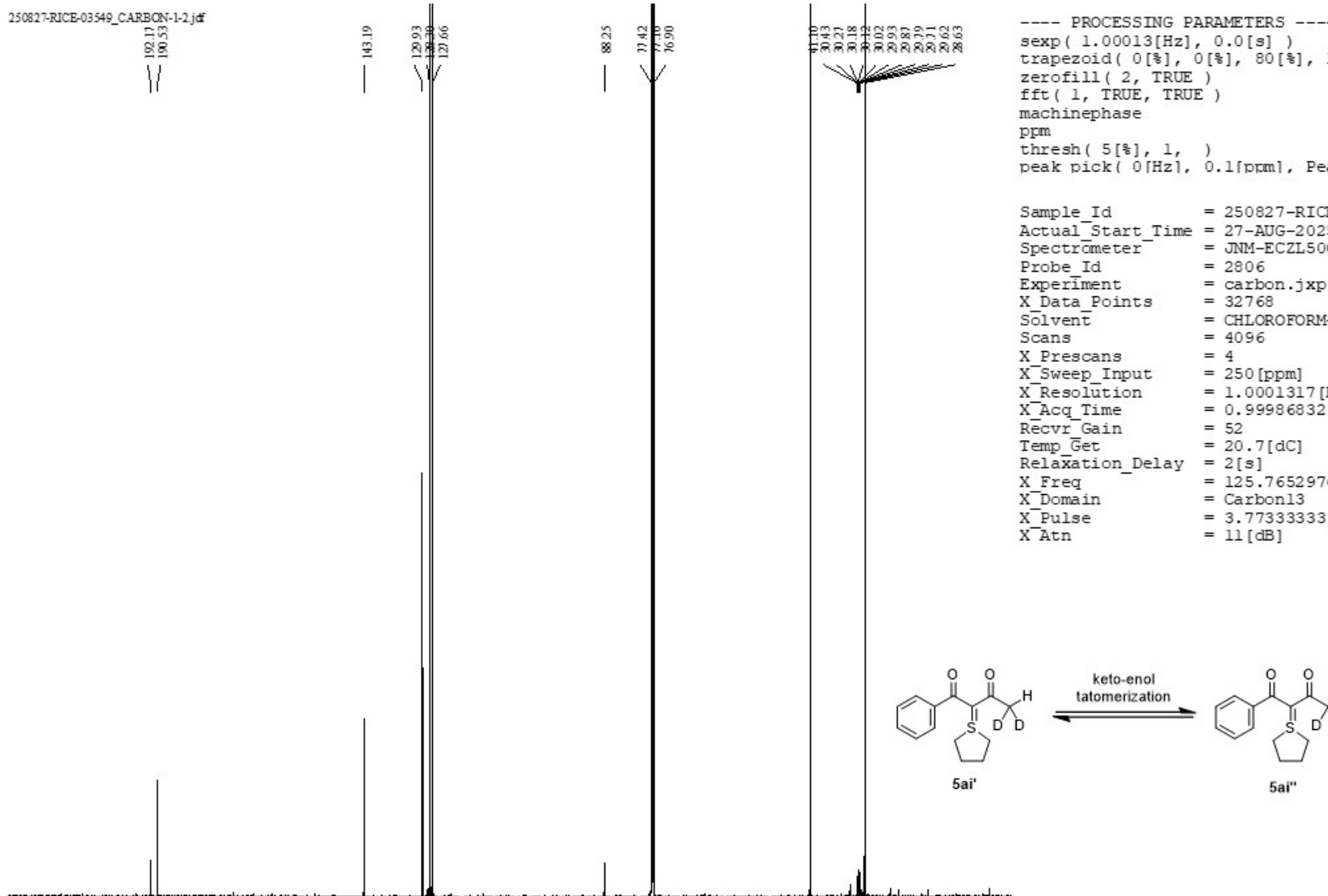


16

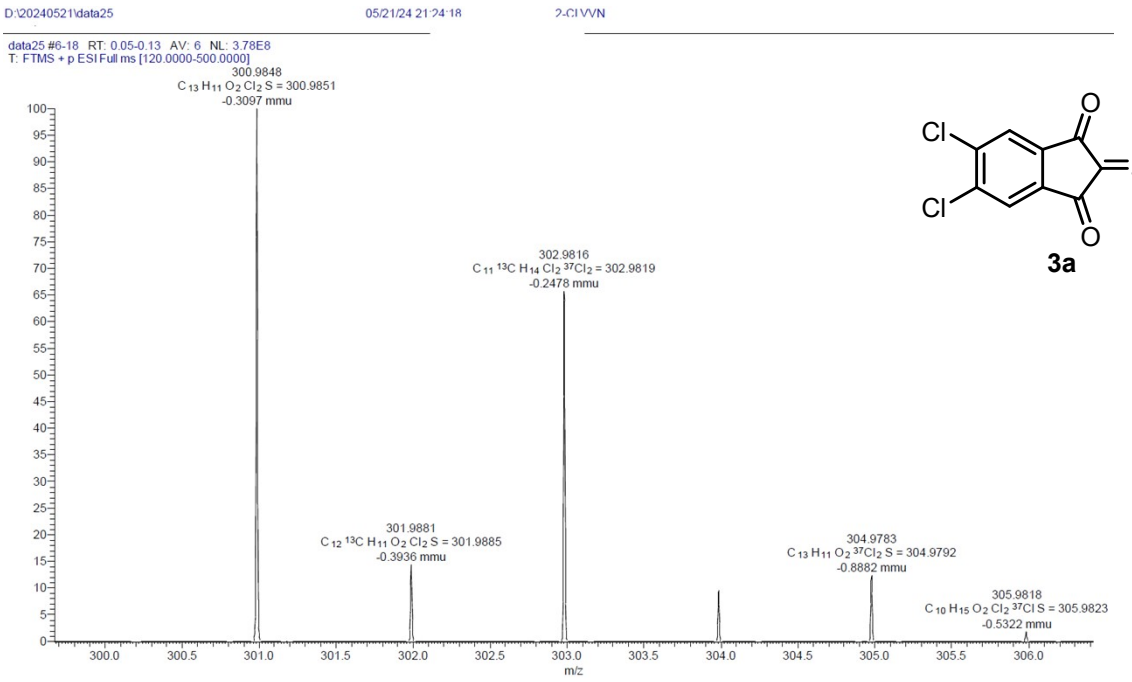

192.84
190.42
143.22
130.05
128.43
127.42
88.99
77.58
77.16
76.73
30.73
26.83
220
200
180
160
140
120
100
80
60
40
20
0 ppm
Current Data Parameters
NAME 5c_13C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20250315
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBO BB-1H/D Z-GRD Z104275/0327
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2756
DS 0
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 219.17
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4756726 MHz
NUC1 13C
P1 10.00 usec
PLW1 28.29999924 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] bi_waltz65_256
PCPD2 90.00 usec
PLW2 8.30000019 W
PLW12 0.20084000 W
PLW13 0.16268000 W
F2 - Processing parameters
SI 32768
SF 75.4677395 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
O
O
CH3
S

5e


250827-RICE-03549_PROTON-1-2.jdf
7.47
7.45
7.42
7.40
7.39
7.38
7.28
3.61
3.60
3.59
3.58
3.56
3.14
3.13
3.12
3.11
3.10
2.73
2.73
2.71
2.23
2.21
1.98
1.97
1.96
1.95
1.26
0.00
---- PROCESSING PARAMETERS ----
sexp(0.24406[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 250827-RICE-0354
Sample_Id = 250827-RIC
Actual_Start_Time = 27-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = single_pul
X_Data_Points = 65536
Solvent = CHLOROFORM
Scans = 32
X_Prescans = 0
X_Sweep_Input = 20[ppm]
X_Resolution = 0.48812173
X_Acq_Time = 2.04866928
Recvr_Gain = 52
Temp_Get = 21.7[dC]
Relaxation_Delay = 2[s]
X_Freq = 500.159915
X_Domain = Proton
X_Pulse = 2.33333333
X_Atn = 7.4[dB]
keto-enol
tatomerization
5ai'
5ai''
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0


