Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information for

Synthesis of cyclic organic carbonates via catalytic oxidative carboxylation of olefins in flow reactors

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Table of Contents

I. General Information

All reagents were obtained from commercial vendors (TCI, Sigma-Aldrich, Alfa-Aesar) and used without purification unless noted. NMR data was collected on Bruker Avance CDPX 300 or DRX 400 MHz instruments. Spectra were referenced internally to tetramethylsilane (TMS) ($CDCl_3$: 0.00 ppm (^1H), 0.0 (^{13}C). Gas chromatography was performed on Agilent 7890A equipped with a HP-5 column and flame ionization detector (GC-FID). The following method was used for analysis. Inlet temperature: 230 °C, carrier gas (Argon) flow rate: 5 mL/min (column), split ratio 38:1, oven program: 50 °C for 1 minute, 10 °C/min to 100 °C, hold at 100 °C for 2.5 minutes, FID temperature: 250 °C, H_2 flow rate: 30 mL/min, air flow rate: 300 mL/min, make-up flow rate: 30 mL/min. Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) measurements were performed on Agilent 700 series instrument. The Re standard (100 ppm Re in 2% HNO_3) for the ICP analysis were purchased from High Purity Standards Ltd. Mass spectrometric measurements were performed at University of Illinois (Champaign, IL) and the Pennsylvania State University Proteomics and Mass Spectrometry Core Facility (University Park, PA). Standard tube fittings were purchased from Swagelok and IDEX health and science.

II. Effect of stirring speed on yield in batch reactor

In a 25 ml round bottom flask equipped with a 1/4 inch stir bar were added methyltrioxorhenium (7.5 mg, 0.03 mmol), dodecane (68 μL, 0.3 mmol), styrene (0.345 mL, 3 mmol), 3-methylpyrazole (58 μL, 0.72 mmol), and dichloromethane (to adjust final volume to 1.5 mL). 30% H_2O_2 (aq) solution (0.64 mL, 6 mmol) was then added to the mixture and the flask was sealed with a rubber septum. The flask was placed on a stir plate and the reaction mixture was stirred at the desired RPM for 1.5 hours at room temperature.

After 1.5 hours the stirring was stopped and approximately 0.5 mL of the organic layer was pipetted into a 2 mL vial. The crude organic layer was analyzed using GC. The styrene conversion was determined by gas chromatography. Figure S1 shows the plot for conversion as a function of stirring rate.

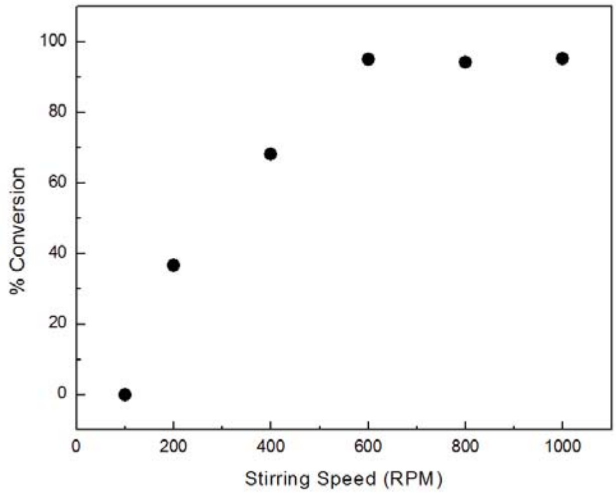


Figure S1. Effect of stirring speed on epoxidation of styrene using MTO and hydrogen peroxide.

III. Optimization of epoxidation flow reactor

a. Preparation of reactant solutions

In a 20 mL scintillation vial, methyltrioxorhenium, dodecane (internal standard) (10 mol%), styrene, 3-methylpyrazole and dichloromethane were added together. The quantity of reactants added depended on the variable being optimized. The mixture was stirred until the catalyst dissolved and subsequently loaded into a 5 mL gas-tight glass syringe after passing through a 0.2 μm PTFE syringe filter. A small aliquot of the solution was analyzed using GC before the reaction. Another 5 mL glass gas tight syringe was filled with 30% H_2O_2 (aq) solution.

b. Reaction procedure and product quantification

The temperature controller was turned on and the epoxidation reactor was set to the desired temperature. After the temperature stabilized the gas tight syringes containing the styrene and H_2O_2 (aq) solutions were loaded onto syringe pumps (New Era NE-510). A 40 psi back pressure regulator from IDEX was attached to the reactor outlet. The pumps were started with their respective flow rates. After constant segmented flow was seen, the system was run for 1.5 residence times. This ensured that the system reached steady state when the reaction mixture was analyzed. For analysis, the reaction mixture was collected in a vial containing MnO_2 to quench the excess peroxide and terminate the reaction. After effervescence ceased, approximately 0.5 mL of DCM was added to the reaction mixture. The organic layer was separated from the aqueous layer using a Pasteur pipette. The crude organic layer was analyzed using GC-FID. The conversion of styrene was determined by comparing the initial and final area ratios of styrene to the internal standard (dodecane).

The conversion of styrene as a function of catalyst loading, co-catalyst loading, oxidant equivalents, residence time, concentration and temperature was studied and the data collected is presented in Figures S2-S7.

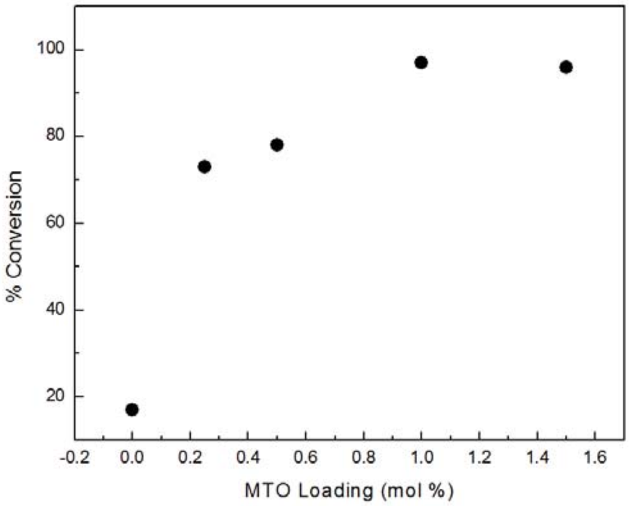


Figure S2. Effect of catalyst loading on styrene epoxidation. Temperature = 40 °C, oxidant = 5 equiv, co-catalyst = 24 mol%, residence time = 30 mins, concentration = 4M, organic flow rate = 0.32 mL/h, aqueous flow rate = 0.68 mL/h.

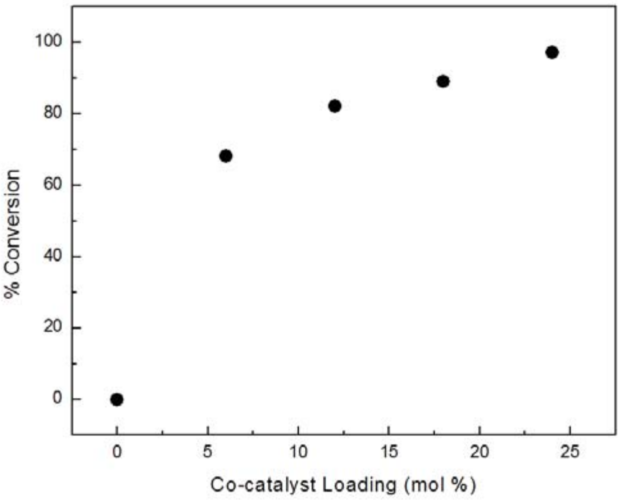


Figure S3. Effect of co-catalyst loading on styrene epoxidation. Temperature = 40 °C, oxidant = 5 equiv, catalyst = 1 mol%, residence time = 30 mins, concentration = 4M, organic flow rate = 0.32 mL/h, aqueous flow rate = 0.68 mL/h.

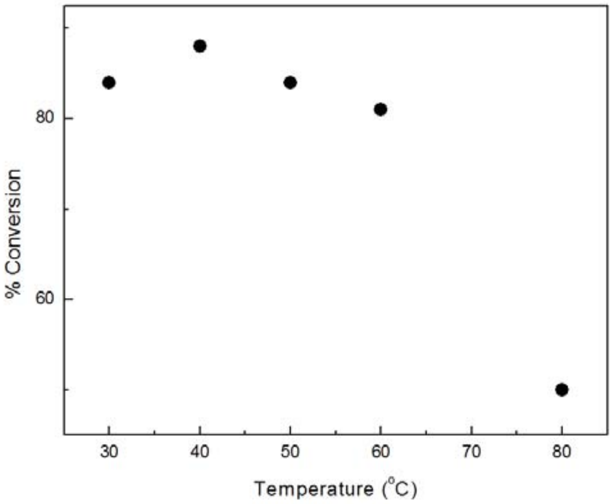


Figure S4. Effect of temperature on styrene epoxidation. Oxidant = 4.7 equiv, co-catalyst = 24 mol%, catalyst = 1 mol%, residence time = 30 mins, concentration = 2M, organic flow rate = 0.5 mL/h, aqueous flow rate = 0.5 mL/h.

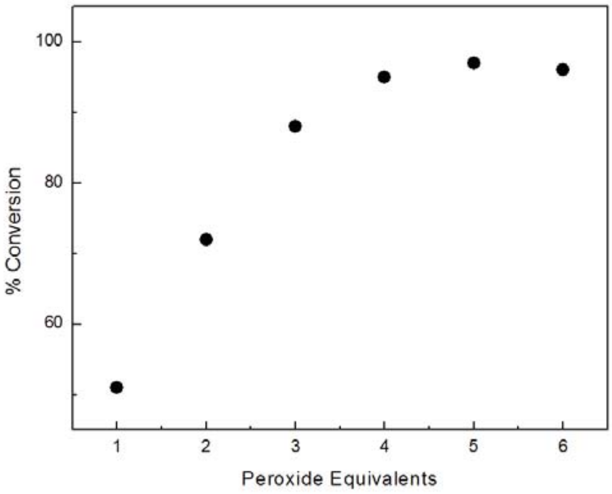


Figure S5. Effect of H_2O_2 equivalents on styrene epoxidation. Temperature = 40 °C, co-catalyst = 24 mol%, catalyst = 1 mol%, residence time = 30 mins, concentration = 4M, total flow rate = 1 mL/h. Note: Oxidant equivalents were varied by changing the ratio of organic to aqueous flow rate.

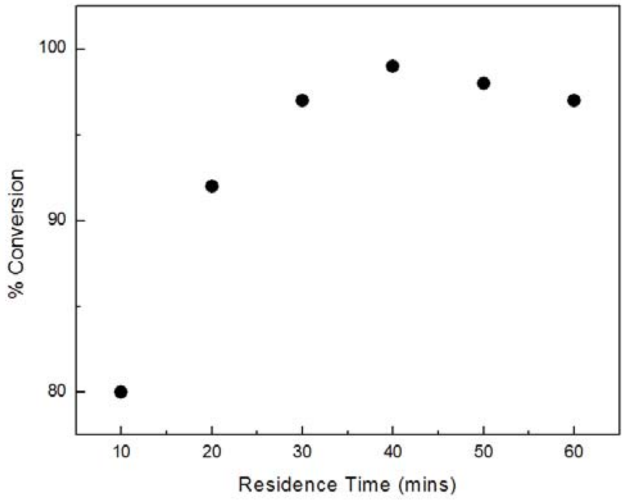


Figure S6. Effect of residence time on styrene epoxidation. Temperature = 40 °C, oxidant = 5 equiv., co-catalyst = 24 mol%, catalyst = 1 mol%, concentration = 4M.

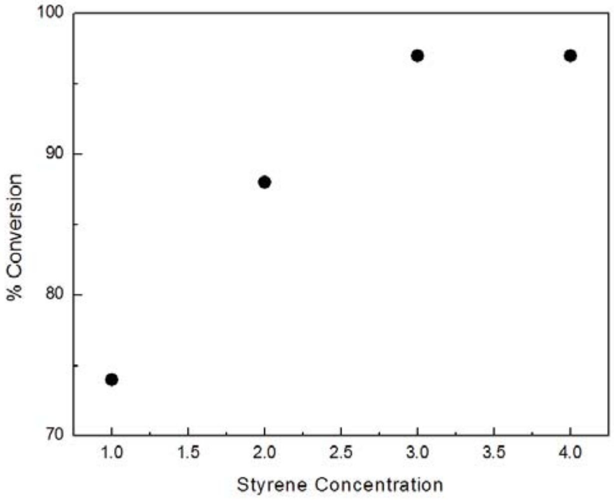


Figure S7. Effect of concentration on styrene epoxidation. Temperature = 40 °C, oxidant = 5 equiv, co-catalyst = 24 mol%, catalyst = 1 mol%, residence time = 30 mins, total flow rate = 1 mL/h. Note: Oxidant equivalents were kept constant by changing the ratio of organic to aqueous flow rate.

IV. Optimization of carboxylation flow reactor

a. Preparation of reactant solutions

In a 20 mL scintillation vial, aluminum catalyst, styrene oxide, tetrabutylammonium iodide, DCM and THF were combined. The mixture was stirred until all the solids dissolved and subsequently transferred into a 5 mL gas-tight glass syringe after passing through a 0.2 µm PTFE syringe filter.

b. Initialization of flow reactor

A syringe containing dichloromethane was loaded onto the syringe pump and the CO_2 cylinder was pressurized to 140 psi, and the Argon cylinder for the back pressure regulator (BPR) was pressurized to 100 psi. The pressure was allowed to equilibrate and the CO_2 mass flow controller was adjusted to the desired setting. The micro metering valve on the BPR was opened to maintain a slow bleed. After the pressure at the CO_2 inlet to the reactor stabilized, the temperature controllers were turned on and adjusted to the desired set point.

c. Reaction procedure and product quantification

After the temperature stabilized the syringes were replaced with those containing the reagent solution. The liquid flow rates were set to 10 mL/h until the liquid pressure just exceeded the system pressure, i.e. when flow starts. The liquid and gas flow rates were adjusted to obtain the desired residence times. After steady state was reached (2 residence times), the reaction mixture was withdrawn using the 6-way valve. Approximately 200 µL of the sample was withdrawn and the solvent removed *in-vacuo*. The crude mixture was analyzed using ^1H NMR (in $CDCl_3$) and the conversion was determined by comparing the ratio of the protons of the styrene oxide to the protons of the cyclic carbonate.

The styrene oxide conversion was studied as a function of residence time (Figure S8), temperature (Figure S9) and co-catalyst loading (Figure S10).

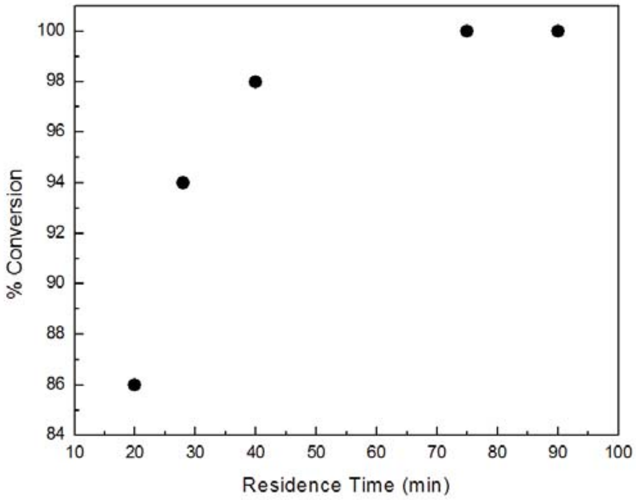


Figure S8. Effect of residence time on conversion of styrene oxide to styrene carbonate. Temperature = 100 °C, Al catalyst loading = 2 mol%, co-catalyst (Bu_4NI) = 10 mol%, concentration = 2M, CO_2 pressure = 110 psi.

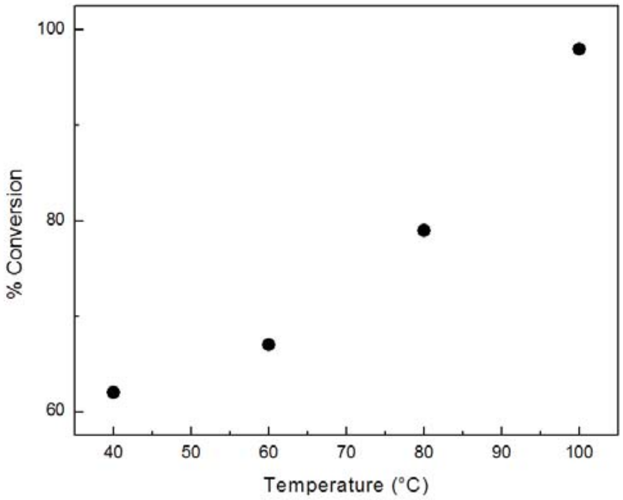


Figure S9. Effect of temperature on conversion of styrene oxide to styrene carbonate. Al catalyst loading = 2 mol%, co-catalyst (Bu_4NI) = 10 mol%, concentration = 2M, CO_2 pressure = 110 psi, residence time = 40 mins.