250827-RICE-03549_CARBON-1-2.jdf
192.17
190.53
143.19
129.93
128.66
127.66
88.25
77.42
77.10
76.90
41.10
30.43
30.27
30.18
30.12
30.02
29.93
29.87
29.79
29.71
29.62
28.63
---- PROCESSING PARAMETERS ----
sexp(1.00013[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%],
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1,)
peak pick(0[Hz], 0.1[ppm], Pe
Sample_Id = 250827-RIC
Actual_Start_Time = 27-AUG-202
Spectrometer = JNM-ECZL50
Probe_Id = 2806
Experiment = carbon.jxp
X_Data_Points = 32768
Solvent = CHLOROFORM
Scans = 4096
X_Prescans = 4
X_Sweep_Input = 250[ppm]
X_Resolution = 1.0001317[
X_Acq_Time = 0.99986832
Recvr_Gain = 52
Temp_Get = 20.7[dC]
Relaxation_Delay = 2[s]
X_Freq = 125.765297
X_Domain = Carbon13
X_Pulse = 3.77333333
X_Atn = 11[dB]
keto-enol
tatomerization
5ai'
5ai''

5. HRMS Spectra



3a

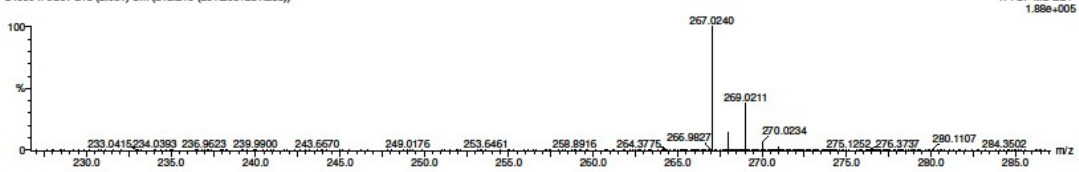
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

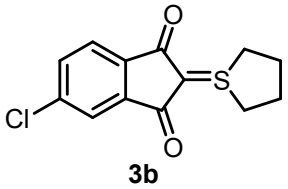
Monoisotopic Mass, Even Electron Ions
178 formula(e) evaluated with 117 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Cl: 1-3

Rice-00473
240904FJU07 213 (2.081) Cm (212:216-(201:205+231:235))

1: TOF MS ES+
1.88e+005



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
267.0240	100.00	267.0247	-0.7	-2.6	7.5	C13 H12 O2 S Cl
		267.0225	1.5	5.6	-1.5	C7 H17 O4 S Cl2
		267.0258	-1.8	-6.7	-6.5	C4 H21 O4 S2 Cl2
		267.0280	-4.0	-15.0	2.5	C10 H16 O2 S2 Cl
		267.0178	6.2	23.2	-6.5	C5 H22 O S2 Cl3
		267.0305	-6.5	-24.3	-1.5	C6 H16 O7 S Cl
		267.0314	-7.4	-27.7	-2.5	C7 H20 O2 S3 Cl
		267.0161	7.9	29.6	-6.5	C3 H20 O5 S3 Cl
		267.0153	8.7	32.6	-5.5	C2 H16 O10 S Cl
		267.0144	9.6	36.0	-1.5	C8 H18 O S Cl3
		267.0339	-9.9	-37.1	-6.5	C3 H20 O7 S2 Cl
		267.0128	11.2	41.9	-1.5	C6 H16 O5 S2 Cl
		267.0355	-11.5	-43.1	-6.5	C5 H22 O3 S Cl3
		267.0377	-13.7	-51.3	2.5	C11 H17 O S Cl2
		267.0094	14.6	54.7	3.5	C9 H12 O5 S Cl
		267.0081	15.9	59.5	-6.5	C4 H21 O2 S3 Cl2
		267.0072	16.8	62.9	-5.5	C3 H17 O7 S Cl2
		267.0411	-17.1	-64.0	-2.5	C8 H21 O S2 Cl2
		267.0047	19.3	72.3	-1.5	C7 H17 O2 S2 Cl2
		267.0436	-19.6	-73.4	-6.5	C4 H21 O6 S Cl2



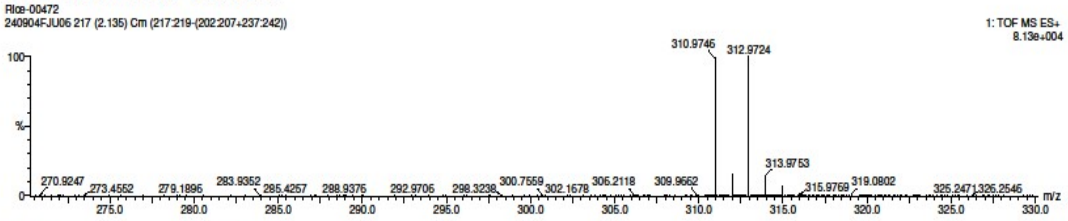
3b

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

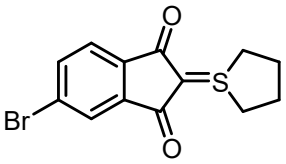
Monoisotopic Mass, Even Electron Ions
107 formula(e) evaluated with 82 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Br: 1-3

Rice-00472
240904FJU06 217 (2.135) Cm (217:219-(202:207+237:242))



Minimum:			-10.0		
Maximum:		10.0	500.0	100.0	

Mass	Calc. Mass	mDa	PPM	DBE	Formula
310.9746	310.9741	0.5	1.6	7.5	C13 H12 O2 S Br
	310.9775	-2.9	-9.3	2.5	C10 H16 O2 S2 Br
	310.9714	3.2	10.3	-8.5	C4 H25 O S2 Br2
	310.9800	-5.4	-17.4	-1.5	C6 H16 O7 S Br
	310.9809	-6.3	-20.3	-2.5	C7 H20 O2 S3 Br
	310.9680	6.6	21.2	-3.5	C7 H21 O S Br2
	310.9834	-8.8	-28.3	-6.5	C3 H20 O7 S2 Br
	310.9656	9.0	28.9	-6.5	C3 H20 O5 S3 Br
	310.9648	9.8	31.5	-5.5	C2 H16 O10 S Br
	310.9623	12.3	39.6	-1.5	C6 H16 O5 S2 Br
	310.9891	-14.5	-46.6	-8.5	C4 H25 O3 S Br2
	310.9589	15.7	50.5	3.5	C9 H12 O5 S Br
	310.9953	-20.7	-66.6	2.5	C10 H16 O4 S Br
	310.9527	21.9	70.4	-7.5	C3 H21 O4 S Br2
	310.9986	-24.0	-77.2	-2.5	C7 H20 O4 S2 Br
	311.0011	-26.5	-85.2	-6.5	C3 H20 O9 S Br
	311.0020	-27.4	-88.1	-7.5	C4 H24 O4 S3 Br
	310.9470	27.6	88.8	-5.5	C2 H16 O8 S2 Br
	310.9445	30.1	96.8	-1.5	C6 H16 O3 S3 Br
	310.9436	31.0	99.7	-0.5	C5 H12 O8 S Br



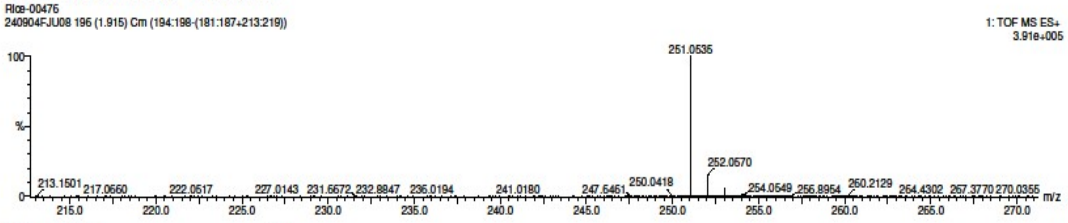
3c

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

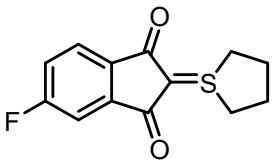
Monoisotopic Mass, Even Electron Ions
207 formula(e) evaluated with 145 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 F: 1-3 S: 1-3

Rice-00476
240904FJU08 196 (1.915) Cm (194:198-(181:187+213:219))