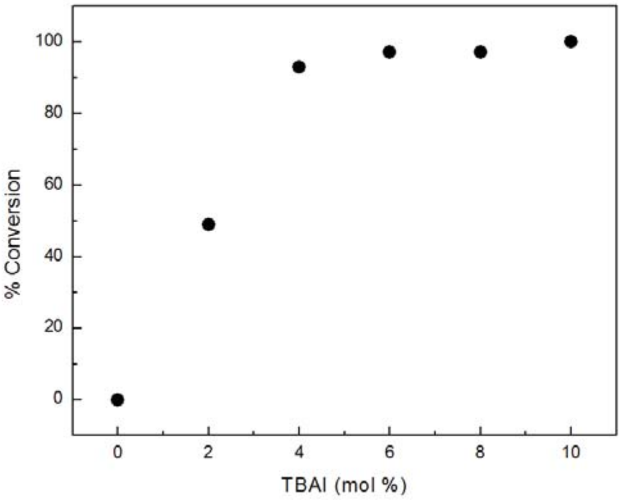


Figure S10. Effect of co-catalyst loading on conversion of styrene oxide to styrene carbonate. Al catalyst loading = 2 mol%, concentration = 2M, CO_2 pressure = 110 psi, residence time = 40 mins.

V. Procedure for sequential batch epoxidation and carboxylation of styrene

To a 20 mL three necked flask equipped with a reflux condensor, methyltrioxorhenium (30 mg), 1,4-dinitrobenzene (internal standard) (50.4 mg), olefin (12 mmol), 3-methylpyrazole (0.232 mL), and dichloromethane (to adjust final volume to 3 mL) were added together. This flask was placed in an ice bath and 6.4 mL of 30% H_2O_2 solution was added dropwise to the vial. Once the addition was complete the flask was removed from the ice bath and transferred to an oil bath set at 40 °C. The reaction was carried out for 30 minutes, after which the contents of the flask were transferred to a separating funnel. The aqueous and organic layer were separated and the organic layer was collected in a 20 mL vial.

To the vial was added the aluminum catalyst (0.124 g, 0.24 mmol), Bu_4NI (0.443g, 1.2mmol), DCM (2.4mL) and THF (0.6 mL). This was then transferred to an autoclave which was subsequently pressurized to 110 psi. The autoclave was placed in an oil bath maintained at 110 °C. After 45 minutes the autoclave was placed in an ice bath and once it cooled down to room temperature was vented.

An aliquot of the reaction mixture was withdrawn for NMR analysis in $CDCl_3$, which indicated a yield of 88% styrene carbonate.

VI. General procedure for the direct oxidative carboxylation of olefins

a. Preparation of reactant solutions

In a 20 mL scintillation vial, methyltrioxorhenium (30 mg), 1,4-dinitrobenzene (internal standard) (50.4 mg), olefin (12 mmol), 3-methylpyrazole (0.232 mL), and dichloromethane (to adjust final volume to 3 mL) were added together. The mixture was stirred until all the solids dissolved and subsequently transferred into a 5 mL gas tight glass syringe. Another 5 mL gas-tight glass syringe was filled with 30% H_2O_2 (aq) solution. In another 20 mL scintillation vial, the aluminum catalyst (0.124 g, 0.24 mmol), Bu_4NI (0.443g, 1.2mmol), DCM (2.4mL) and THF (0.6 mL) were combined. The mixture was stirred until all the solids were dissolved, and the solution loaded into a 5 mL gas-tight glass syringe after passing through a 0.2 μm PTFE syringe filter.

b. Initialization of flow reactor

The syringe pumps were initially loaded with syringes containing pure solvents, dichloromethane for the organic reaction streams and distilled water for the aqueous stream. All three pumps were started with an initial flow rate of 6 mL/h. The CO_2 cylinder was pressurized to 140 psi, and the Argon cylinder for the back pressure regulator (BPR) was pressurized to 100 psi. The pressure was allowed to equilibrate and the CO_2 mass flow controller was adjusted to the desired setting (1 sccm). The micro metering valve on the BPR was opened to maintain a slow bleed. After the pressure at the CO_2 inlet to the reactor stabilized, the temperature controllers were turned on and the epoxidation reactor was set to 40 °C and the carboxylation reactor was set to 100 °C.

c. Reaction procedure and product quantification

After the temperature stabilized the syringes were swapped with those containing the reagent solutions. The liquid flow rates were set to 10 mL/h until the liquid pressure reached the system pressure i.e. when flow starts. The liquid flow rates were then adjusted as follows: olefin – 0.32 mL/h; peroxide – 0.68 mL/h; and the carboxylation catalyst – 0.32 mL/h. The CO_2 flow rate was set at 1 sccm.

After steady segmented flow was seen, the system was run for 7 h. This ensures that the system is at steady-state when analyzing the reaction mixture. The reaction mixture was then withdrawn using a 6 way valve. Approximately 200 μL of the sample was withdrawn and the solvent removed *in-vacuo*. The crude mixture was analyzed using ^{1}H NMR (in $CDCl_3$) and the yield of the reaction is determined by comparing the ratio of the protons of the internal standard (1,4-dinitrobenzene) to the protons of the cyclic carbonate.

Once the reaction was completed, the flow reactor was depressurized by turning off the gas inlets and opening the micro metering valve to vent the BPR. The product collected in the BPR was chromatographed on silica gel using ethyl acetate/hexanes on a Combiflash Rf+.

VI. Procedure for ICP analysis of Re in reactor effluent.

50 μL of reactor effluent (aqueous or organic) was taken in a 20 mL scintillation vial. It was evaporated to dryness under vacuum. To the residue was added 2 mL of conc. HNO_3 which was subsequently boiled off to digest all the Re. To this solution was added 10 mL of 2% HNO_3 solution and the resulting solution was filtered through a 0.2 μm PTFE syringe filter. The solution was analyzed by ICP-OES to determine the concentration of the rhenium in each phase.

It was found that the Re partitioned to 56% in the aqueous and 44% in the organic phase.

VII. Reactor Setup

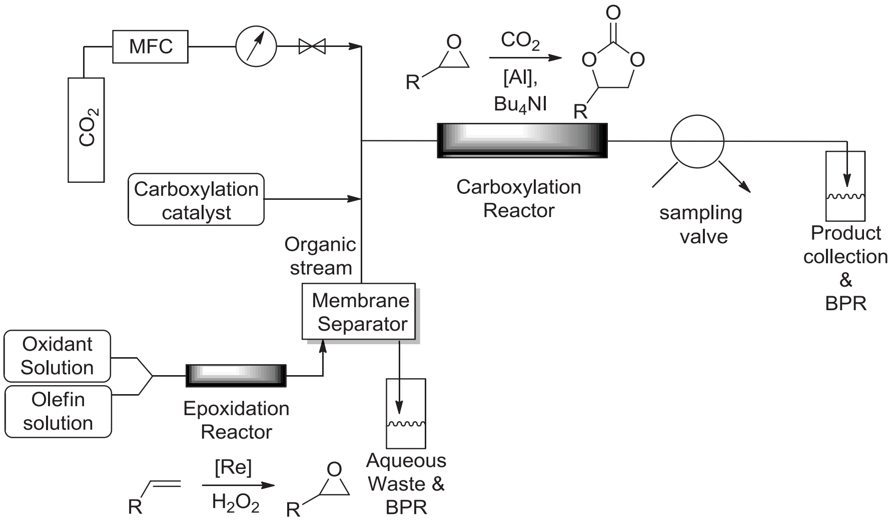


Figure S11. Reactor setup for oxidative carboxylation of olefins.

The oxidative carboxylation reactor was setup as shown in Figure S11. The organic solution, containing the olefin, catalyst and co-catalyst, and the aqueous peroxide solution were loaded into gas-tight syringes and introduced into the system using syringe pumps. The fluidic connections were made using either flat bottom or compression fittings. The streams were mixed using a T-mixer before entering the epoxidation reactor, which was made from 1/8" PTFE tubing and packed with sand. A PTFE membrane based separator was utilized to partition the aqueous and organic phases coming out of the epoxidation reactor. The aqueous phase was sent to a bulk collection vessel and the separator outlet containing the organic stream was mixed with the carboxylation catalyst solution in another T-mixer. This solution was then mixed with CO_2 gas which was introduced from a mass flow controller. The gas-liquid segmented flow then entered the carboxylation reactor, made from 1/8" stainless steel tubing and packed with sand. The back pressure of the system was set by pressurizing the bulk collection vessels with Argon. The temperature of both reactors was maintained using heat tape and a PID temperature controller. Effluent sampling from the carboxylation reactor was done using a 6-way valve.

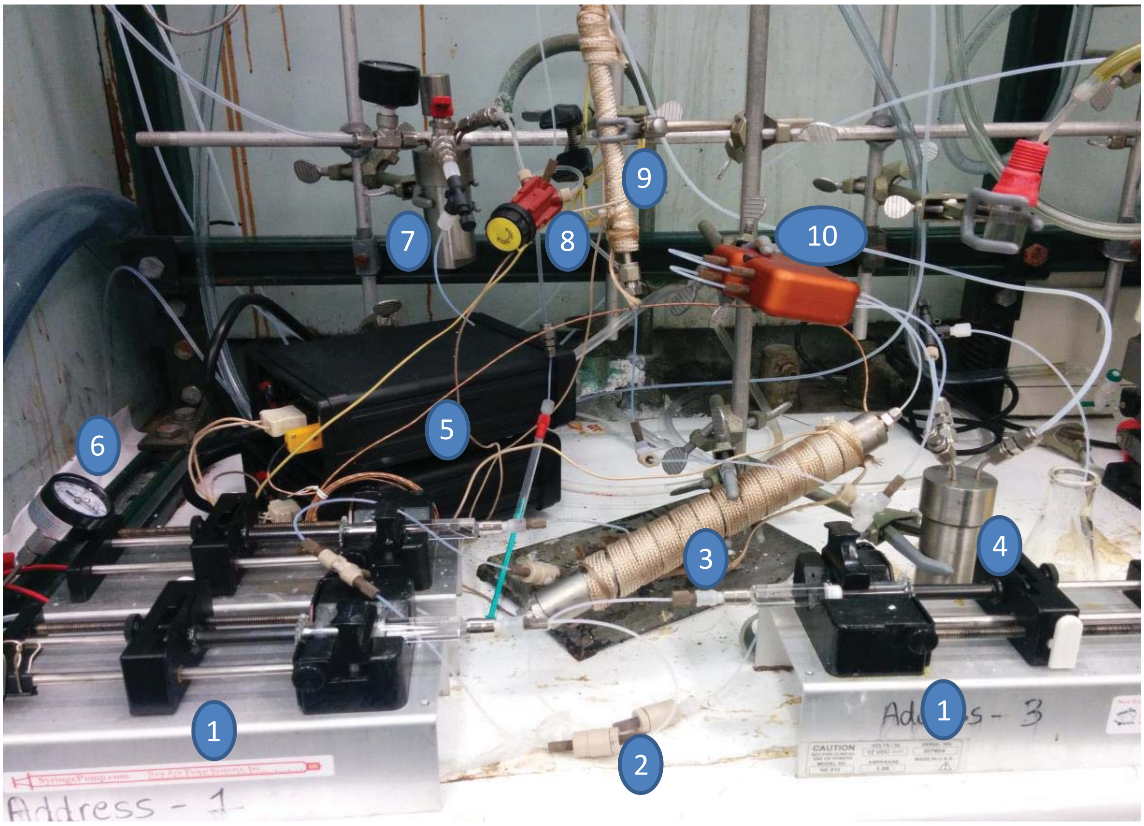


Figure S12. Reactor set-up: (1) syringe pumps, (2) check valves, (3) epoxidation reactor, (4) BPR and aqueous waste, (5) temperature controller, (6) pressure gauge, (7) BPR and product collection, (8) sampling valve, (9) carboxylation reactor, (10) membrane separator.

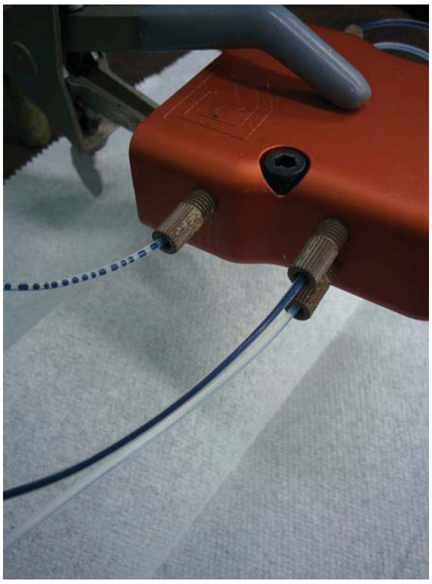


Figure S13: The membrane separator splitting an inlet stream of food dye (aqueous) and dichloromethane (organic) into respective components.

VIII. Reactor parts list

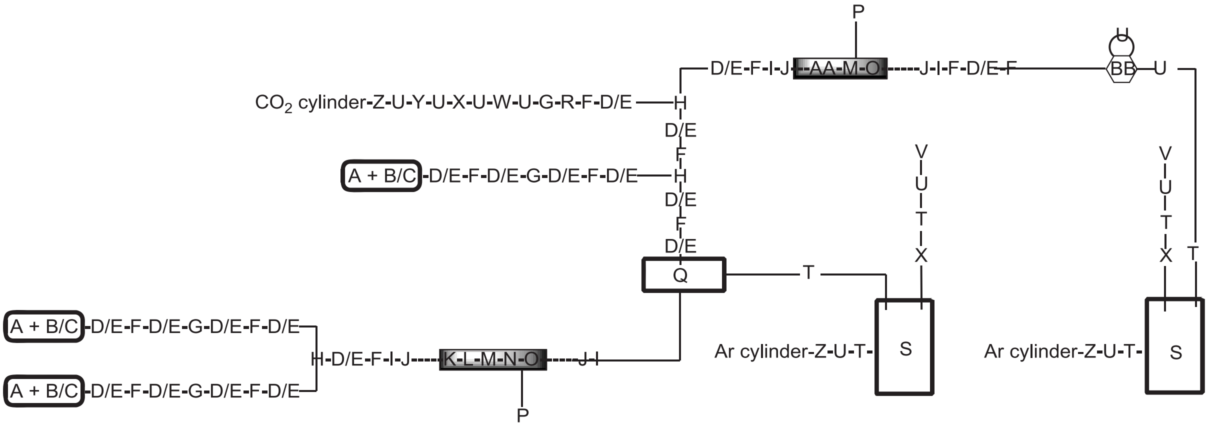
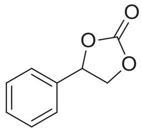


Figure S14. Components used for construction of the reactor set-up in Figure S12. For details on vendors and part numbers, see Table S1.

Table S1: Oxidative carboxylation reactor parts list

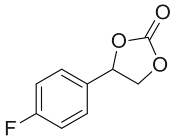
Item	Vendor	Part #	Part description
A	New Era Pump Systems Inc.	NE-510	Syringe pump
B	Hamilton	81520	5 mL glass syringe
C	IDEX H&S	P-628/P-678	Luer adapter
D	IDEX H&S	P-287	Super flangeless nut for 1/16” tubing
E	IDEX H&S	P-250	Super flangeless ferrule for 1/16” tubing
F	Zeus tubing	IWTT-063-C	1/16” PTFE tubing (1/32” ID)
G	IDEX H&S	CV-3330	Check valve
H	IDEX H&S	P-632	Mixing tee
I	Swagelok	SS-400-6-1	Steel reducing union, 1/4" x 1/16”
J	Sigma Aldrich	18421	Glass wool
K	Saint Gobain	TSPF35-0250-062-25	1/4” PTFE tubing (1/8” ID) (epoxidation reactor)
L	Fischer Scientific	S23-3	Sand for packed bed reactor
M	Fischer Scientific	S25-500	Sand for heating reactor
N	McMaster Carr		Aluminum tube for heating reactor
O	N/A	N/A	Heat tape
P	Auber Instruments	WS-1510DPM	PID temperature controller & thermocouple
Q	Zaiput Flow Technologies	SEP10	Membrane Separator with 0.2 µm membrane from sterlitech
R	Swagelok	SS-200-6-1	Steel reducing union, 1/8” x 1/16”
S	PSU ChE Machine Shop	N/A	Autoclave
T	Swagelok	SS-200-6	Steel union, 1/8”
U	McMaster Carr	5239K24	1/8” PTFE tubing (1/16” ID)
V	IDEX H&S	P-445	Micro metering valve
W	Hoke	7155G2Y	Shut off valve
X	McMaster Carr	2227T44	Pressure gauge
Y	Tylan	FC-260V/AA9304091	MFC (0-10 sccm CO_2)
Z	Air Gas		Gas regulators
AA	Swagelok	89785K824	1/4" steel tubing (0.18” ID) (carboxylation reactor)
BB	IDEX H&S	V-540	6-way valve

IX. Characterization Data



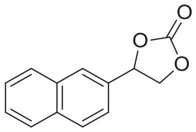
(a) 4-phenyl-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.47-7.26 (m, 5H), 5.70 (t, 1H, J = 8 Hz), 4.82 (t, 1H, J = 8.4 Hz), 4.35 (t, 1H, J = 8 Hz); ^{13}C ($CDCl_3$, 75 MHz) δ = 154.9, 135.8, 129.7, 129.2, 125.9, 78.0, 71.2. HRMS calculated for $C_9H_{12}NO_3$ $[M+NH_4]^+$: 182.0817. Found: 182.0831. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.35



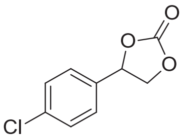
(b) 4-(4-fluorophenyl)-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.40-7.35 (m, 2H), 7.15-7.09 (m, 2H), 5.72 (t, 1H, J = 8 Hz), 4.84 (t, 1H, J = 8.5 Hz), 4.36 (t, 1H, J = 8.3 Hz); ^{13}C ($CDCl_3$, 75 MHz) δ = 165.0, 161.7, 154.8, 131.7, 131.7, 128.2, 128.1, 116.4, 116.1, 77.6, 71.2. HRMS: calculated for $C_9H_7O_3F$: 182.0379. Found: 182.0370. Rf (silica gel with 30% EtOAc in Hexanes as eluent): 0.28



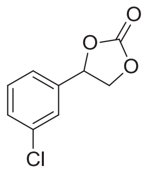
(c) 4-(naphthalen-2-yl)-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.87-7.77 (m, 4H), 7.52-7.49 (m, 2H), 7.37 (dd, 1H, J = 8.5, 1.6 Hz), 5.78 (t, 1H, J = 8 Hz), 4.81 (t, 1H, J = 9 Hz), 4.38 (t, 1H, J = 9 Hz); ^{13}C ($CDCl_3$, 75 MHz) δ = 155.0, 133.6, 132.9, 132.8, 129.4, 128.1, 127.8, 127.1, 126.9, 125.9, 122.5, 78.2, 71.0. HRMS calculated for $C_{13}H_{14}NO_3$ $[M+NH_4]^+$: 232.0974. Found: 232.0955. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.28



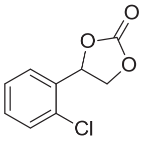
(d) 4-(4-chlorophenyl)-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.40 (d, 2H, J = 9 Hz), 7.32 (d, 2H, J = 9 Hz), 5.71 (t, 1H, J = 9 Hz), 4.85 (t, 1H, J = 9 Hz), 4.33 (t, 1H, J = 9 Hz); ^{13}C ($CDCl_3$, 75 MHz) δ = 154.8, 135.5, 134.4, 129.4, 127.5, 77.3, 71.0. HRMS: calculated for $C_9H_7O_3Cl$: 198.0084. Found: 198.0074.. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.36



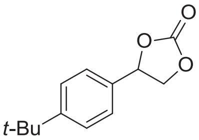
(e) 4-(3-chlorophenyl)-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.39-7.37 (m, 3H), 7.27-7.24 (m, 1H), 5.70 (t, 1H, J = 7.9 Hz), 4.86 (t, 1H, J = 8.5 Hz), 4.34 (t, 1H, J = 8.2 Hz); ^{13}C ($CDCl_3$, 75 MHz) δ = 154.6, 137.9, 135.1, 130.6, 129.8, 126.0, 123.9, 77.0, 71.0. HRMS: calculated for $C_9H_7O_3Cl$: 198.0084. Found: 198.0074. Rf (silica gel with 30% EtOAc in Hexanes as eluent): 0.42



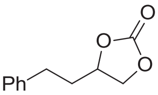
(f) 4-(2-chlorophenyl)-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.50-7.47 (m, 1H), 7.41-7.33 (m, 3H), 6.00 (t, 1H, *J* = 9 Hz), 4.99 (t, 1H, *J* = 8.5 Hz), 4.27 (t, 1H, *J* = 8 Hz); ^{13}C ($CDCl_3$, 75 MHz) δ = 154.7, 134.5, 131.1, 130.4, 129.9, 127.6, 126.2, 75.0, 70.4. HRMS calculated for $C_9H_{11}ClNO_3$ $[M+NH_4]^+$: 216.0427. Found: 216.0436. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.38



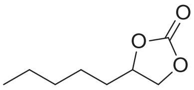
(g) 4-(4-(tert-butyl)phenyl)-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 400 MHz) δ = 7.45 (d, 2H, *J* = 8.4 Hz), 7.31 (d, 2H, *J* = 8 Hz), 5.66 (t, 1H, *J* = 8 Hz), 4.77 (t, 1H, *J* = 8.4 Hz), 4.33 (t, 1H, *J* = 8 Hz), 1.31 (s, 9H); ^{13}C ($CDCl_3$, 75 MHz) δ = 155.0, 152.9, 132.8, 126.1, 125.9, 78.0, 71.1, 34.7, 31.2. HRMS calculated for $C_{13}H_{20}NO_3$ $[M+NH_4]^+$: 238.1443. Found: 238.1438. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.45



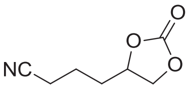
(h) 4-phenethyl-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 7.29-7.13 (m, 5H), 4.61-4.57 (m, 1H), 4.39 (t, 1H, *J* = 9 Hz), 3.97 (t, 1H, *J* = 9 Hz), 2.76-2.63 (m, 2H), 2.03-1.88 (m, 2H); ^{13}C ($CDCl_3$, 75 MHz) δ = 155.1, 140.0, 128.6, 128.4, 126.4, 76.2, 69.3, 35.3, 30.7. HRMS calculated for $C_{11}H_{16}NO_3$ $[M+NH_4]^+$: 210.1130. Found: 210.1132. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.30



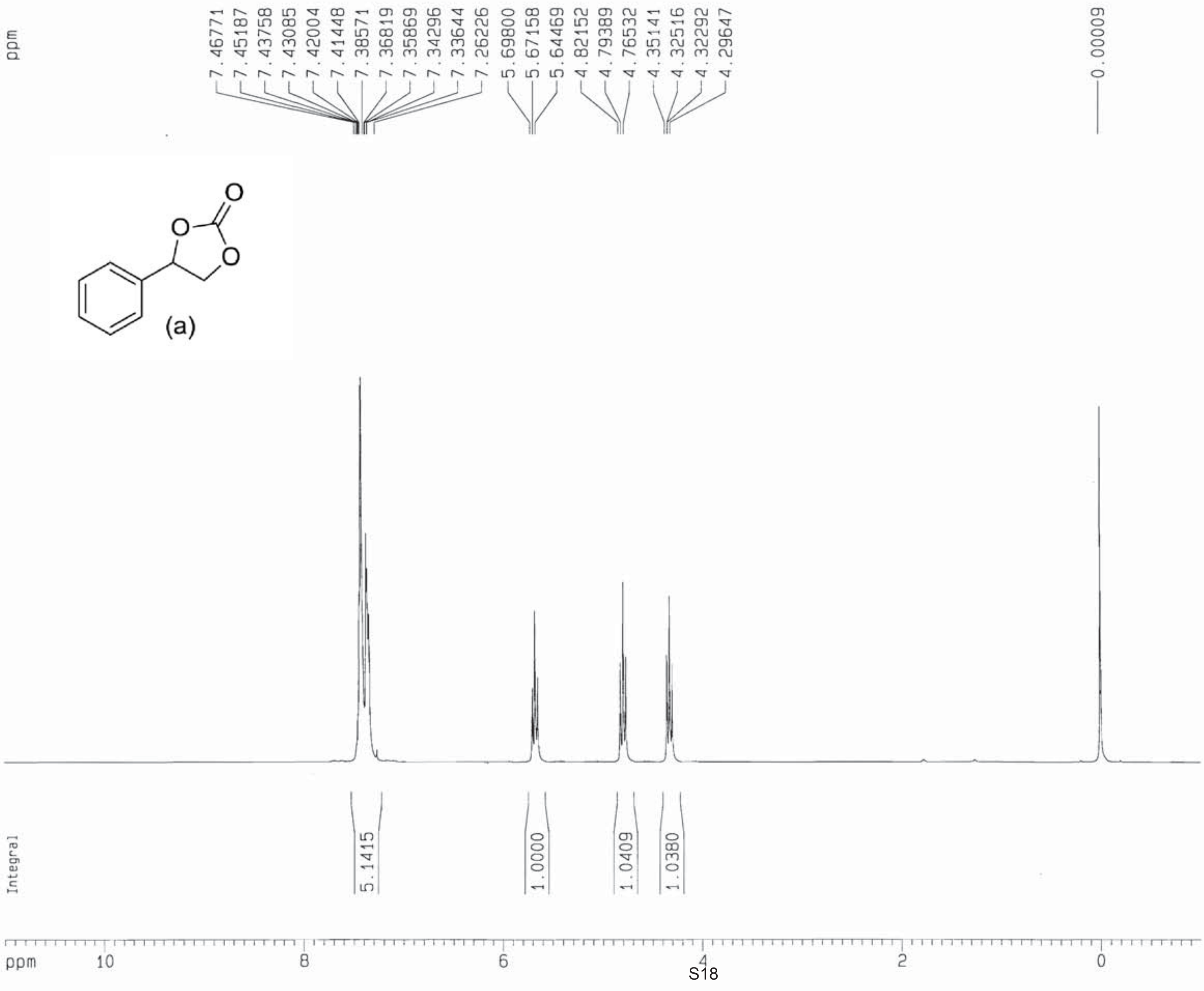
(i) 4-pentyl-1,3-dioxolan-2-one

^{1}H ($CDCl_3$, 300 MHz) δ = 4.74-4.70 (m, 1H), 4.57 (t, 1H, *J* = 9 Hz), 4.10 (t, 1H, *J* = 9 Hz), 1.82-1.65 (m, 2H), 1.48-1.30 (m, 8H), 0.89 (t, 3H); ^{13}C ($CDCl_3$, 75 MHz) δ = 155.2, 69.5, 33.9, 31.5, 28.8, 24.4, 22.5, 14.0. HRMS calculated for $C_8H_{18}NO_3$ $[M+NH_4]^+$: 176.1287. Found: 176.1269. R_f (silica gel with 30% EtOAc in Hexanes as eluent): 0.31