Minimum:	80.00			-10.0		
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
251.0535	100.00	251.0542	-0.7	-2.8	7.5	C13 H12 O2 F S
		251.0553	-1.8	-7.2	3.5	C10 H13 O3 F2 S
		251.0565	-3.0	-11.9	-0.5	C7 H14 O4 F3 S
		251.0576	-4.1	-16.3	2.5	C10 H16 O2 F S2
		251.0587	-5.2	-20.7	-1.5	C7 H17 O3 F2 S2
		251.0599	-6.4	-25.5	-5.5	C4 H18 O4 F3 S2
		251.0601	-6.6	-26.3	-1.5	C6 H16 O7 F S
		251.0609	-7.4	-29.5	-2.5	C7 H20 O2 F S3
		251.0612	-7.7	-30.7	-5.5	C3 H17 O8 F2 S
		251.0457	7.8	31.1	-6.5	C3 H20 O5 F S3
		251.0621	-8.6	-34.3	-6.5	C4 H21 O3 F2 S3
		251.0448	8.7	34.7	-5.5	C2 H16 O10 F S
		251.0634	-9.9	-39.4	-6.5	C3 H20 O7 F S2
		251.0435	10.0	39.8	-5.5	C3 H17 O6 F2 S2
		251.0423	11.2	44.6	-1.5	C6 H16 O5 F S2
		251.0421	11.4	45.4	-5.5	C4 H18 O2 F3 S3
		251.0412	12.3	49.0	-4.5	C3 H14 O7 F3 S
		251.0410	12.5	49.8	-1.5	C7 H17 O F2 S3
		251.0401	13.4	53.4	-0.5	C6 H13 O6 F2 S
		251.0389	14.6	58.2	3.5	C9 H12 O5 F S



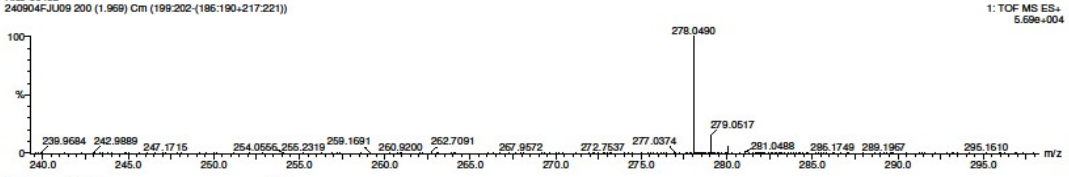
3d

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

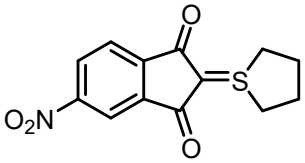
Monoisotopic Mass, Even Electron Ions
651 formula(e) evaluated with 242 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 S: 1-3

Rice-00482
240904FJU09 200 (1.969) Cm (199:202-(186:190+217:221))



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
278.0490	100.00	278.0487	0.3	1.1	8.5	C13 H12 N O4 S
		278.0494	-0.4	-1.4	4.5	C6 H12 N7 O2 S2
		278.0481	0.9	3.2	-0.5	C5 H16 N3 O6 S2
		278.0514	-2.4	-8.6	-5.5	C2 H20 N3 O6 S3
		278.0519	-2.9	-10.4	0.5	C2 H12 N7 O7 S
		278.0460	3.0	10.8	9.5	C9 H8 N7 O2 S
		278.0521	-3.1	-11.1	3.5	C10 H16 N O4 S2
		278.0455	3.5	12.6	3.5	C9 H16 N3 O S3
		278.0454	3.6	12.9	0.5	C H12 N9 O4 S2
		278.0528	-3.8	-13.7	-0.5	C3 H16 N7 O2 S3
		278.0447	4.3	15.5	4.5	C8 H12 N3 O6 S
		278.0546	-5.6	-20.1	-0.5	C6 H16 N O9 S
		278.0554	-6.4	-23.0	-1.5	C7 H20 N O4 S3
		278.0422	6.8	24.5	8.5	C12 H12 N3 O S2
		278.0559	-6.9	-24.8	4.5	C7 H12 N5 O5 S
		278.0420	7.0	25.2	5.5	C4 H8 N9 O4 S
		278.0415	7.5	27.0	-0.5	C4 H16 N5 O3 S3
		278.0407	8.3	29.9	0.5	C3 H12 N5 O8 S
		278.0573	-8.3	-29.9	9.5	C8 H8 N9 O S
		278.0402	8.8	31.6	-5.5	C3 H20 N O7 S3



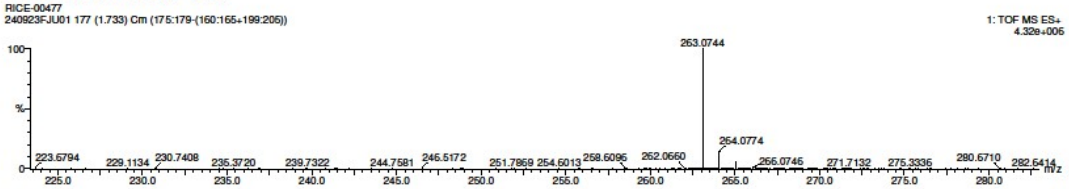
3e

Elemental Composition Report **Page 1**

Tolerance = 10.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

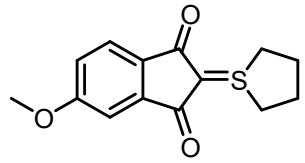
Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 6 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

RICE-00477
240923FJU01 177 (1.733) Cm (175:179-(160:165+199:205))



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
263.0744	100.00	263.0742	0.2	0.8	7.5	C14 H15 O3 S
		263.0776	-3.2	-12.2	2.5	C11 H19 O3 S2
		263.0801	-5.7	-21.7	-1.5	C7 H19 O8 S
		263.0809	-6.5	-24.7	-2.5	C8 H23 O3 S3
		263.0657	8.7	33.1	-6.5	C4 H23 O6 S3
		263.0834	-9.0	-34.2	-6.5	C4 H23 O8 S2



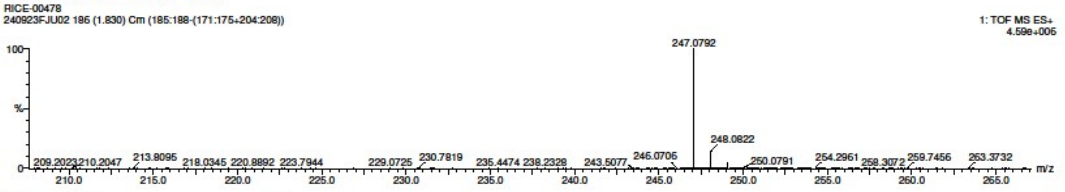
3f

Elemental Composition Report **Page 1**

Tolerance = 10.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

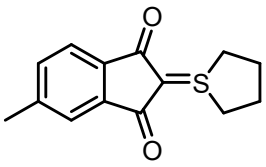
Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 7 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

RICE-00478
240923FJU02 186 (1.830) Cm (185:188-(171:175+204:208))



Minimum: 80.00
Maximum: 100.00 10.0 500.0 -10.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
247.0792	100.00	247.0793	-0.1	-0.4	7.5	C14 H15 O2 S
		247.0826	-3.4	-13.8	2.5	C11 H19 O2 S2
		247.0851	-5.9	-23.9	-1.5	C7 H19 O7 S
		247.0860	-6.8	-27.5	-2.5	C8 H23 O2 S3
		247.0708	8.4	34.0	-6.5	C4 H23 O5 S3
		247.0885	-9.3	-37.6	-6.5	C4 H23 O7 S2
		247.0699	9.3	37.6	-5.5	C3 H19 O10 S



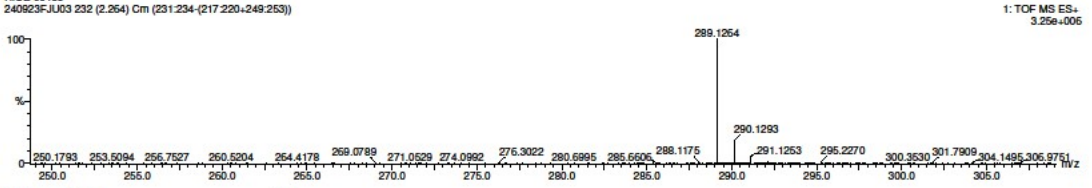
3g

Elemental Composition Report **Page 1**

Tolerance = 10.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

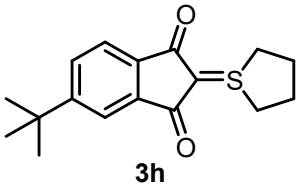
Monoisotopic Mass, Even Electron Ions
116 formula(e) evaluated with 7 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

RICE-00488
240923FJU03 232 (2.254) Cm (231:234-(217:220+249:253))