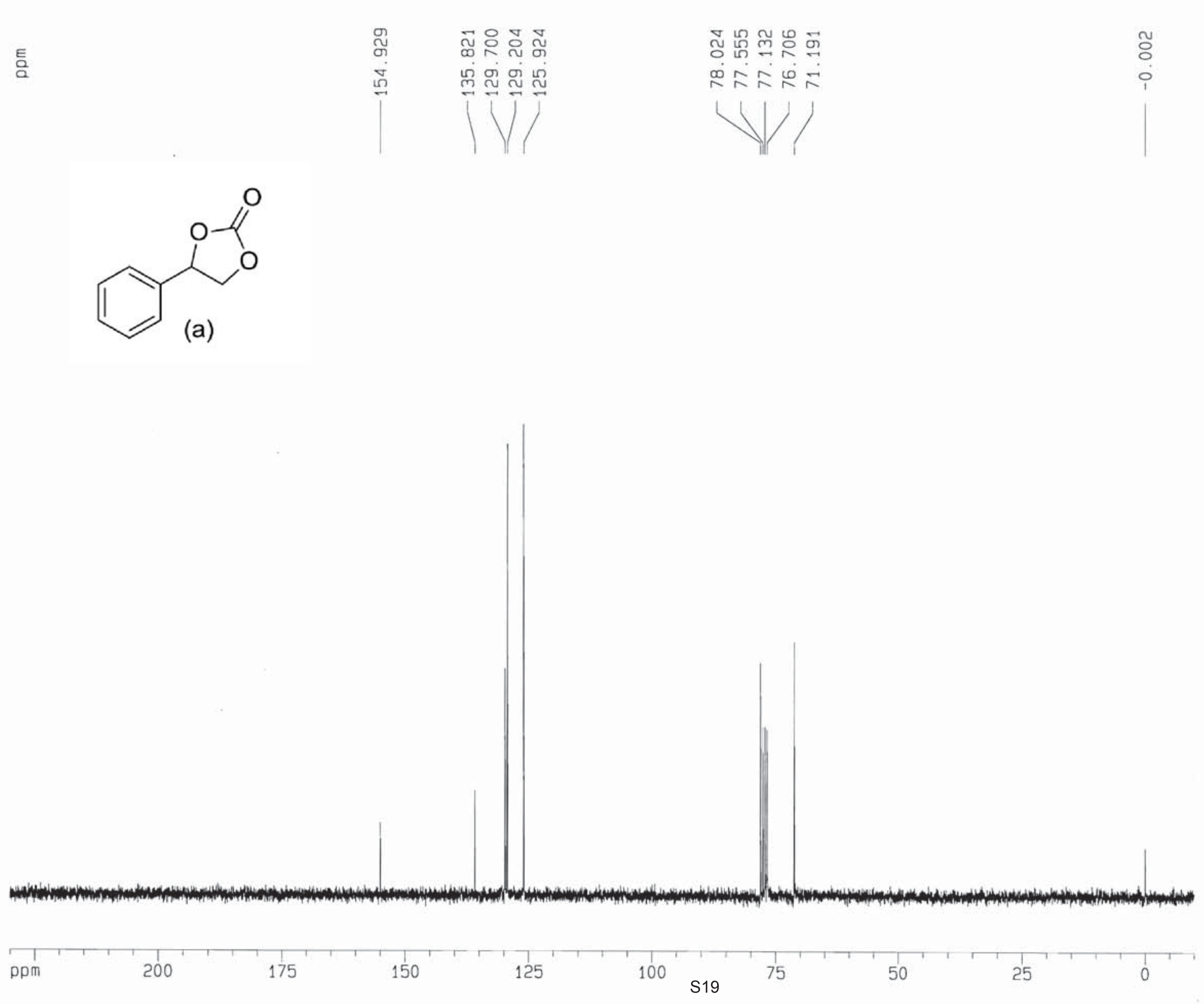


(j) 4-(2-oxo-1,3-dioxolan-4-yl)butanenitrile

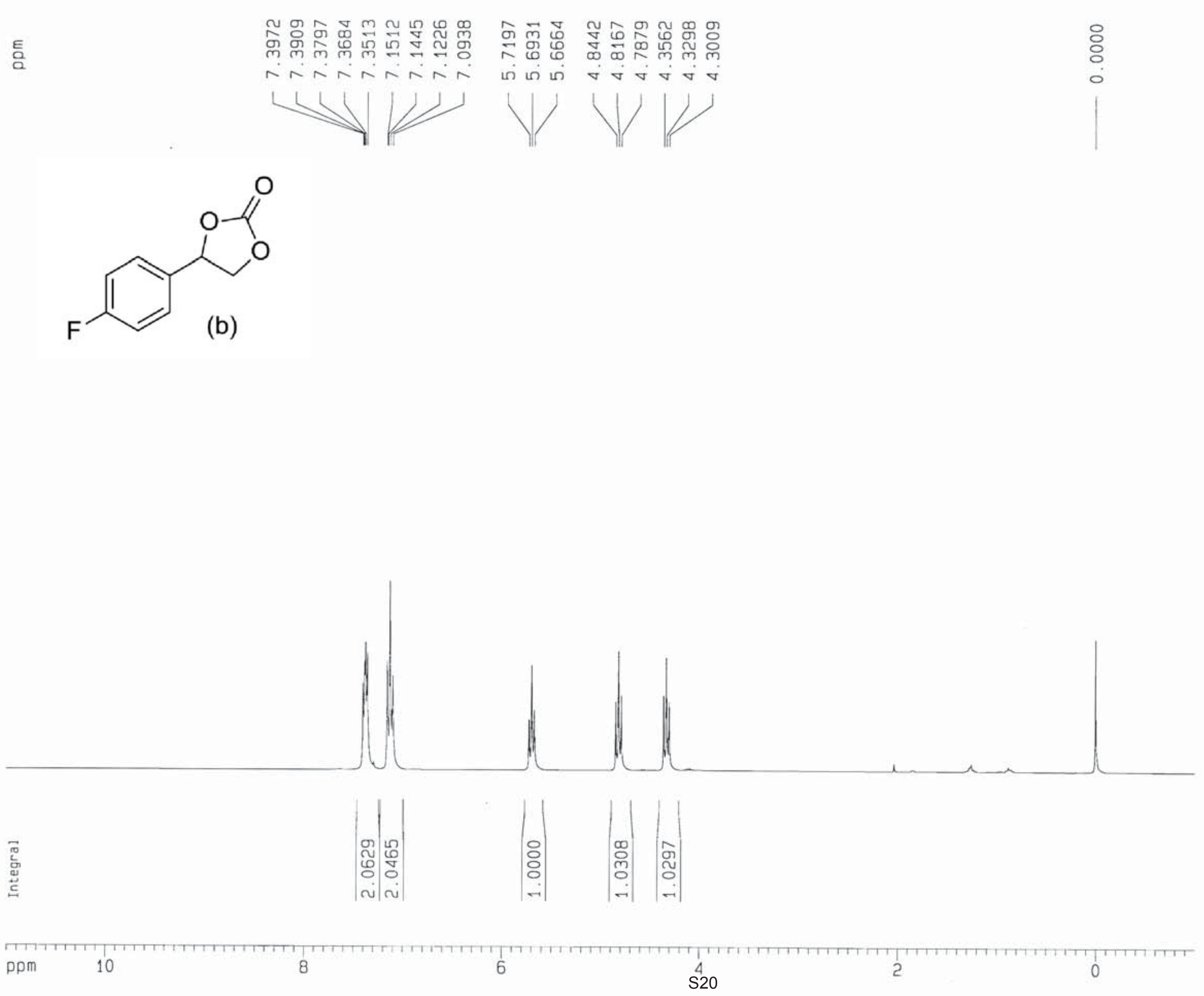
^{1}H ($CDCl_3$, 300 MHz) δ = 4.80 (t, 1H, *J* = 6 Hz), 4.61 (t, 1H, *J* = 8.2 Hz), 4.14 (t, 1H, *J* = 8 Hz), 2.49-2.45 (m, 2H), 1.91-1.75 (m, 4H); ^{13}C ($CDCl_3$, 75 MHz) δ = 155.0, 119.6, 76.4, 69.3, 32.5, 20.9, 16.6. HRMS calculated for $C_7H_{13}N_2O_3$ $[M+NH_4]^+$: 173.0926. Found: 173.0919. R_f (silica gel with 50% EtOAc in Hexanes as eluent): 0.23



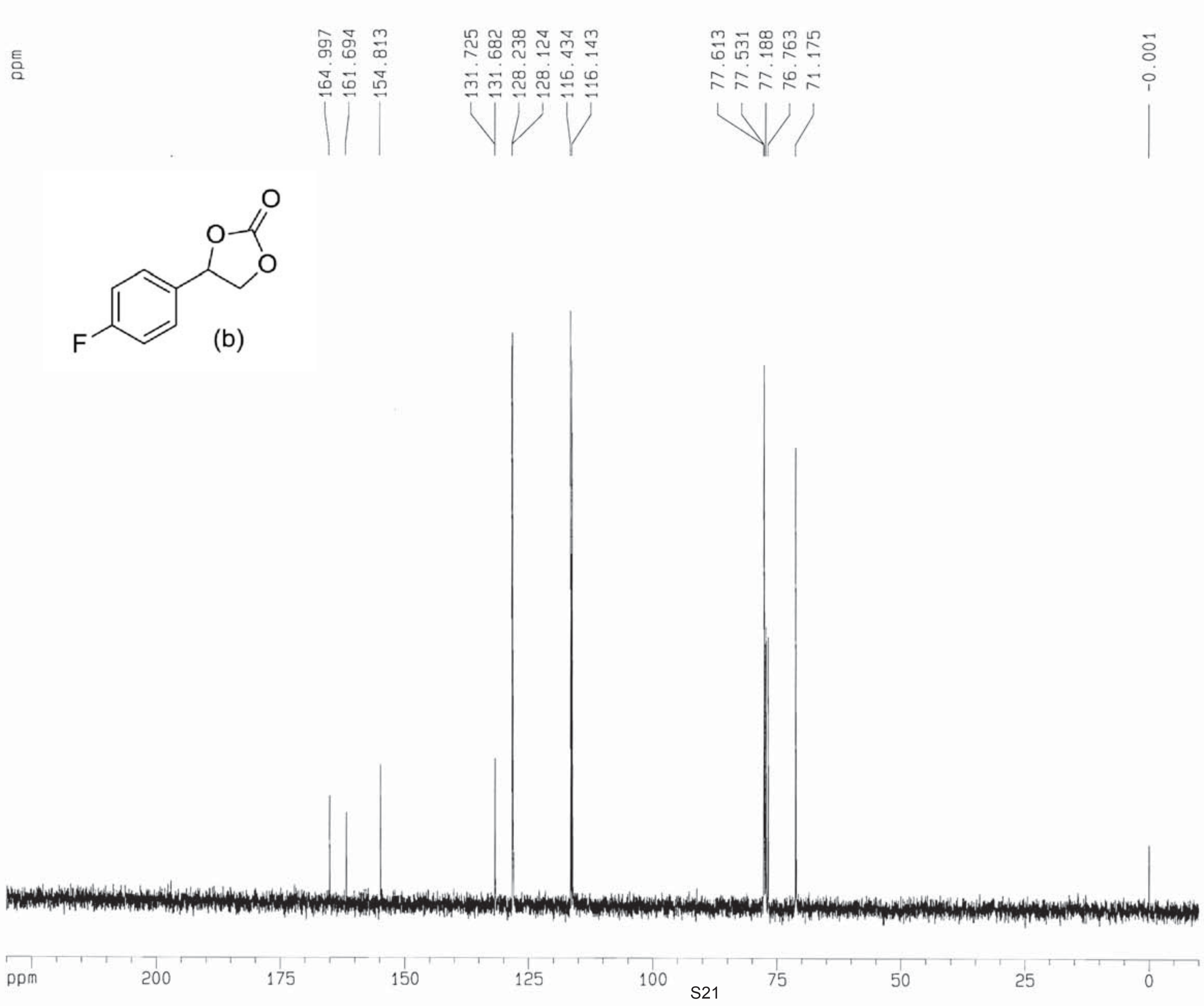
```
Current Data Parameters
NAME          styrenecarb
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151207
Time                17.45
INSTRUM             spect
PROBHD    5 mm QNP 1H/1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ            5.3084660 sec
RG                   80.6
DW               81.000 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec

============ CHANNEL f1 ========
NUC1                   1H
P1                  12.10 usec
PL1                  0.00 dB
SFO1          299.8718518 MHz

F2 - Processing parameters
SI                  32768
SF            299.8700089 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
F1P                11.000 ppm
F1                3298.57 Hz
F2P                -1.000 ppm
F2                -299.87 Hz
PPMCM             0.60000 ppm/cm
HZCM            179.92200 Hz/cm
```



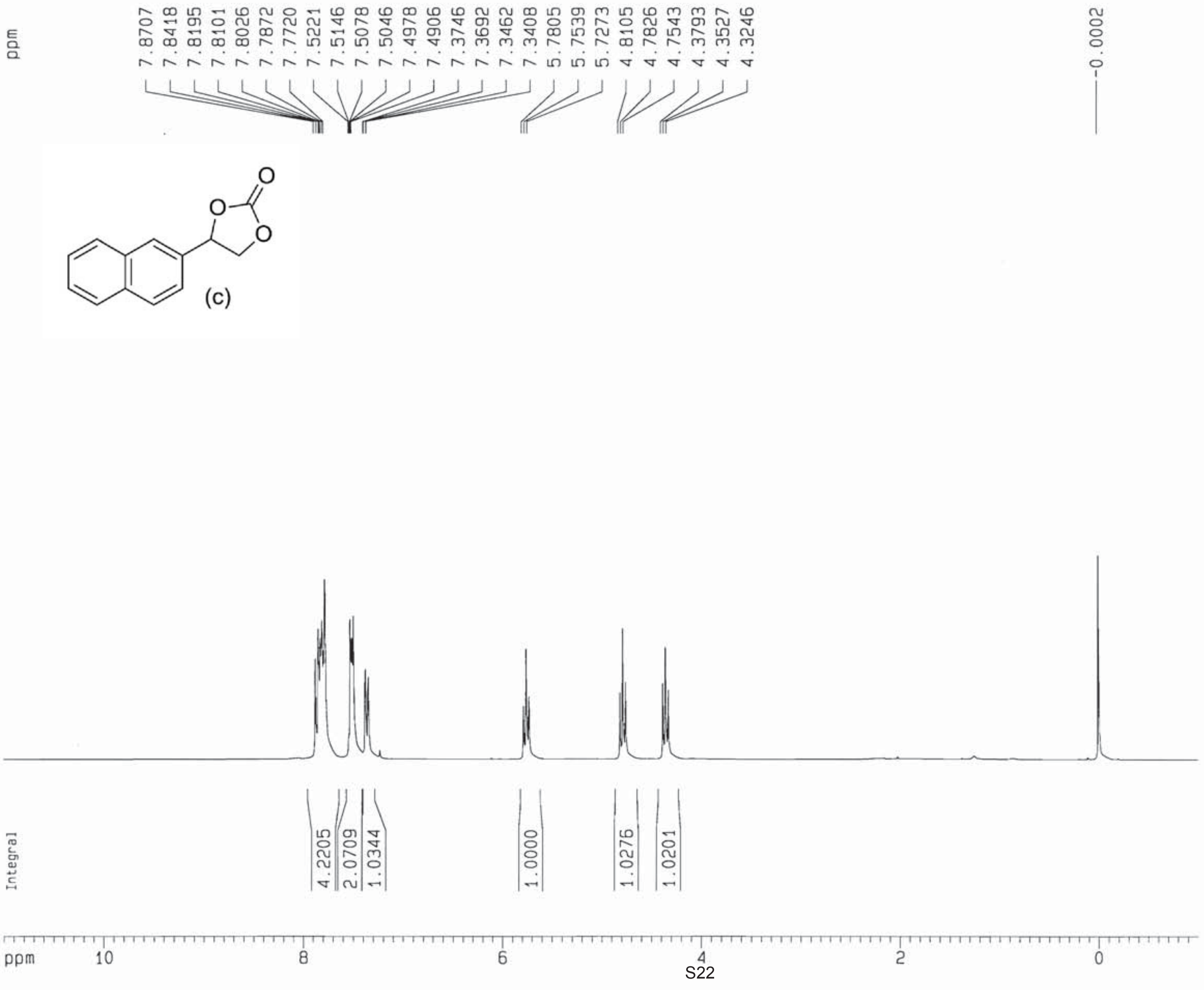
```
Current Data Parameters
NAME          styrenecarb
EXPNO                   8
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151207
Time               17.49
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    28
DS                     4
SWH            18796.992 Hz
FIDRES          0.286819 Hz
AQ             1.7433076 sec
RG                  4096
DW                26.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                  5.25 usec
PL1                -6.00 dB
SFO1         75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             115.00 usec
PL2                 0.00 dB
PL12               19.70 dB
PL13               19.70 dB
SFO2        299.8711995 MHz

F2 - Processing parameters
SI                 32768
SF            75.4023753 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              230.000 ppm
F1              17342.54 Hz
F2P              -10.000 ppm
F2               -754.02 Hz
PPMCM           12.00000 ppm/cm
HZCM           904.82849 Hz/cm
```



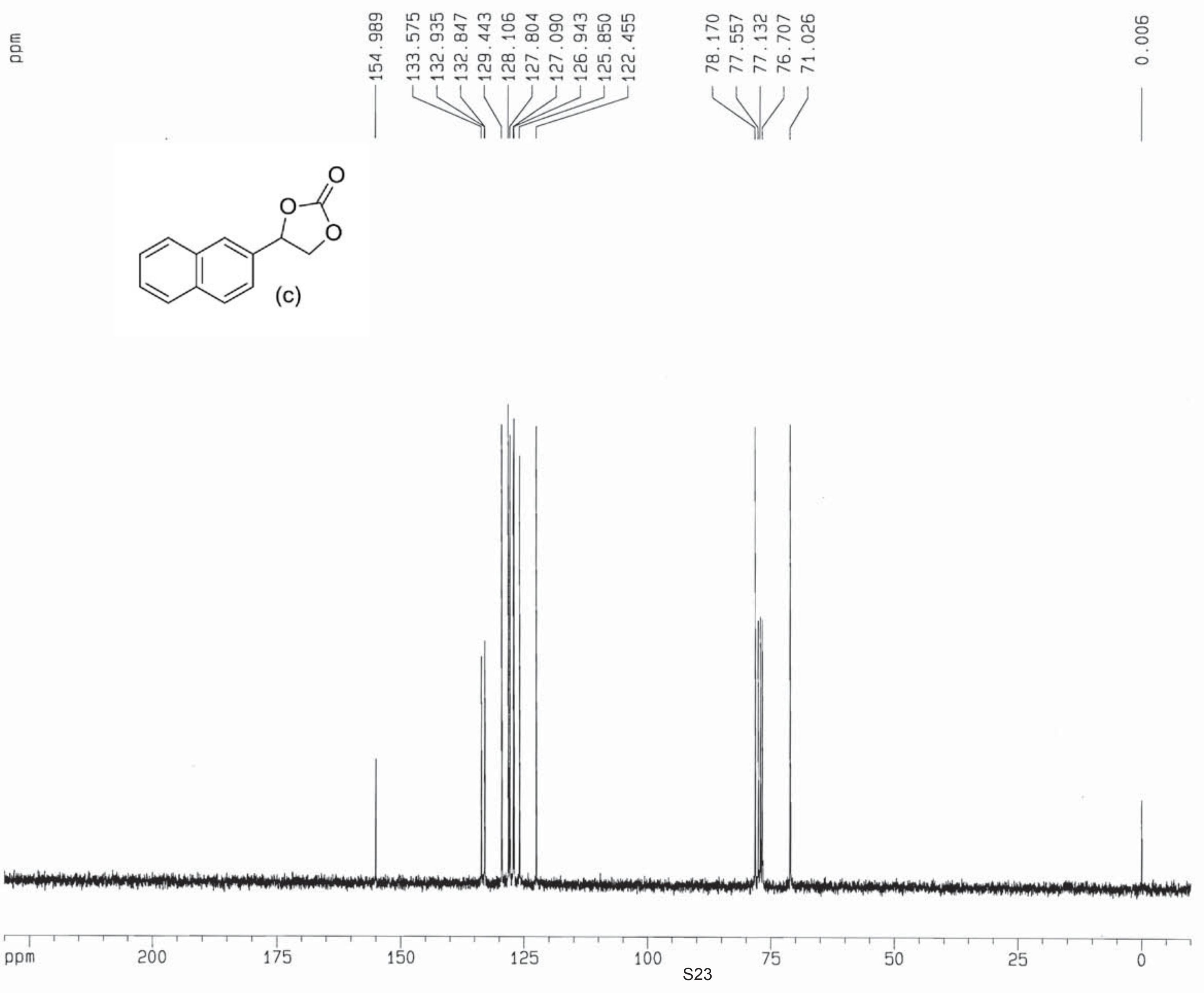
```
Current Data Parameters
NAME          4_Fstycarb
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151207
Time               10.07
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ           5.3084660 sec
RG                  80.6
DW              81.000 usec
DE                6.00 usec
TE               300.0 K
D1          1.00000000 sec

============ CHANNEL f1 ========
NUC1                  1H
P1               12.10 usec
PL1               0.00 dB
SF01        299.8718518 MHz

F2 - Processing parameters
SI                 32768
SF          299.8700006 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
F1P               11.000 ppm
F1               3298.57 Hz
F2P               -1.000 ppm
F2               -299.87 Hz
PPMCM            0.60000 ppm/cm
HZCM           179.92200 Hz/cm
```