Minimum: 80.00
Maximum: 100.00 10.0 500.0 -10.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
289.1264	100.00	289.1262	0.2	0.7	7.5	C17 H21 O2 S
		289.1296	-3.2	-11.1	2.5	C14 H25 O2 S2
		289.1321	-5.7	-19.7	-1.5	C10 H25 O7 S
		289.1330	-6.6	-22.8	-2.5	C11 H29 O2 S3
		289.1177	8.7	30.1	-6.5	C7 H29 O5 S3
		289.1355	-9.1	-31.5	-6.5	C7 H29 O7 S2
		289.1168	9.6	33.2	-5.5	C6 H25 O10 S



3h

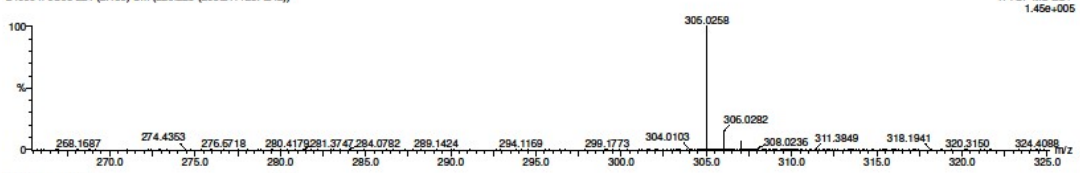
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
365 formula(e) evaluated with 267 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 F: 1-4 S: 1-3

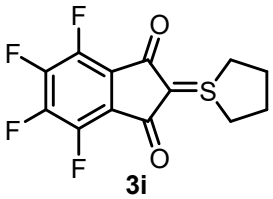
LA-01069
240904FJU03 221 (2.169) Cm (220:223-(205:211+237:242))

1: TOF MS ES+
1.45e+005



Minimum:	80.00			-10.0	
Maximum:	100.00		10.0	500.0	100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
305.0258	100.00	305.0259	-0.1	-0.3	7.5	C13 H9 O2 F4 S
		305.0248	1.0	3.3	11.5	C16 H8 O F3 S
		305.0282	-2.4	-7.9	6.5	C13 H12 O F3 S2
		305.0284	-2.6	-8.5	10.5	C15 H10 O4 F S
		305.0293	-3.5	-11.5	2.5	C10 H13 O2 F4 S2
		305.0295	-3.7	-12.1	6.5	C12 H11 O5 F2 S
		305.0210	4.8	15.7	-7.5	C2 H19 O8 F2 S3
		305.0307	-4.9	-16.1	2.5	C9 H12 O6 F3 S
		305.0315	-5.7	-18.7	1.5	C10 H16 O F3 S3
		305.0199	5.9	19.3	-3.5	C5 H18 O7 F S3
		305.0318	-6.0	-19.7	5.5	C12 H14 O4 F S2
		305.0318	-6.0	-19.7	-1.5	C6 H13 O7 F4 S
		305.0327	-6.9	-22.6	-2.5	C7 H17 O2 F4 S3
		305.0188	7.0	22.9	-6.5	C2 H16 O9 F3 S2
		305.0329	-7.1	-23.3	1.5	C9 H15 O5 F2 S2
		305.0176	8.2	26.9	-2.5	C5 H15 O8 F2 S2
		305.0340	-8.2	-26.9	-2.5	C6 H16 O6 F3 S2
		305.0174	8.4	27.5	-6.5	C3 H17 O5 F4 S3
		305.0343	-8.5	-27.9	1.5	C8 H14 O9 F S
		305.0166	9.2	30.2	-5.5	C2 H13 O10 F4 S



3i

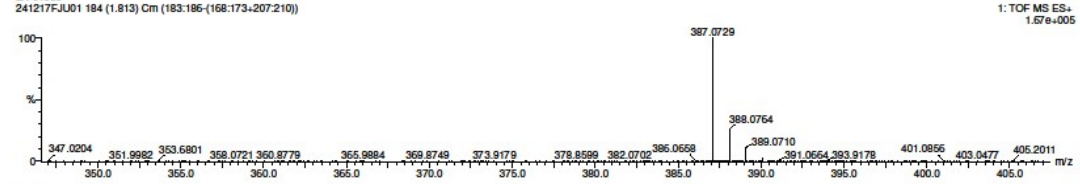
Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
146 formula(e) evaluated with 105 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

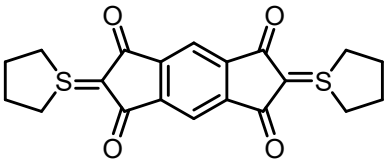
LA-01066
241217FJU01 184 (1.813) Cm (183:186-(168:173+207:210))

1: TOF MS ES+
1.57e+005



Minimum:	80.00			-10.0	
Maximum:	100.00		10.0	500.0	100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
387.0729	100.00	387.0725	0.4	1.0	11.5	C20 H19 O4 S2
		387.0750	-2.1	-5.4	7.5	C16 H19 O9 S
		387.0758	-2.9	-7.5	6.5	C17 H23 O4 S3
		387.0691	3.8	9.8	16.5	C23 H15 O4 S
		387.0783	-5.4	-14.0	2.5	C13 H23 O9 S2
		387.0817	-8.8	-22.7	-2.5	C10 H27 O9 S3
		387.0844	-11.5	-29.7	20.5	C27 H15 O S
		387.0606	12.3	31.8	2.5	C13 H23 O7 S3
		387.0877	-14.8	-38.2	15.5	C24 H19 O S2
		387.0572	15.7	40.6	7.5	C16 H19 O7 S2



3j

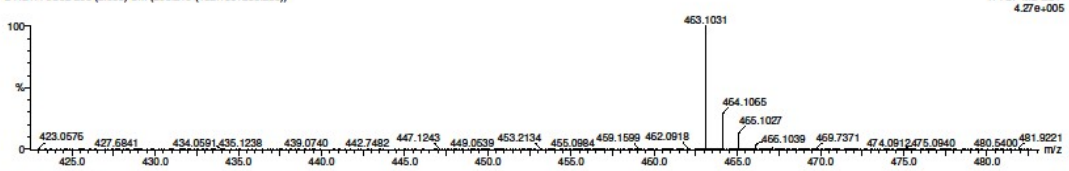
Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
173 formula(e) evaluated with 130 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

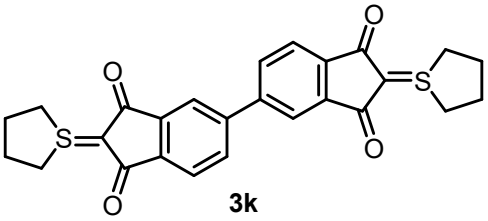
LA-01076
241217FJU02 208 (2.038) Cm (206:210-(182:188+235:239))

1: TOF MS ES+
4.27e+005



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
463.1031	100.00	463.1038	-0.7	-1.5	15.5	C26 H23 O4 S2
		463.1004	2.7	5.8	20.5	C29 H19 O4 S
		463.1063	-3.2	-6.9	11.5	C22 H23 O9 S
		463.1071	-4.0	-8.6	10.5	C23 H27 O4 S3
		463.1096	-6.5	-14.0	6.5	C19 H27 O9 S2
		463.1130	-9.9	-21.4	1.5	C16 H31 O9 S3
		463.0919	11.2	24.2	6.5	C19 H27 O7 S3
		463.1157	-12.6	-27.2	24.5	C33 H19 O S
		463.0885	14.6	31.5	11.5	C22 H23 O7 S2
		463.1190	-15.9	-34.3	19.5	C30 H23 O S2



3k

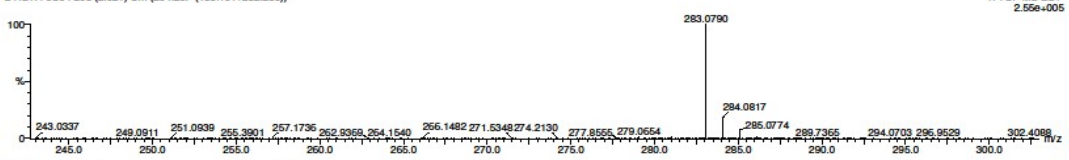
Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
106 formula(e) evaluated with 76 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

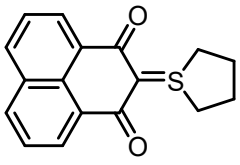
LA-01090
241217FJU04 206 (2.021) Cm (204:207-(185:191+232:235))