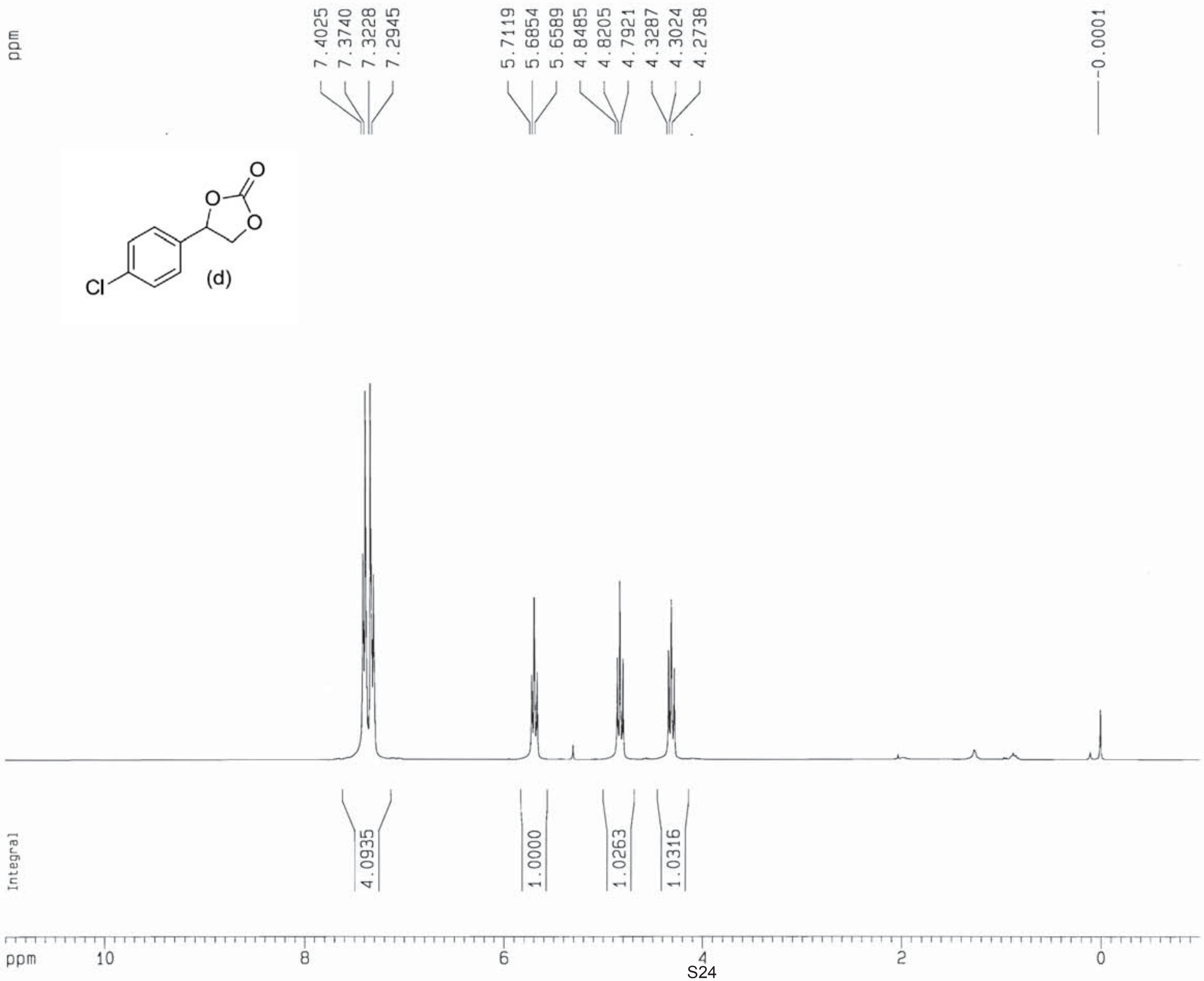
```
Current Data Parameters
NAME          4_Fstycarb
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151207
Time               10.09
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    42
DS                     4
SWH           18796.992 Hz
FIDRES         0.286819 Hz
AQ            1.7433076 sec
RG                  2048
DW                26.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ===========
NUC1                 13C
P1                  5.25 usec
PL1                -6.00 dB
SFO1         75.4106357 MHz

============ CHANNEL f2 ===========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             115.00 usec
PL2                 0.00 dB
PL12               19.70 dB
PL13               19.70 dB
SFO2        299.8711995 MHz

F2 - Processing parameters
SI                 32768
SF            75.4023713 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              230.000 ppm
F1              17342.54 Hz
F2P              -10.000 ppm
F2               -754.02 Hz
PPMCM           12.00000 ppm/cm
HZCM           904.82849 Hz/cm
```



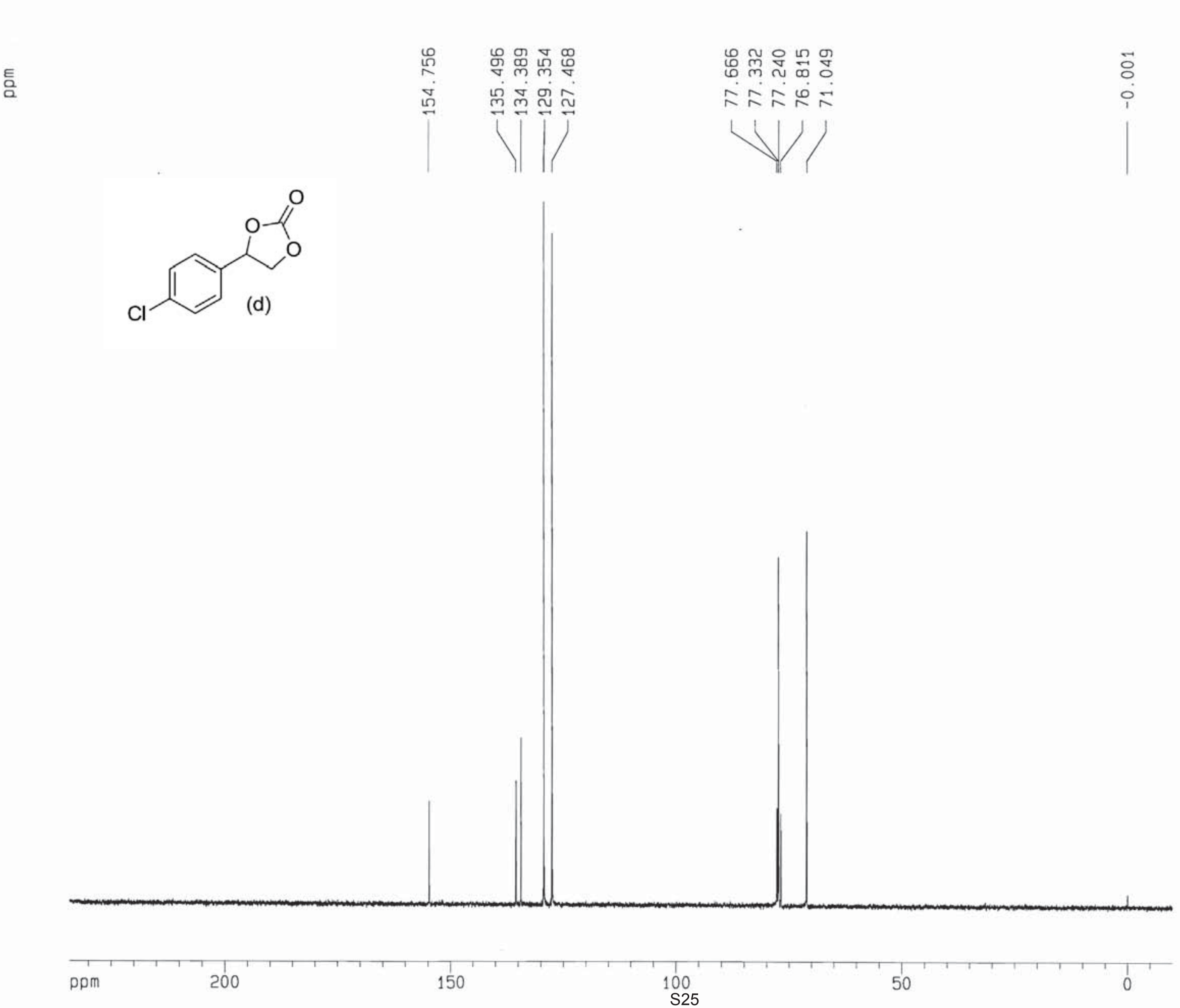
```
Current Data Parameters
NAME              nap_carb
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20151128
Time                 14.32
INSTRUM              spect
PROBHD    5 mm QNP 1H/1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ           5.3084660 sec
RG                    80.6
DW            81.000 usec
DE              6.00 usec
TE               300.0 K
D1        1.00000000 sec

============ CHANNEL f1 ========
NUC1                    1H
P1             12.10 usec
PL1               0.00 dB
SFO1    299.8718518 MHz

F2 - Processing parameters
SI                   32768
SF        299.8700196 MHz
WDW                     no
SSB                      0
LB                 0.00 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                20.00 cm
F1P             11.000 ppm
F1             3298.57 Hz
F2P             -1.000 ppm
F2             -299.87 Hz
PPMCM      0.60000 ppm/cm
HZCM     179.92201 Hz/cm
```



```
Current Data Parameters
NAME            nap_carb
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151128
Time               14.45
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   165
DS                     4
SWH            18796.992 Hz
FIDRES          0.286819 Hz
AQ             1.7433076 sec
RG                3649.1
DW                26.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                  5.25 usec
PL1                -6.00 dB
SFO1         75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             115.00 usec
PL2                 0.00 dB
PL12               19.70 dB
PL13               19.70 dB
SFO2         299.8711995 MHz

F2 - Processing parameters
SI                 32768
SF            75.4023794 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              230.000 ppm
F1              17342.55 Hz
F2P              -10.000 ppm
F2               -754.02 Hz
PPMCM           12.00000 ppm/cm
HZCM           904.82861 Hz/cm
```

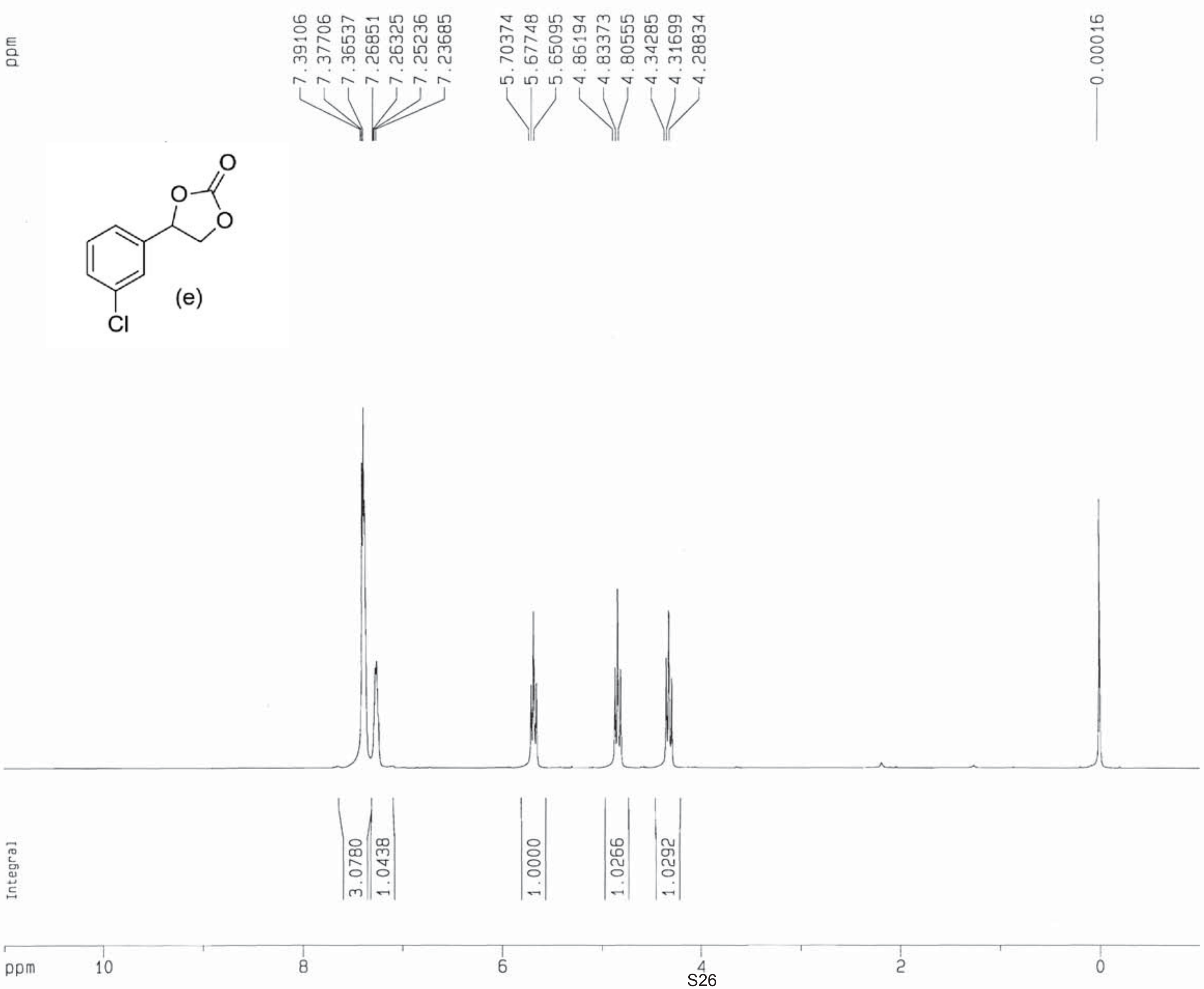


```
Current Data Parameters
NAME       4_Cl_stycarbo
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151111
Time               15.21
INSTRUM            spect
PROBHD    5 mm QNP 1H/1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ            5.3084660 sec
RG                    57
DW               81.000 usec
DE                 6.00 usec
TE                300.0 K
D1          1.00000000 sec

============ CHANNEL f1 ========
NUC1                  1H
P1                 12.10 usec
PL1                 0.00 dB
SFO1         299.8718518 MHz

F2 - Processing parameters
SI                 32768
SF           299.8699974 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
F1P               11.000 ppm
F1               3298.57 Hz
F2P               -1.000 ppm
F2               -299.87 Hz
PPMCM            0.60000 ppm/cm
HZCM           179.92200 Hz/cm
```

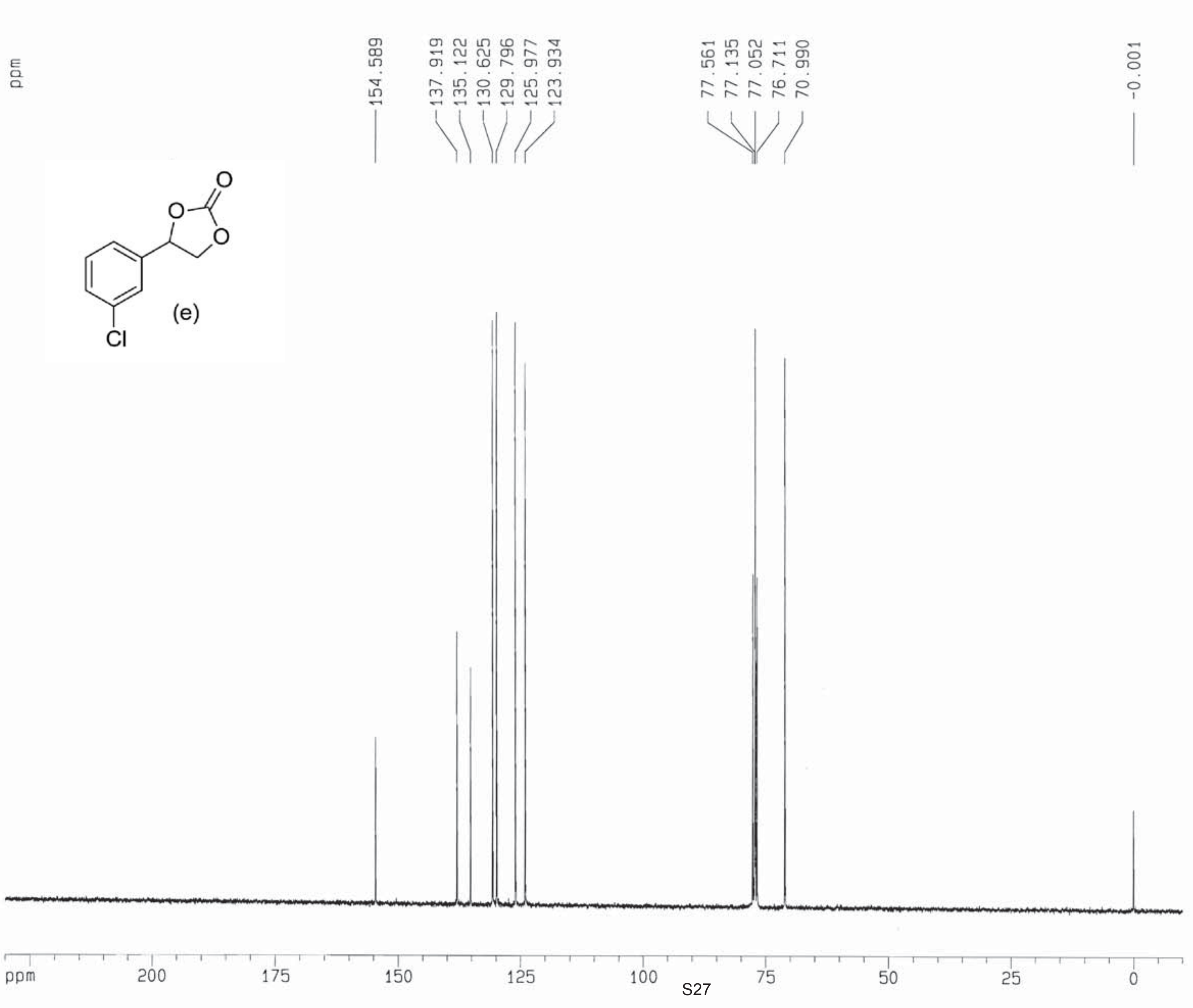


(d)