1: TOF MS ES+
2.55e+005



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
283.0790	100.00	283.0793	-0.3	-1.1	10.5	C17 H15 O2 S
		283.0826	-3.6	-12.7	5.5	C14 H19 O2 S2
		283.0733	5.7	20.1	-7.5	C3 H23 O10 S2
		283.0851	-6.1	-21.5	1.5	C10 H19 O7 S
		283.0860	-7.0	-24.7	0.5	C11 H23 O2 S3
		283.0708	8.2	29.0	-3.5	C7 H23 O5 S3
		283.0699	9.1	32.1	-2.5	C6 H19 O10 S
		283.0885	-9.5	-33.6	-3.5	C7 H23 O7 S2
		283.0674	11.6	41.0	1.5	C10 H19 O5 S2
		283.0919	-12.9	-45.6	-8.5	C4 H27 O7 S3



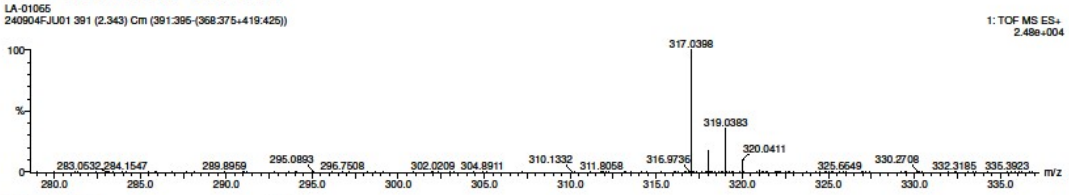
3l

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

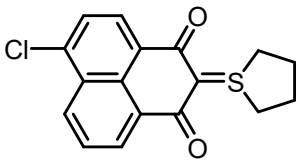
Monoisotopic Mass, Even Electron Ions
252 formula(e) evaluated with 186 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Cl: 1-3

LA-01065
240904FJU01 391 (2.343) Cm (391:395-(368:375+419:425))



Minimum: 80.00 -10.0
Maximum: 100.00 10.0 500.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
317.0398	100.00	317.0403	-0.5	-1.6	10.5	C17 H14 O2 S Cl
		317.0381	1.7	5.4	1.5	C11 H19 O4 S C12
		317.0415	-1.7	-5.4	-3.5	C8 H23 O4 S2 C12
		317.0368	3.0	9.5	-8.5	C6 H26 O S3 C13
		317.0437	-3.9	-12.3	5.5	C14 H18 O2 S2 C1
		317.0359	3.9	12.3	-7.5	C5 H24 O6 S C13
		317.0440	-4.2	-13.2	-7.5	C4 H23 O9 S C12
		317.0449	-5.1	-16.1	-8.5	C5 H27 O4 S3 C12
		317.0343	5.5	17.3	-7.5	C3 H22 O10 S2 C1
		317.0462	-6.4	-20.2	1.5	C10 H18 O7 S C1
		317.0334	6.4	20.2	-3.5	C9 H24 O S2 C13
		317.0470	-7.2	-22.7	0.5	C11 H22 O2 S3 C1
		317.0318	8.0	25.2	-3.5	C7 H22 O5 S3 C1
		317.0309	8.9	28.1	-2.5	C6 H18 O10 S C1
		317.0495	-9.7	-30.6	-3.5	C7 H22 O7 S2 C1
		317.0300	9.8	30.9	1.5	C12 H20 O S C13
		317.0512	-11.4	-36.0	-3.5	C9 H24 O3 S C13
		317.0284	11.4	36.0	1.5	C10 H18 O5 S2 C1
		317.0529	-13.1	-41.3	-8.5	C4 H26 O7 S3 C1
		317.0262	13.6	42.9	-7.5	C4 H23 O7 S2 C12



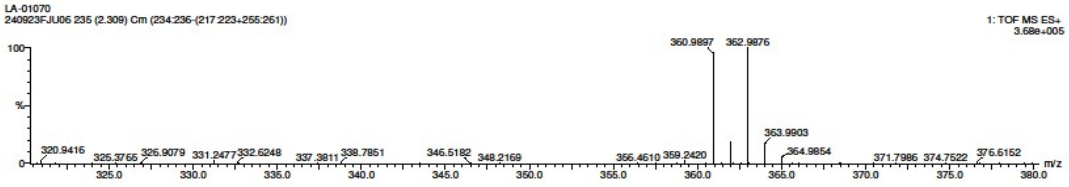
3m

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

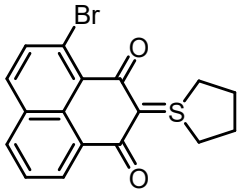
Monoisotopic Mass, Even Electron Ions
176 formula(e) evaluated with 11 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Br: 1-3

LA-01070
240923FJU06 235 (2.309) Cm (234:236-(217:223+255:261))



Minimum: -10.0
Maximum: 10.0 500.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
360.9897	360.9898	-0.1	-0.3	10.5	C17 H14 O2 S Br
	360.9895	0.2	0.6	-9.5	C4 H27 O6 S Br2
	360.9870	2.7	7.5	-5.5	C8 H27 O S2 Br2
	360.9932	-3.5	-9.7	5.5	C14 H18 O2 S2 Br
	360.9838	5.9	16.3	-7.5	C3 H22 O10 S2 Br
	360.9957	-6.0	-16.6	1.5	C10 H18 O7 S Br
	360.9836	6.1	16.9	-0.5	C11 H23 O S Br2
	360.9965	-6.8	-18.8	0.5	C11 H22 O2 S3 Br
	360.9813	8.4	23.3	-3.5	C7 H22 O5 S3 Br
	360.9990	-9.3	-25.8	-3.5	C7 H22 O7 S2 Br
	360.9804	9.3	25.8	-2.5	C6 H18 O10 S Br



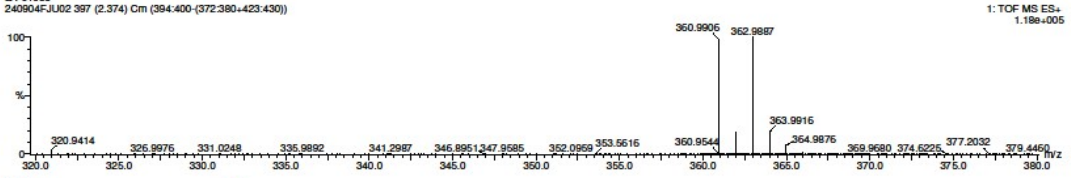
3n

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

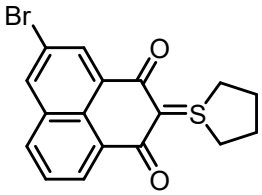
Monoisotopic Mass, Even Electron Ions
176 formula(e) evaluated with 131 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Br: 1-3

LA-01068
240904FJU02 397 (2.374) Cm (394:400-(372:380+423:430))



Minimum: -10.0
Maximum: 10.0 500.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
360.9906	360.9898	0.8	2.2	10.5	C17 H14 O2 S Br
	360.9895	1.1	3.0	-9.5	C4 H27 O6 S Br2
	360.9932	-2.6	-7.2	5.5	C14 H18 O2 S2 Br
	360.9870	3.6	10.0	-5.5	C8 H27 O S2 Br2
	360.9957	-5.1	-14.1	1.5	C10 H18 O7 S Br
	360.9965	-5.9	-16.3	0.5	C11 H22 O2 S3 Br
	360.9838	6.8	18.8	-7.5	C3 H22 O10 S2 Br
	360.9836	7.0	19.4	-0.5	C11 H23 O S Br2
	360.9990	-8.4	-23.3	-3.5	C7 H22 O7 S2 Br
	360.9813	9.3	25.8	-3.5	C7 H22 O5 S3 Br
	360.9804	10.2	28.3	-2.5	C6 H18 O10 S Br
	361.0024	-11.8	-32.7	-8.5	C4 H26 O7 S3 Br
	360.9779	12.7	35.2	1.5	C10 H18 O5 S2 Br
	361.0048	-14.2	-39.3	-5.5	C8 H27 O3 S Br2
	360.9745	16.1	44.6	6.5	C13 H14 O5 S Br
	360.9718	18.8	52.1	-9.5	C4 H27 O4 S2 Br2
	361.0109	-20.3	-56.2	5.5	C14 H18 O4 S Br
	360.9684	22.2	61.5	-4.5	C7 H23 O4 S Br2
	361.0143	-23.7	-65.7	0.5	C11 H22 O4 S2 Br
	360.9660	24.6	68.1	-7.5	C3 H22 O8 S3 Br



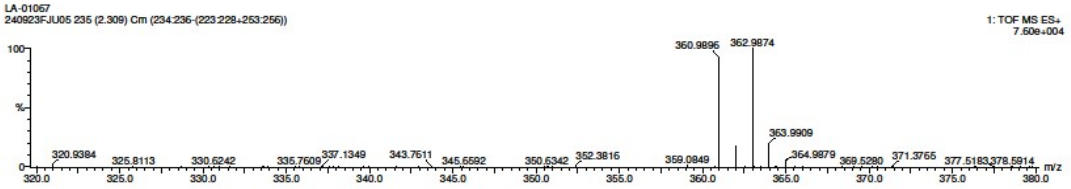
3o

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

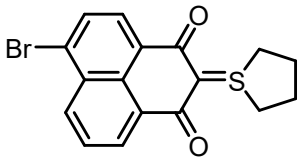
Monoisotopic Mass, Even Electron Ions
176 formula(e) evaluated with 11 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Br: 1-3

LA-01067
240923FJU05 235 (2.309) Cm (234:236-(223:228+253:256))



Minimum: -10.0
Maximum: 10.0 500.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
360.9896	360.9898	-0.2	-0.6	10.5	C17 H14 O2 S Br
	360.9895	0.1	0.3	-9.5	C4 H27 O6 S Br2
	360.9957	-6.1	-16.9	1.5	C10 H18 O7 S Br
	360.9836	6.0	16.6	-0.5	C11 H23 O S Br2
	360.9804	9.2	25.5	-2.5	C6 H18 O10 S Br
	360.9990	-9.4	-26.0	-3.5	C7 H22 O7 S2 Br
	360.9932	-3.6	-10.0	5.5	C14 H18 O2 S2 Br
	360.9838	5.8	16.1	-7.5	C3 H22 O10 S2 Br
	360.9870	2.6	7.2	-5.5	C8 H27 O S2 Br2
	360.9813	8.3	23.0	-3.5	C7 H22 O5 S3 Br
	360.9965	-6.9	-19.1	0.5	C11 H22 O2 S3 Br



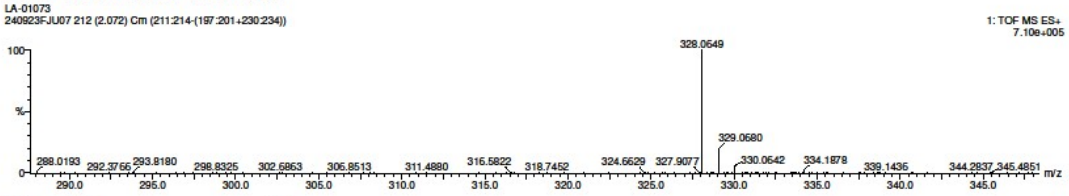
3p

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

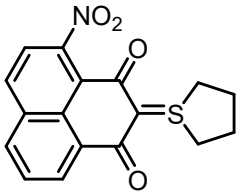
Monoisotopic Mass, Even Electron Ions
966 formula(e) evaluated with 26 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 S: 1-3

LA-01073
240923FJU07 212 (2.072) Cm (211:214-(197:201+230:234))



Minimum: 80.00 -10.0
Maximum: 100.00 10.0 500.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
328.0649	100.00	328.0644	0.5	1.5	11.5	C17 H14 N O4 S
		328.0702	-5.3	-16.2	2.5	C10 H18 N O9 S
		328.0677	-2.8	-8.5	6.5	C14 H18 N O4 S2
		328.0711	-6.2	-18.9	1.5	C11 H22 N O4 S3
		328.0603	4.6	14.0	7.5	C12 H14 N3 O6 S
		328.0612	3.7	11.3	6.5	C13 H18 N3 O S3
		328.0637	1.2	3.7	2.5	C9 H18 N3 O6 S2
		328.0578	7.1	21.6	11.5	C16 H14 N3 O S2
		328.0671	-2.2	-6.7	-2.5	C6 H22 N3 O6 S3
		328.0630	1.9	5.8	-6.5	C H22 N5 O8 S3
		328.0716	-6.7	-20.4	7.5	C11 H14 N5 O5 S
		328.0597	5.2	15.9	-1.5	C4 H18 N5 O8 S2
		328.0650	-0.1	-0.3	7.5	C10 H14 N7 O2 S2
		328.0709	-6.0	-18.3	-1.5	C3 H18 N7 O7 S2
		328.0617	3.2	9.8	12.5	C13 H10 N7 O2 S
		328.0675	-2.6	-7.9	3.5	C6 H14 N7 O7 S
		328.0684	-3.5	-10.7	2.5	C7 H18 N7 O2 S3
		328.0635	1.4	4.3	-0.5	C H14 N9 O9 S
		328.0610	3.9	11.9	3.5	C5 H14 N9 O4 S2
		328.0644	0.5	1.5	-1.5	C2 H18 N9 O4 S3



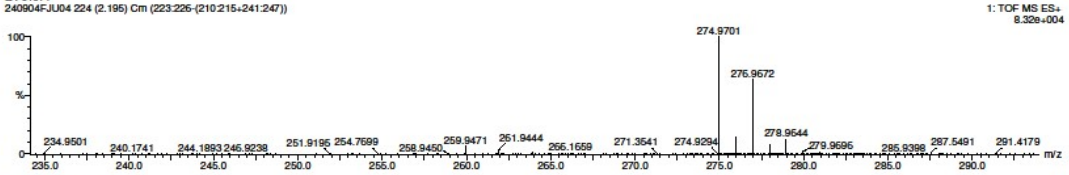
3q

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

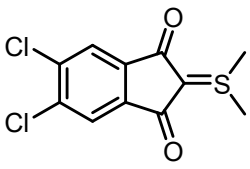
Monoisotopic Mass, Even Electron Ions
185 formula(e) evaluated with 136 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Cl: 1-3

LA-01071
240904FJU04 224 (2.195) Cm (223:226-(210:215+241:247))



Minimum: 80.00 -10.0
Maximum: 100.00 10.0 500.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
274.9701	100.00	274.9700	0.1	0.4	6.5	C11 H9 O2 S Cl2
		274.9712	-1.1	-4.0	-7.5	C2 H18 O4 S2 Cl3
		274.9678	2.3	8.4	-2.5	C5 H14 O4 S Cl3
		274.9734	-3.3	-12.0	1.5	C8 H13 O2 S2 Cl2
		274.9662	3.9	14.2	-2.5	C3 H12 O8 S2 Cl
		274.9759	-5.8	-21.1	-2.5	C4 H13 O7 S Cl2
		274.9637	6.4	23.3	1.5	C7 H12 O3 S3 Cl
		274.9768	-6.7	-24.4	-3.5	C5 H17 O2 S3 Cl2
		274.9628	7.3	26.5	2.5	C6 H8 O8 S Cl
		274.9781	-8.0	-29.1	6.5	C10 H8 O5 S Cl
		274.9615	8.6	31.3	-7.5	C H17 O5 S3 Cl2
		274.9793	-9.2	-33.5	-7.5	C H17 O7 S2 Cl2
		274.9603	9.8	35.6	6.5	C10 H8 O3 S2 Cl
		274.9815	-11.4	-41.5	1.5	C7 H12 O5 S2 Cl
		274.9581	12.0	43.6	-2.5	C4 H13 O5 S2 Cl2
		274.9831	-13.0	-47.3	1.5	C9 H14 O S Cl3
		274.9570	13.1	47.6	11.5	C13 H4 O3 S Cl
		274.9840	-13.9	-50.6	-2.5	C3 H12 O10 S Cl
		274.9848	-14.7	-53.5	-3.5	C4 H16 O5 S3 Cl
		274.9548	15.3	55.6	2.5	C7 H9 O5 S Cl2

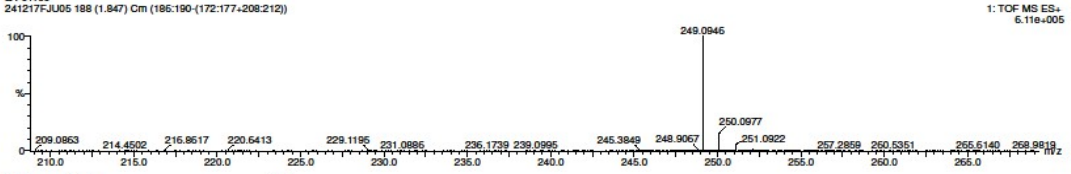


3r

Elemental Composition Report **Page 1**

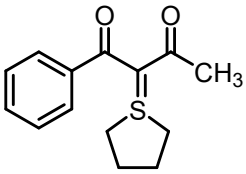
Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
96 formula(e) evaluated with 59 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3
LA-01100
241217FJU05 188 (1.847) Cm (186:190-(172:177+208:212))