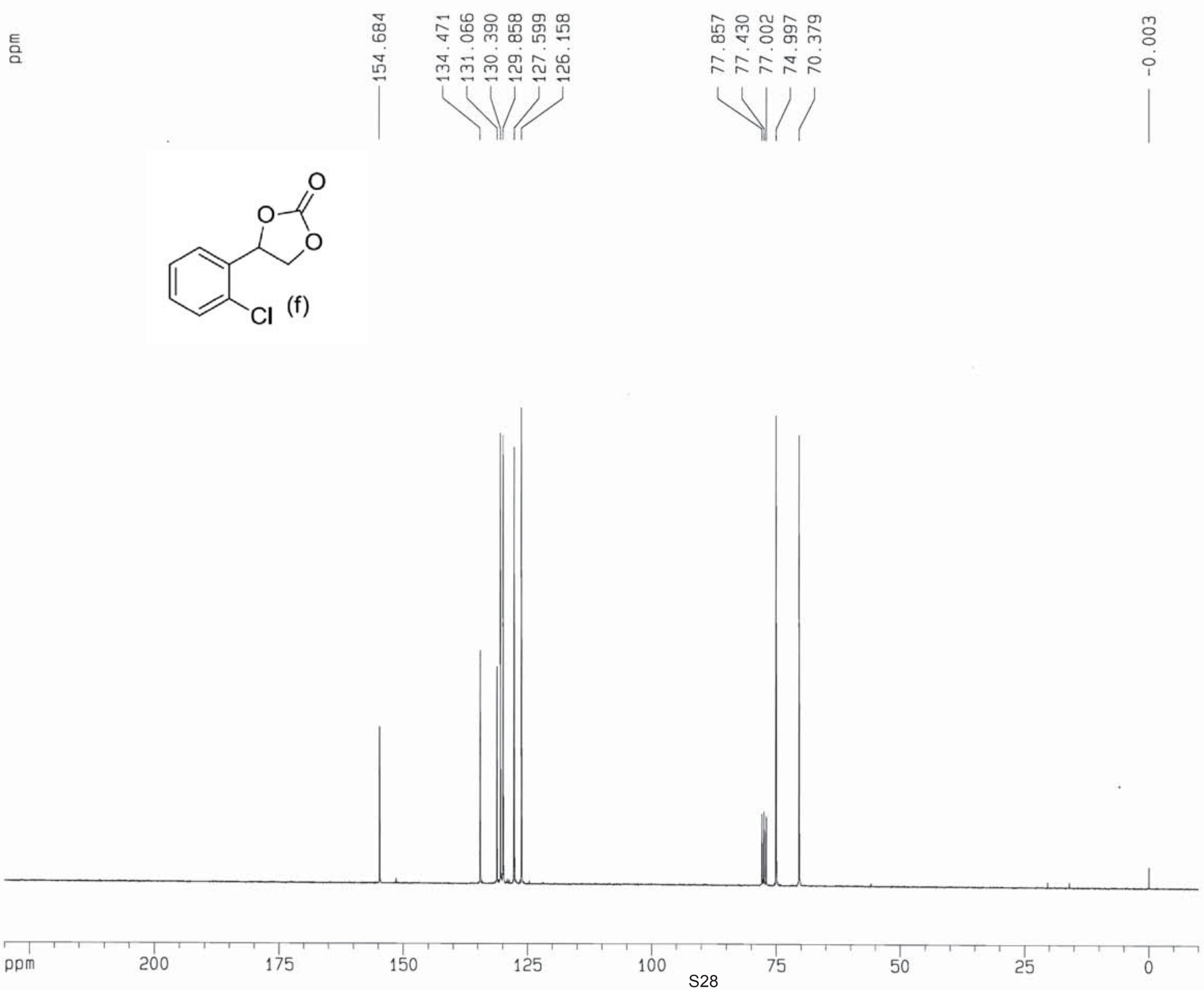
```
Current Data Parameters
NAME       4_Cl_stycarbo
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151111
Time               15.31
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   102
DS                     4
SWH           18796.992 Hz
FIDRES         0.286819 Hz
AQ            1.7433076 sec
RG                  4096
DW                26.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                  5.25 usec
PL1                -6.00 dB
SFO1          75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2           waltz16
NUC2                  1H
PCPD2             115.00 usec
PL2                 0.00 dB
PL12               19.70 dB
PL13               19.70 dB
SFO2         299.8711995 MHz

F2 - Processing parameters
SI                 32768
SF            75.4023753 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              250.000 ppm
F1              18850.59 Hz
F2P              -10.000 ppm
F2               -754.02 Hz
PPMCM           13.00000 ppm/cm
HZCM           980.23083 Hz/cm
```



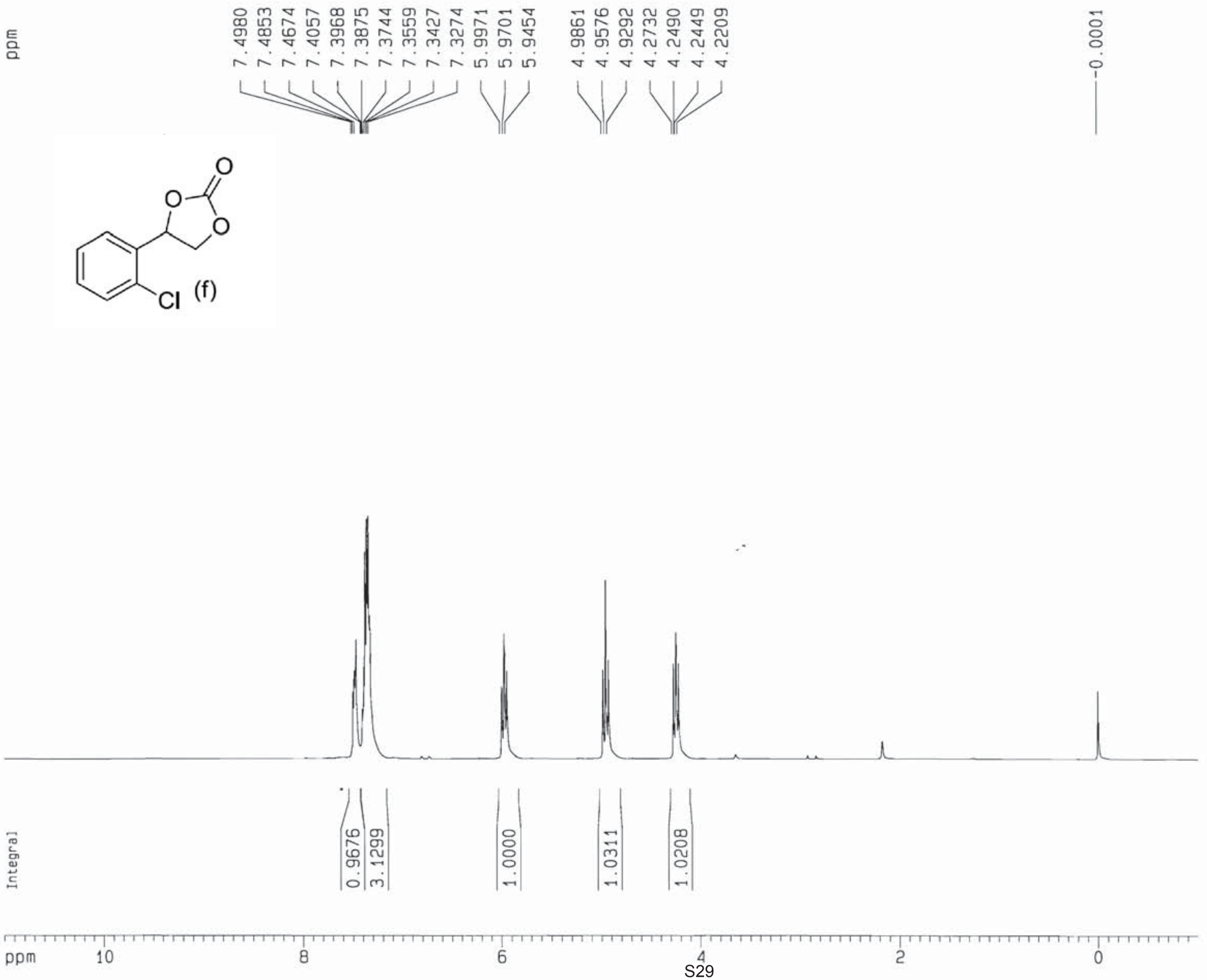
```
Current Data Parameters
NAME        3_Cl_sty_OC
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20151116
Time              17.27
INSTRUM           spect
PROBHD   5 mm QNP 1H/1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ            5.3084660 sec
RG                 80.6
DW               81.000 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec

============ CHANNEL f1 ========
NUC1                 1H
P1                12.10 usec
PL1                0.00 dB
SFO1        299.8718518 MHz

F2 - Processing parameters
SI                32768
SF          299.8700029 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
F1P              11.000 ppm
F1              3298.57 Hz
F2P              -1.000 ppm
F2              -299.87 Hz
PPMCM           0.60000 ppm/cm
HZCM          179.92200 Hz/cm
```



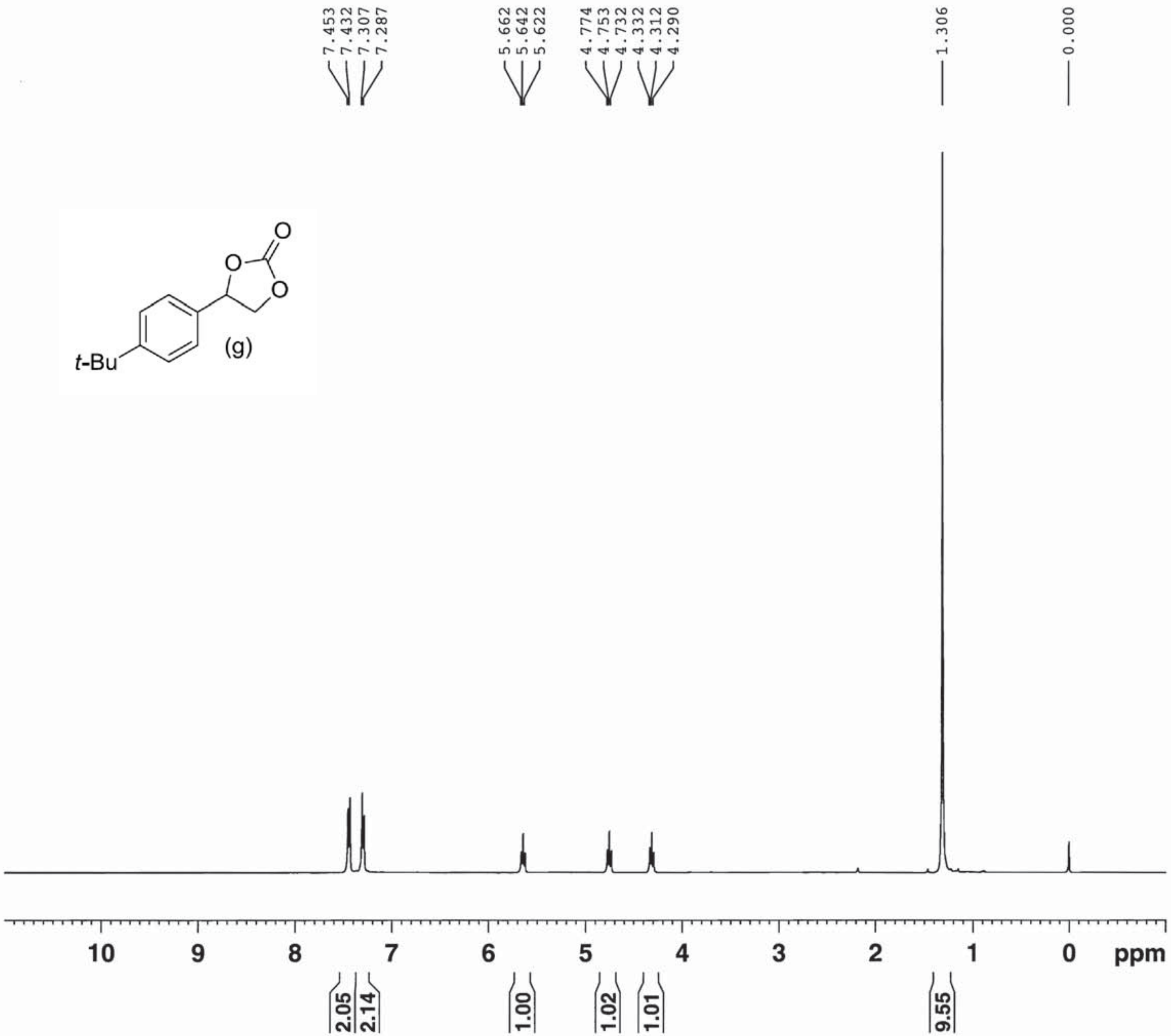
```
Current Data Parameters
NAME          3_Cl_sty_OC
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151116
Time                18.32
INSTRUM             spect
PROBHD    5 mm QNP 1H/1
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH            18796.992 Hz
FIDRES          0.286819 Hz
AQ             1.7433076 sec
RG                   2048
DW                 26.600 usec
DE                   6.00 usec
TE                  300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ===========
NUC1                  13C
P1                   5.25 usec
PL1                 -6.00 dB
SFO1          75.4106357 MHz

============ CHANNEL f2 ===========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              115.00 usec
PL2                  0.00 dB
PL12                19.70 dB
PL13                19.70 dB
SFO2         299.8711995 MHz

F2 - Processing parameters
SI                  32768
SF            75.4023748 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
F1P               230.000 ppm
F1               17342.54 Hz
F2P               -10.000 ppm
F2                -754.02 Hz
PPMCM            12.00000 ppm/cm
HZCM            904.82849 Hz/cm
```



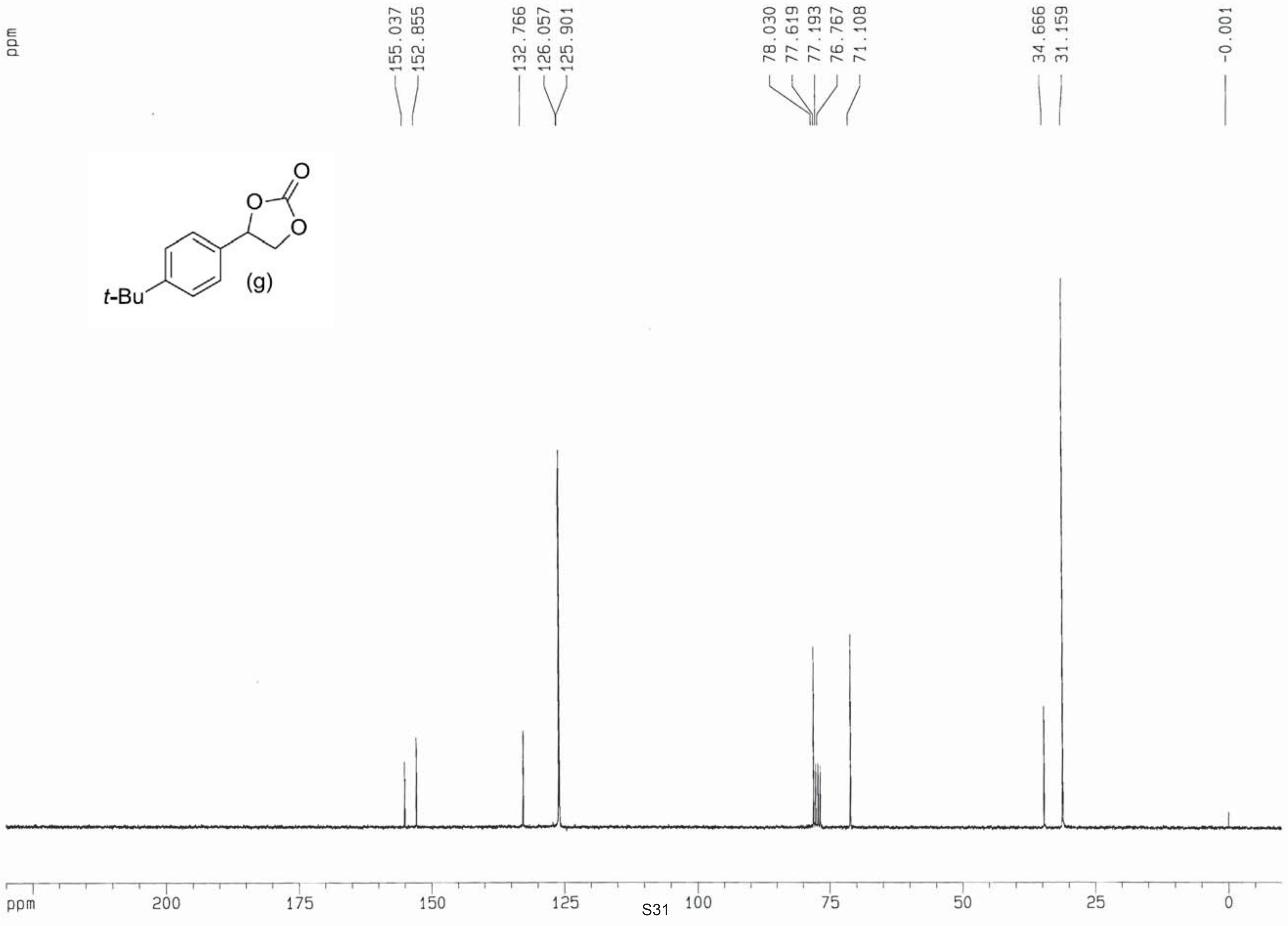
```
Current Data Parameters
NAME       2_Cl_Sty_carb
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151128
Time               14.27
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  961
DS                    4
SWH          18796.992 Hz
FIDRES        0.286819 Hz
AQ           1.7433076 sec
RG                 1024
DW               26.600 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec

============ CHANNEL f1 ============
NUC1                13C
P1                 5.25 usec
PL1               -6.00 dB
SFO1        75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2         waltz16
NUC2                 1H
PCPD2            115.00 usec
PL2                0.00 dB
PL12              19.70 dB
PL13              19.70 dB
SFO2       299.8711995 MHz

F2 - Processing parameters
SI                32768
SF          75.4023731 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
F1P             230.000 ppm
F1             17342.54 Hz
F2P             -10.000 ppm
F2              -754.02 Hz
PPMCM          12.00000 ppm/cm
HZCM          904.82849 Hz/cm
```



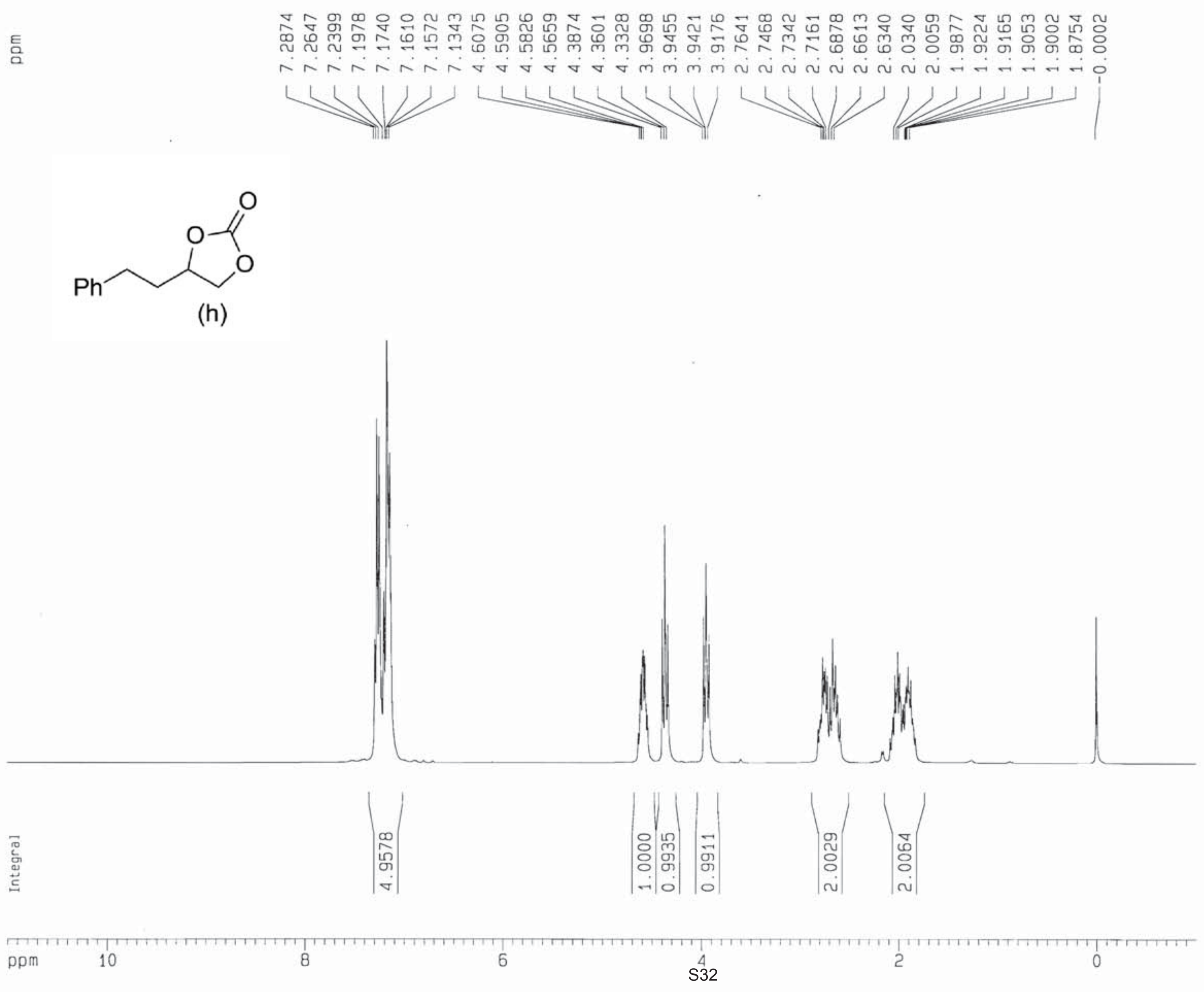
```
Current Data Parameters
NAME       2_Cl_Sty_carb
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151128
Time               13.21
INSTRUM            spect
PROBHD     5 mm QNP 1H/1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ             5.3084660 sec
RG                  35.9
DW                81.000 usec
DE                  6.00 usec
TE                 300.0 K
D1            1.00000000 sec

============ CHANNEL f1 ========
NUC1                  1H
P1                 12.10 usec
PL1                 0.00 dB
SFO1         299.8718518 MHz

F2 - Processing parameters
SI                 32768
SF           299.8699872 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
F1P               11.000 ppm
F1               3298.57 Hz
F2P               -1.000 ppm
F2               -299.87 Hz
PPMCM            0.60000 ppm/cm
HZCM           179.92200 Hz/cm
```



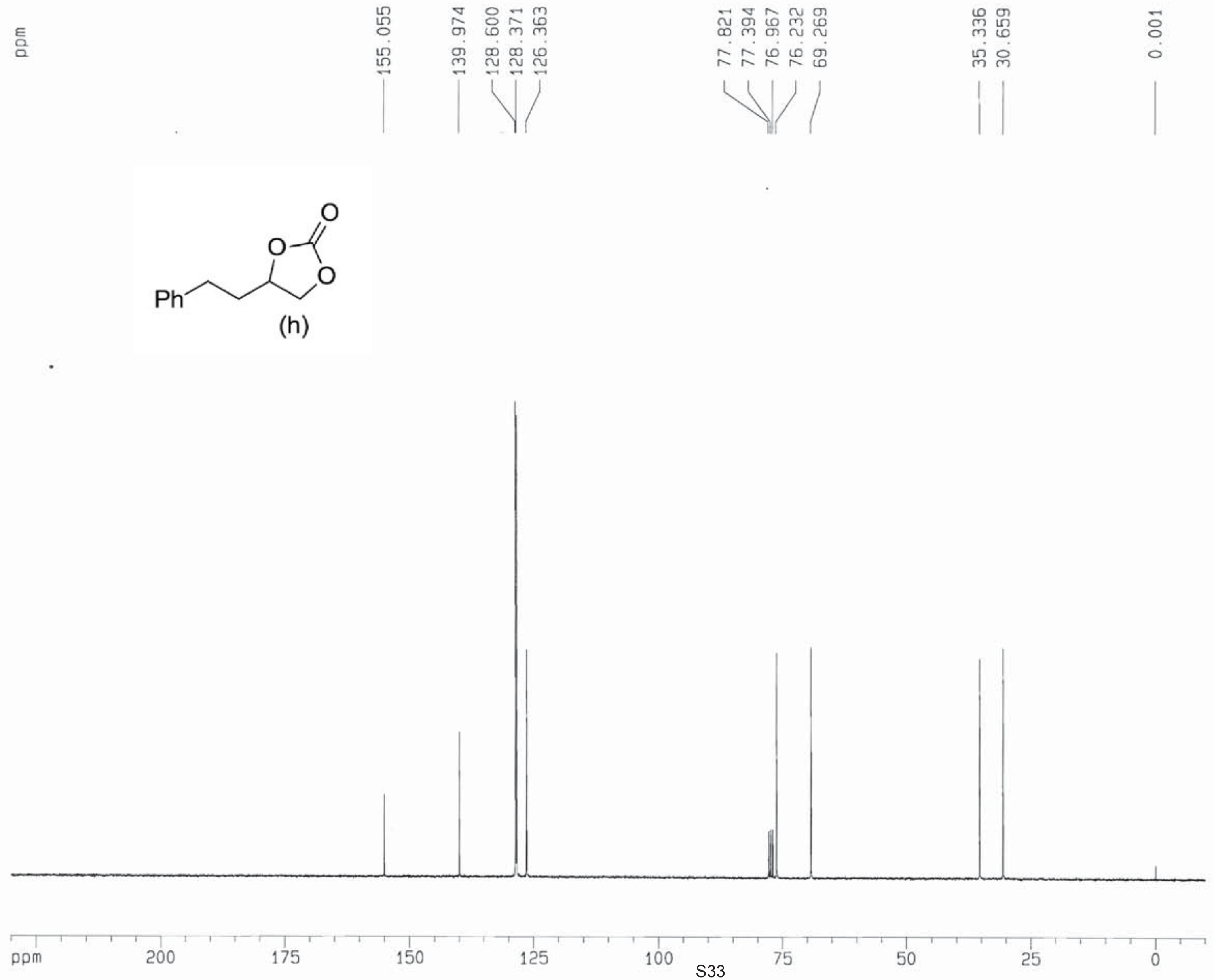
```
Current Data Parameters
NAME        4_tBusty_carb
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151128
Time                14.25
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG              zg30
TD                  54634
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             8278.146 Hz
FIDRES          0.151520 Hz
AQ             3.2999437 sec
RG                   90.5
DW                 60.400 usec
DE                   6.00 usec
TE                  294.6 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
PL1                  1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF            400.1300144 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```



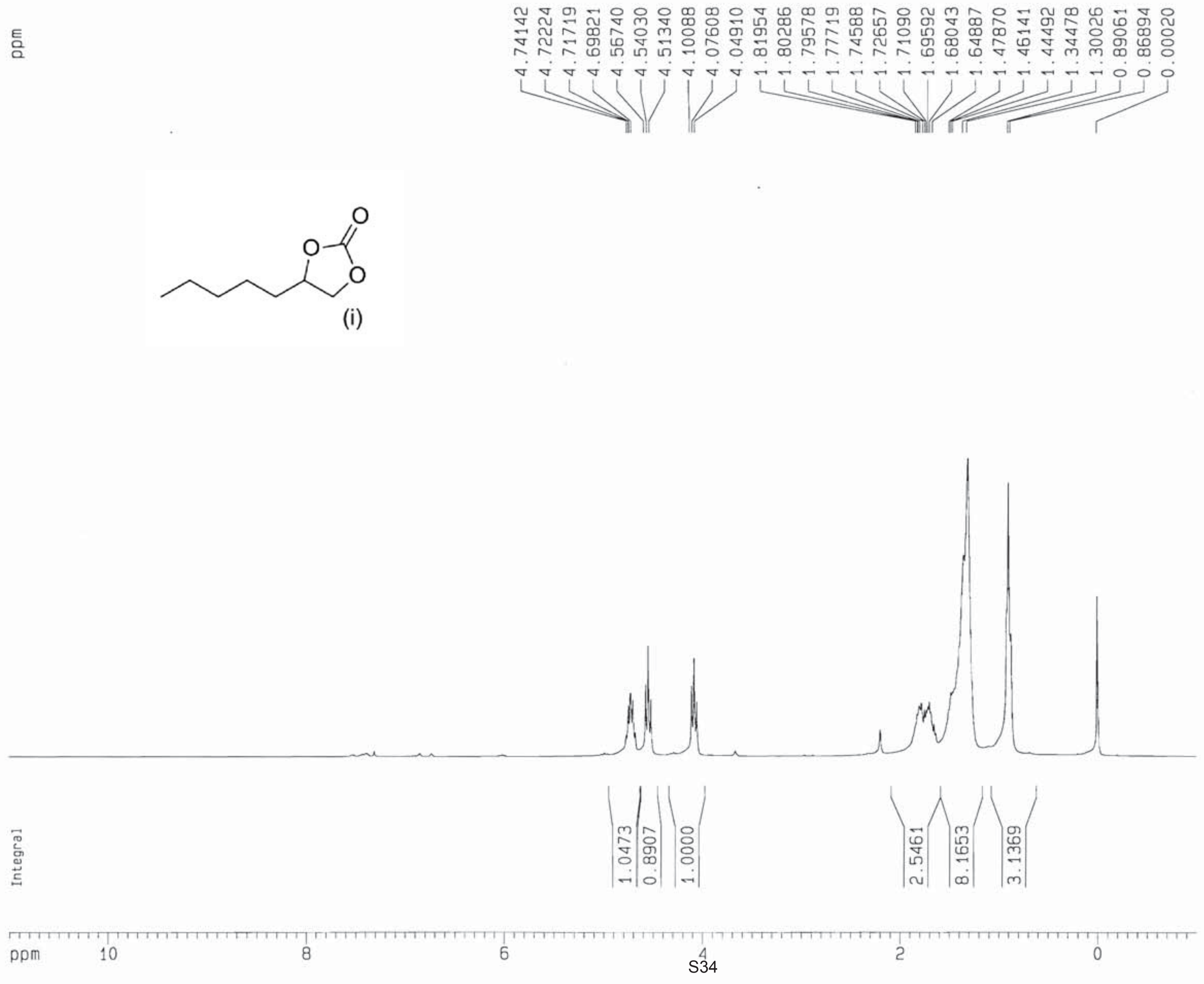
```
Current Data P
NAME      4_tb
EXPNO
PROCNO

F2 - Acquisiti
Date_
Time
INSTRUM
PROBHD    5 mm
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1           2
D11          0
D12          0