Minimum: 80.00
Maximum: 100.00 10.0 500.0 -10.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
249.0946	100.00	249.0949	-0.3	-1.2	6.5	C14 H17 O2 S
		249.0983	-3.7	-14.9	1.5	C11 H21 O2 S2
		249.1008	-6.2	-24.9	-2.5	C7 H21 O7 S
		249.1017	-7.1	-28.5	-3.5	C8 H25 O2 S3
		249.0864	8.2	32.9	-7.5	C4 H25 O5 S3
		249.0855	9.1	36.5	-6.5	C3 H21 O10 S
		249.1042	-9.6	-38.5	-7.5	C4 H25 O7 S2
		249.0830	11.6	46.6	-2.5	C7 H21 O5 S2
		249.0797	14.9	59.8	2.5	C10 H17 O5 S
		249.1161	-21.5	-86.3	1.5	C11 H21 O4 S

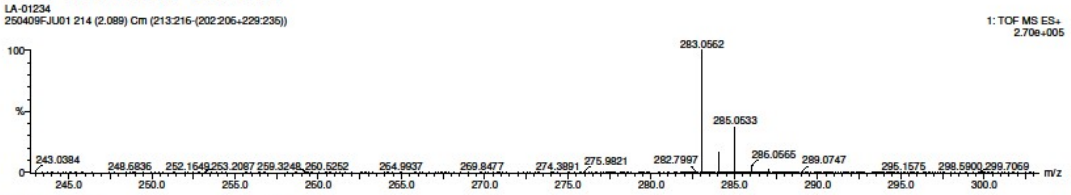


5a

Elemental Composition Report **Page 1**

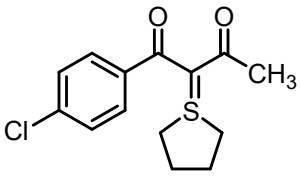
Single Mass Analysis
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
205 formula(e) evaluated with 125 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 Cl: 1-3
LA-01234
250409FJU01 214 (2.089) Cm (213:216-(202:206+229:235))



Minimum: 80.00
Maximum: 100.00 10.0 500.0 -10.0 100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
283.0562	100.00	283.0560	0.2	0.7	6.5	C14 H16 O2 S Cl
		283.0571	-0.9	-3.2	-7.5	C5 H25 O4 S2 Cl2
		283.0538	2.4	8.5	-2.5	C8 H21 O4 S Cl2
		283.0593	-3.1	-11.0	1.5	C11 H20 O2 S2 Cl
		283.0618	-5.6	-19.8	-2.5	C7 H20 O7 S Cl
		283.0627	-6.5	-23.0	-3.5	C8 H24 O2 S3 Cl
		283.0491	7.1	25.1	-7.5	C6 H26 O S2 Cl3
		283.0474	8.8	31.1	-7.5	C4 H24 O5 S3 Cl
		283.0652	-9.0	-31.8	-7.5	C4 H24 O7 S2 Cl
		283.0466	9.6	33.9	-6.5	C3 H20 O10 S Cl
		283.0457	10.5	37.1	-2.5	C9 H22 O S Cl3
		283.0668	-10.6	-37.4	-7.5	C6 H26 O3 S Cl3
		283.0441	12.1	42.7	-2.5	C7 H20 O5 S2 Cl
		283.0690	-12.8	-45.2	1.5	C12 H21 O S Cl2
		283.0407	15.5	54.8	2.5	C10 H16 O5 S Cl
		283.0724	-16.2	-57.2	-3.5	C9 H25 O S2 Cl2
		283.0394	16.8	59.4	-7.5	C5 H25 O2 S3 Cl2
		283.0385	17.7	62.5	-6.5	C4 H21 O7 S Cl2
		283.0749	-18.7	-66.1	-7.5	C5 H25 O6 S Cl2
		283.0758	-19.6	-69.2	-8.5	C6 H29 O S3 Cl2



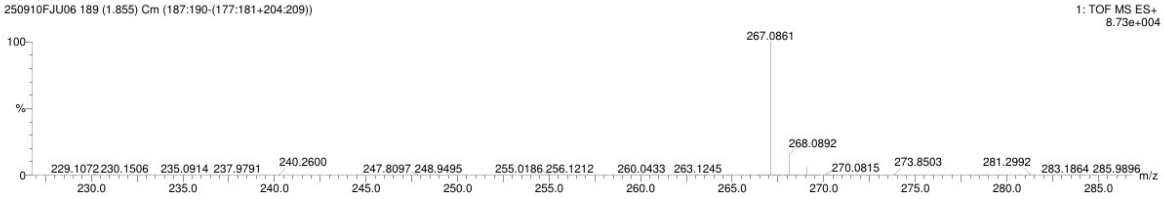
5b

Elemental Composition Report **Page 1**

Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

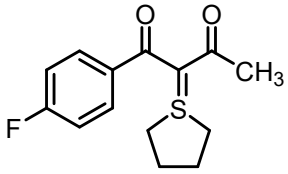
Monoisotopic Mass, Even Electron Ions
236 formula(e) evaluated with 159 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3 F: 1-3

RICE-03552
250910FJU06 189 (1.855) Cm (187:190-(177:181+204:209))



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
267.0861	100.00	267.0855	0.6	2.2	6.5	C14 H16 O2 S F
		267.1030	-16.9	-63.3	2.5	C12 H18 O S F3
		267.0667	19.4	72.6	3.5	C11 H14 O2 S F3
		267.0725	13.6	50.9	-5.5	C4 H18 O7 S F3
		267.0866	-0.5	-1.9	2.5	C11 H17 O3 S F2
		267.0925	-6.4	-24.0	-6.5	C4 H21 O8 S F2
		267.0702	15.9	59.5	2.5	C10 H16 O5 S F
		267.0714	14.7	55.0	-1.5	C7 H17 O6 S F2
		267.0914	-5.3	-19.8	-2.5	C7 H20 O7 S F
		267.0878	-1.7	-6.4	-1.5	C8 H18 O4 S F3
		267.0761	10.0	37.4	-6.5	C3 H20 O10 S F
		267.0889	-2.8	-10.5	1.5	C11 H20 O2 S2 F
		267.0900	-3.9	-14.6	-2.5	C8 H21 O3 S2 F2
		267.0700	16.1	60.3	-1.5	C8 H18 O2 S2 F3
		267.1064	-20.3	-76.0	-2.5	C9 H22 O S2 F3
		267.0736	12.5	46.8	-2.5	C7 H20 O5 S2 F
		267.0947	-8.6	-32.2	-7.5	C4 H24 O7 S2 F
		267.0912	-5.1	-19.1	-6.5	C5 H22 O4 S2 F3
		267.0689	17.2	64.4	2.5	C11 H17 O S2 F2
		267.0748	11.3	42.3	-6.5	C4 H21 O6 S2 F2
		267.0770	9.1	34.1	-7.5	C4 H24 O5 S3 F
		267.0734	12.7	47.6	-6.5	C5 H22 O2 S3 F3
		267.0723	13.8	51.7	-2.5	C8 H21 O S3 F2
		267.0922	-6.1	-22.8	-3.5	C8 H24 O2 S3 F
		267.0934	-7.3	-27.3	-7.5	C5 H25 O3 S3 F2



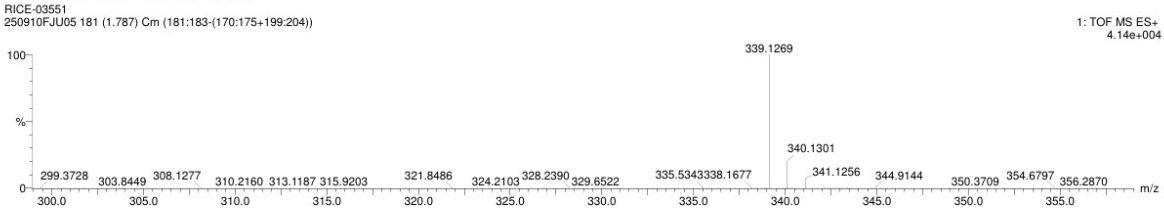
5c

Elemental Composition Report **Page 1**

Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

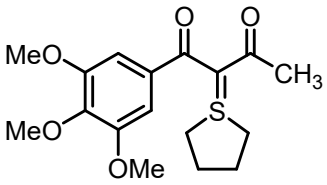
Monoisotopic Mass, Even Electron Ions
128 formula(e) evaluated with 94 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