============ C
NUC1
P1
PL1
SF01         7

============ C
CPDPRG2
NUC2
PCPD2
PL2
PL12
PL13
SF02        29

F2 - Processin
SI
SF           7
WDW
SSB
LB
GB
PC

1D NMR plot pa
CX
F1P
F1
F2P
F2
PPMCM
HZCM
```



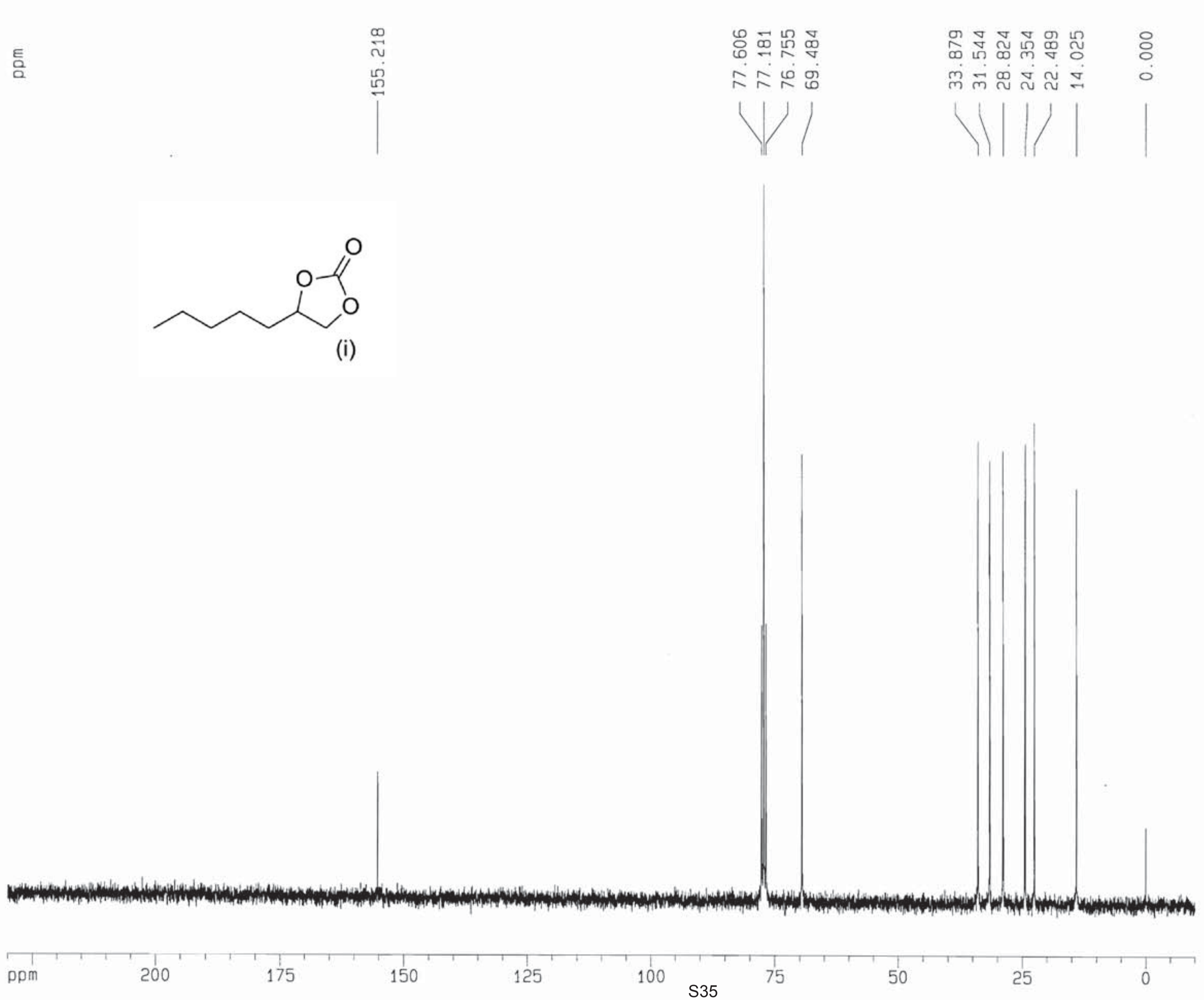
```
Current Data Parameters
NAME       4_Ph_But_Carb
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151130
Time               14.09
INSTRUM            spect
PROBHD    5 mm QNP 1H/1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ           5.3084660 sec
RG                  25.4
DW             81.000 usec
DE               6.00 usec
TE               300.0 K
D1         1.00000000 sec

============ CHANNEL f1 ========
NUC1                  1H
P1              12.10 usec
PL1              0.00 dB
SFO1      299.8718518 MHz

F2 - Processing parameters
SI                 32768
SF        299.8700225 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                20.00 cm
F1P              11.000 ppm
F1              3298.57 Hz
F2P              -1.000 ppm
F2              -299.87 Hz
PPMCM           0.60000 ppm/cm
HZCM          179.92201 Hz/cm
```



```
Current Data Parameters
NAME       4_Ph_But_Carb
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151130
Time               14.16
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    81
DS                     4
SWH           18796.992 Hz
FIDRES         0.286819 Hz
AQ            1.7433076 sec
RG                  1024
DW                26.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                  5.25 usec
PL1                -6.00 dB
SFO1         75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             115.00 usec
PL2                 0.00 dB
PL12               19.70 dB
PL13               19.70 dB
SFO2        299.8711995 MHz

F2 - Processing parameters
SI                 32768
SF           75.4023822 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              230.000 ppm
F1              17342.55 Hz
F2P              -10.000 ppm
F2               -754.02 Hz
PPMCM           12.00000 ppm/cm
HZCM           904.82861 Hz/cm
```



```
Current Data Parameters
NAME          octene_carb
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151130
Time                13.54
INSTRUM             spect
PROBHD    5 mm QNP 1H/1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6172.839 Hz
FIDRES           0.094190 Hz
AQ              5.3084660 sec
RG                   50.8
DW                 81.000 usec
DE                   6.00 usec
TE                  300.0 K
D1             1.00000000 sec

============ CHANNEL f1 ========
NUC1                   1H
P1                  12.10 usec
PL1                  0.00 dB
SFO1         299.8718518 MHz

F2 - Processing parameters
SI                  32768
SF           299.8699963 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
F1P                11.000 ppm
F1                3298.57 Hz
F2P                -1.000 ppm
F2                -299.87 Hz
PPMCM             0.60000 ppm/cm
HZCM            179.92200 Hz/cm
```



```
Current Data Parameters
NAME             octene_carb
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20151130
Time                   14.03
INSTRUM                spect
PROBHD     5 mm QNP 1H/1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       108
DS                         4
SWH               18796.992 Hz
FIDRES             0.286819 Hz
AQ                1.7433076 sec
RG                      4096
DW                    26.600 usec
DE                      6.00 usec
TE                     300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec

============ CHANNEL f1 ============
NUC1                     13C
P1                      5.25 usec
PL1                    -6.00 dB
SF01             75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2              waltz16
NUC2                      1H
PCPD2                 115.00 usec
PL2                     0.00 dB
PL12                   19.70 dB
PL13                   19.70 dB
SF02             299.8711995 MHz

F2 - Processing parameters
SI                     32768
SF                75.4023690 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     20.00 cm
F1P                  230.000 ppm
F1                  17342.54 Hz
F2P                  -10.000 ppm
F2                   -754.02 Hz
PPMCM               12.00000 ppm/cm
HZCM               904.82837 Hz/cm
```

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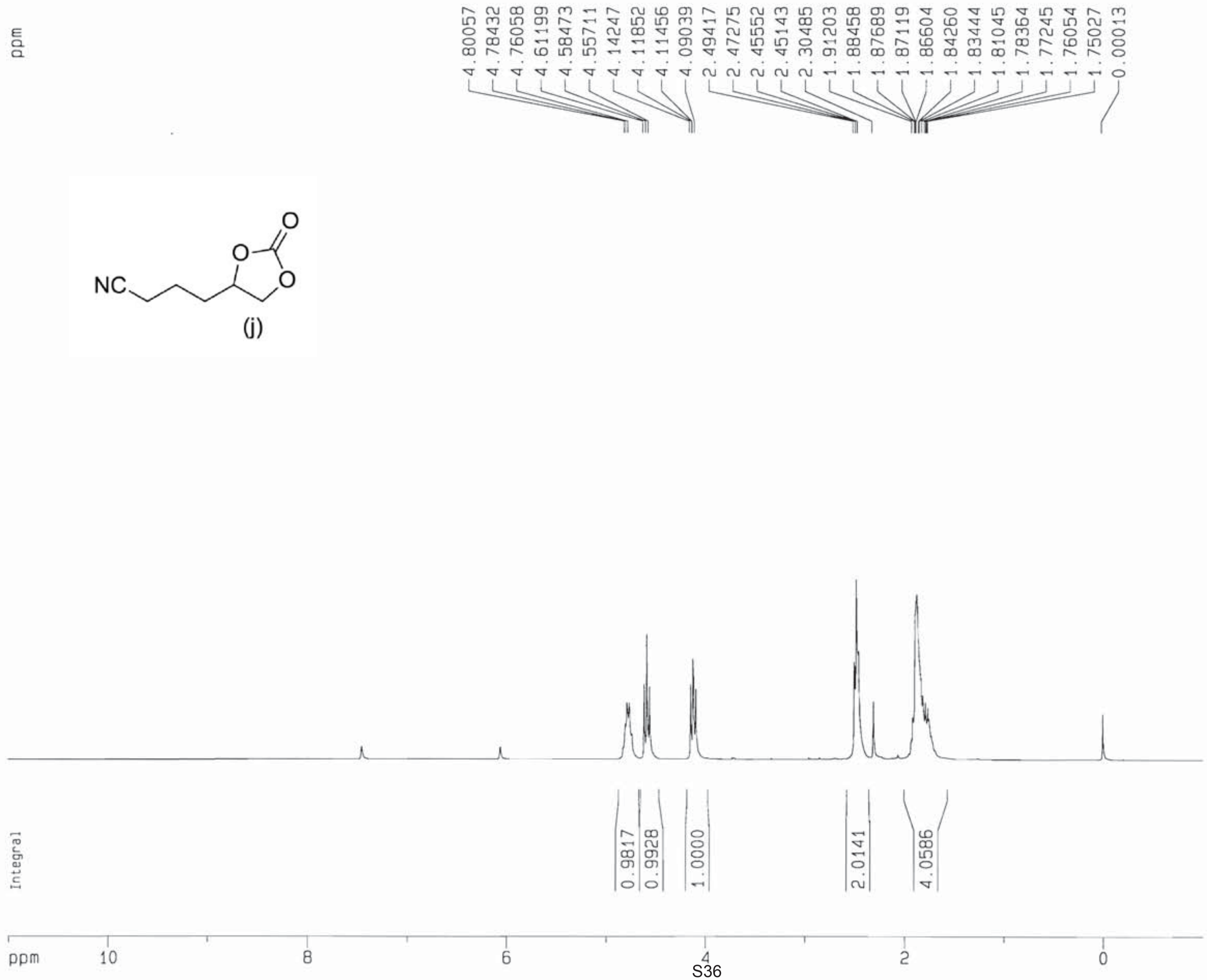


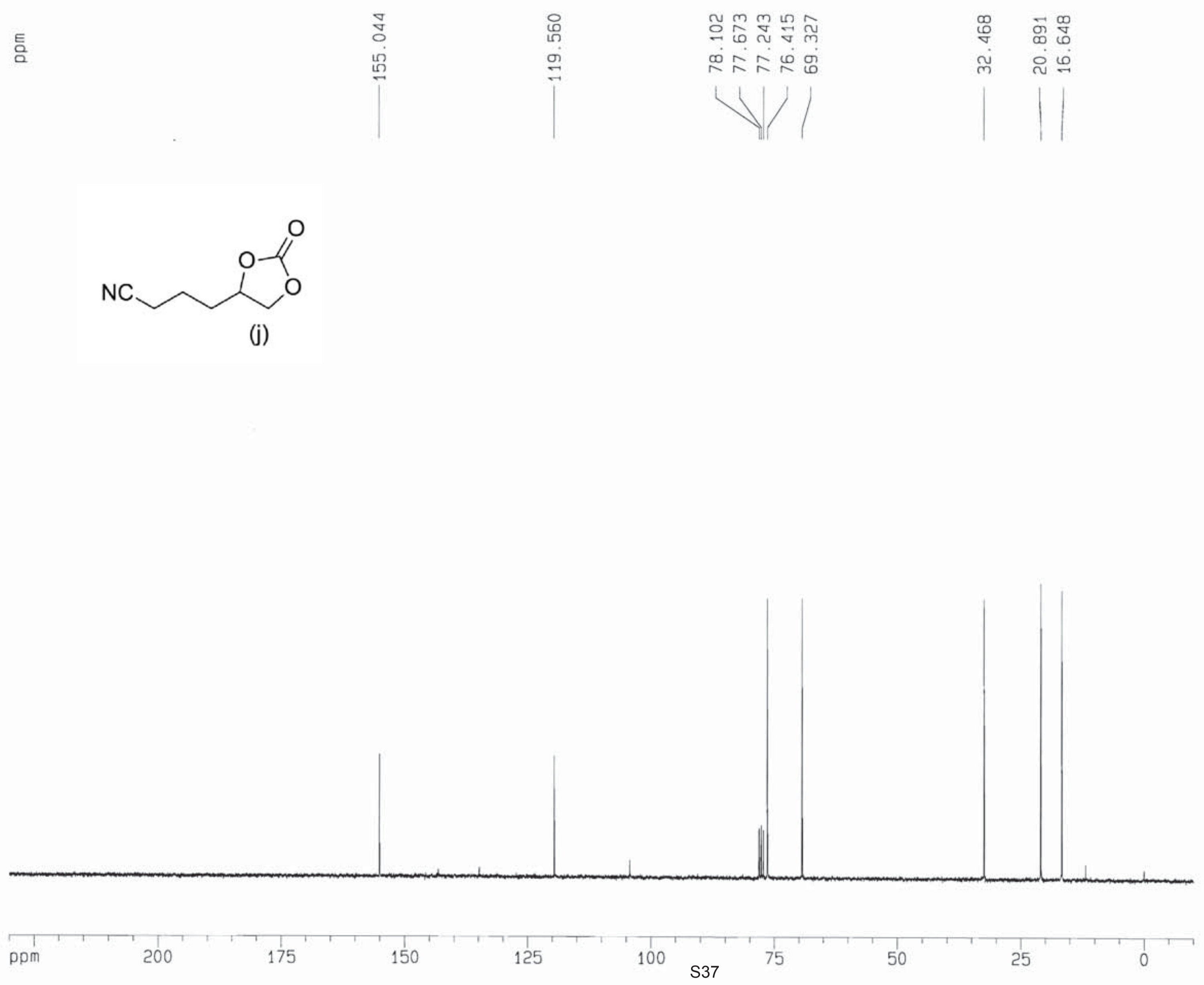
```
Current Data Parameters
NAME       6_CN_hex_carb
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151207
Time                9.56
INSTRUM            spect
PROBHD     5 mm QNP 1H/1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH          6172.839 Hz
FIDRES       0.094190 Hz
AQ          5.3084660 sec
RG                  25.4
DW            81.000 usec
DE              6.00 usec
TE               300.0 K
D1        1.00000000 sec

============ CHANNEL f1 ========
NUC1                  1H
P1             12.10 usec
PL1               0.00 dB
SF01      299.8718518 MHz

F2 - Processing parameters
SI                 32768
SF        299.8699575 MHz
WDW                   no
SSB                    0
LB               0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX              20.00 cm
F1P            11.000 ppm
F1            3298.57 Hz
F2P            -1.000 ppm
F2            -299.87 Hz
PPMCM      0.60000 ppm/cm
HZCM      179.92198 Hz/cm
```



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```
Current Data Parameters
NAME       6_CN_hex_carb
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151207
Time               10.00
INSTRUM            spect
PROBHD   5 mm QNP 1H/1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    30
DS                     4
SWH           18796.992 Hz
FIDRES         0.286819 Hz
AQ            1.7433076 sec
RG                  1024
DW                26.600 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                  5.25 usec
PL1                -6.00 dB
SFO1         75.4106357 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             115.00 usec
PL2                 0.00 dB
PL12               19.70 dB
PL13               19.70 dB
SFO2        299.8711995 MHz

F2 - Processing parameters
SI                 32768
SF           75.4023667 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              230.000 ppm
F1              17342.54 Hz
F2P              -10.000 ppm
F2               -754.02 Hz
PPMCM           12.00000 ppm/cm
HZCM           904.82837 Hz/cm
```