RICE-03551
250910FJU05 181 (1.787) Cm (181:183-(170:175+199:204))



Minimum:	80.00				-10.0	
Maximum:	100.00		10.0	500.0	100.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
339.1269	100.00	339.1266	0.3	0.9	6.5	C17 H23 O5 S
		339.1300	-3.1	-9.1	1.5	C14 H27 O5 S2
		339.1325	-5.6	-16.5	-2.5	C10 H27 O10 S
		339.1334	-6.5	-19.2	-3.5	C11 H31 O5 S3
		339.1181	8.8	25.9	-7.5	C7 H31 O8 S3
		339.1359	-9.0	-26.5	-7.5	C7 H31 O10 S2
		339.1147	12.2	36.0	-2.5	C10 H27 O8 S2
		339.1122	14.7	43.3	1.5	C14 H27 O3 S3
		339.1419	-15.0	-44.2	10.5	C21 H23 O2 S
		339.1114	15.5	45.7	2.5	C13 H23 O8 S
		339.1089	18.0	53.1	6.5	C17 H23 O3 S2
		339.1452	-18.3	-54.0	5.5	C18 H27 O2 S2
		339.1477	-20.8	-61.3	1.5	C14 H27 O7 S
		339.1055	21.4	63.1	11.5	C20 H19 O3 S
		339.1486	-21.7	-64.0	0.5	C15 H31 O2 S3
		339.1511	-24.2	-71.4	-3.5	C11 H31 O7 S2
		339.1545	-27.6	-81.4	-8.5	C8 H35 O7 S3
		339.0970	29.9	88.2	-2.5	C10 H27 O6 S3
		339.0936	33.3	98.2	2.5	C13 H23 O6 S2
		339.0911	35.8	105.6	6.5	C17 H23 O S3
		339.1630	-36.1	-106.4	5.5	C18 H27 O4 S
		339.0902	36.7	108.2	7.5	C16 H19 O6 S
		339.0877	39.2	115.6	11.5	C20 H19 O S2
		339.1664	-39.5	-116.5	0.5	C15 H31 O4 S2
		339.1689	-42.0	-123.8	-3.5	C11 H31 O9 S



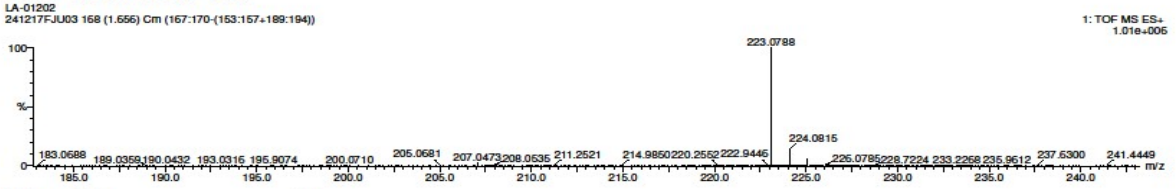
5d

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

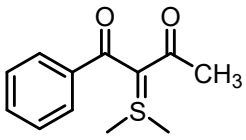
Monoisotopic Mass, Even Electron Ions
75 formula(e) evaluated with 48 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 S: 1-3

LA-01202
241217FJU03 168 (1.656) Cm (167:170-(153:157+189:194))



Minimum:	80.00			-10.0	
Maximum:	100.00		10.0	500.0	100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
223.0788	100.00	223.0793	-0.5	-2.2	5.5	C12 H15 O2 S
		223.0826	-3.8	-17.0	0.5	C9 H19 O2 S2
		223.0851	-6.3	-28.2	-3.5	C5 H19 O7 S
		223.0860	-7.2	-32.3	-4.5	C6 H23 O2 S3
		223.0708	8.0	35.9	-8.5	C2 H23 O5 S3
		223.0699	8.9	39.9	-7.5	C H19 O10 S
		223.0885	-9.7	-43.5	-8.5	C2 H23 O7 S2
		223.0674	11.4	51.1	-3.5	C5 H19 O5 S2
		223.0640	14.8	66.3	1.5	C8 H15 O5 S
		223.1004	-21.6	-96.8	0.5	C9 H19 O4 S



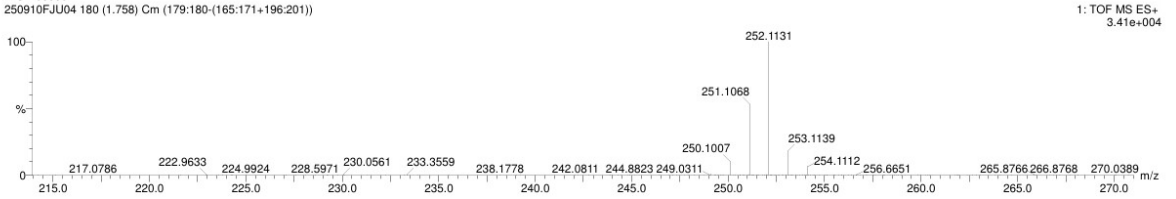
5e

Elemental Composition Report **Page 1**

Tolerance = 500.0 PPM / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

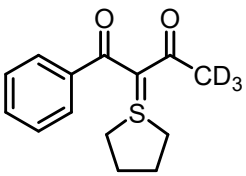
Monoisotopic Mass, Even Electron Ions
4474 formula(e) evaluated with 269 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 O: 1-10 S: 1-3 1H: 1-100 2H: 1-10

RICE-03550
250910FJU04 180 (1.758) Cm (179:180-(165:171+196:201))



Minimum:	80.00			-10.0	
Maximum:	100.00		10.0	500.0	100.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
252.1131	100.00	252.1138	-0.7	-2.8	6.5	C14 O2 S 1H14 2H3
		252.1076	5.5	21.8	8.5	C14 O2 S 1H6 2H7
		252.1169	-3.8	-15.1	5.5	C14 O2 S 1H18 2H
		252.1107	2.4	9.5	7.5	C14 O2 S 1H10 2H5
		252.1202	-7.1	-28.2	0.5	C11 O2 S2 1H22 2H
		252.1078	5.3	21.0	4.5	C11 O2 S2 1H6 2H9
		252.1171	-4.0	-15.9	1.5	C11 O2 S2 1H18 2H3
		252.1140	-0.9	-3.6	2.5	C11 O2 S2 1H14 2H5
		252.1109	2.2	8.7	3.5	C11 O2 S2 1H10 2H7
		252.1205	-7.4	-29.4	-3.5	C8 O2 S3 1H22 2H3
		252.1174	-4.3	-17.1	-2.5	C8 O2 S3 1H18 2H5
		252.1112	1.9	7.5	-0.5	C8 O2 S3 1H10 2H9
		252.1143	-1.2	-4.8	-1.5	C8 O2 S3 1H14 2H7
		252.1050	8.1	32.1	-3.5	C7 O5 S2 1H22 2H
		252.1134	-0.3	-1.2	-0.5	C7 O7 S 1H10 2H7
		252.1165	-3.4	-13.5	-1.5	C7 O7 S 1H14 2H5
		252.1196	-6.5	-25.8	-2.5	C7 O7 S 1H18 2H3
		252.1103	2.8	11.1	0.5	C7 O7 S 1H6 2H9
		252.1083	4.8	19.0	-8.5	C4 O5 S3 1H26 2H
		252.1052	7.9	31.3	-7.5	C4 O5 S3 1H22 2H3
		252.1199	-6.8	-27.0	-6.5	C4 O7 S2 1H18 2H5
		252.1137	-0.6	-2.4	-4.5	C4 O7 S2 1H10 2H9
		252.1168	-3.7	-14.7	-5.5	C4 O7 S2 1H14 2H7
		252.1075	5.6	22.2	-7.5	C3 O10 S 1H22 2H
		252.1171	-4.0	-15.9	-9.5	C O7 S3 1H14 2H9



5ai"

6. References

1) Allen, A.D.; Andraos, J.; Tidwell, T.T.; Vukovic, S., 2014. Ketene reactions with tertiary amines. *J. Org. Chem.* **2014**, *79*, 679-685.