Electronic Supplementary Information

Electrocatalytic synthesis of *α,α-gem*-dihalide ketones from *α-mono*-halide ketones and unexpected dimer condensation

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CONTENTS

1. General experiment

1.1 Experimental details

Electro-catalysis experiments were performed in an argon atmosphere. Chemical reagents were obtained from commercial suppliers (Sigma-Aldrich, Adamas, Shanghai Titan Technology Co., LTD, et al.) and used without further purification. Purified water was purchased from the local market. Reactions were monitored by thin-layer chromatography (TLC) on 0.25 mm silica gel GF254 plate (Merck Silica gel 60-F254) using UV light as a visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. Silica gel (300-400 mesh) was used for flash column chromatography. Yields refer to chromatographically and spectroscopically homogeneous materials unless otherwise noted. Switching DC voltage regulator for electrolysis is a triple display potentiostat (KORAD-KA3305D, made in China). The anodic electrode was carbon plate (10 mm×10 mm×2 mm), and the cathodic electrode was platinum plate (10 mm×10 mm×0.2 mm).

1.2 Characterizations

^{1}H-NMR, ***^{13}C-NMR,*** and ***^{19}F-NMR*** were recorded with Bruker Advance (300, 400, 500 & 600 MHz) spectrometers. All chemical shifts were reported as δ values in parts per million (ppm) and coupling constants (J) in Hz. Tetramethylsilane (TMS) was used as the internal standard for $CDCl_3$ (7.26 ppm for ^{1}H, 77.00 ppm for ^{13}C), respectively.

IR spectra were recorded on a Bruker Bio-Rad FTS-135 spectrometer with KBr pellets.

Mass spectra: **(1)** ***HR-MS (ESI)*** was taken on AB QSTAR Pulsar mass spectrometer or Agilent LC/MSD TOF mass spectrometer. HR-MS data were recorded via electron impact mass spectrometry using a time-of-flight analyzer. ***(2) GC–MS*** was performed on a Hewlett-Packard 6890 N gas chromatograph (equipped with the same HP-5MS capillary column) under identical operating conditions used in Mass Spectral Library by R. P. Adams (Adams, 2007).

Electrochemistry (**CVs**): cyclic voltammograms were obtained on a Metrohm PGSTAT302N potentiostat.

1.3 Electrocatalysis apparatus

Switching DC voltage regulator for electrolysis is a triple display potentiostat (KORAD-KA3305D, made in China). In an oven-dried undivided two-necked (or three-necked) flask (50 mL) equipped with a stir bar. The flask was equipped with a platinum plate (10 mm×10 mm×0.2 mm) as the cathodic electrode and a carbon plate (10 mm×10 mm×2 mm) as the anodic electrode. The reaction was in an argon atmosphere. The reaction was conducted at room temperature.

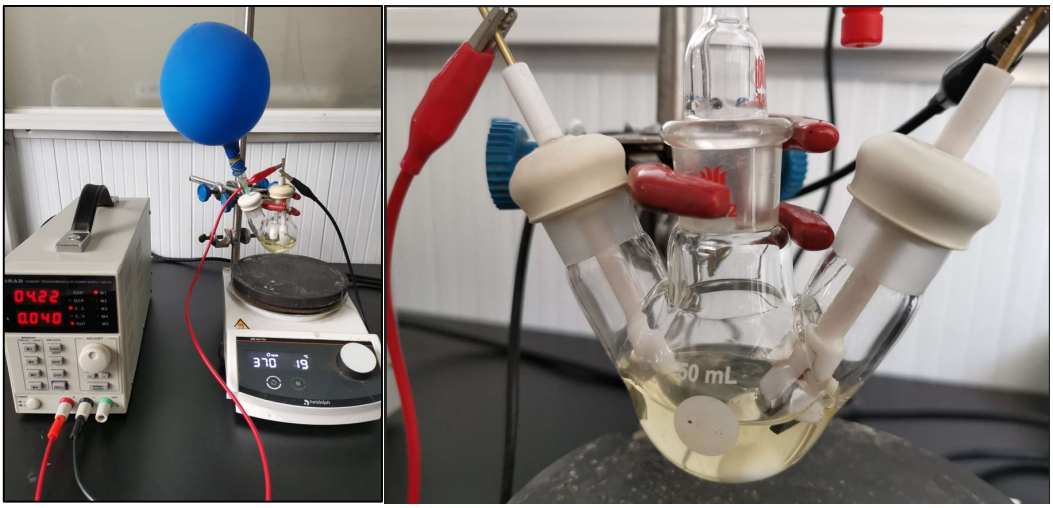
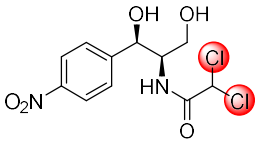
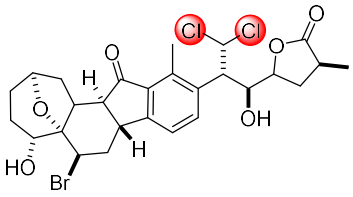


Figure S1. Electrochemical reaction cell apparatus and electrodes

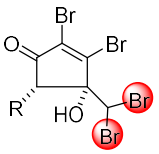
1.4 Bio-active *α,α-gem*-dihalide natural products



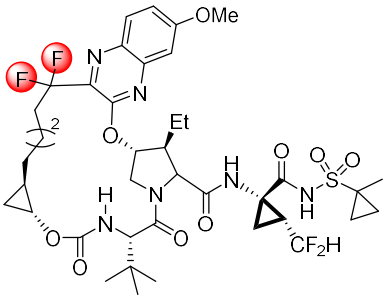
Chloramphenicol
antibacterial activity



Nakiterpiosin
anticancer activity



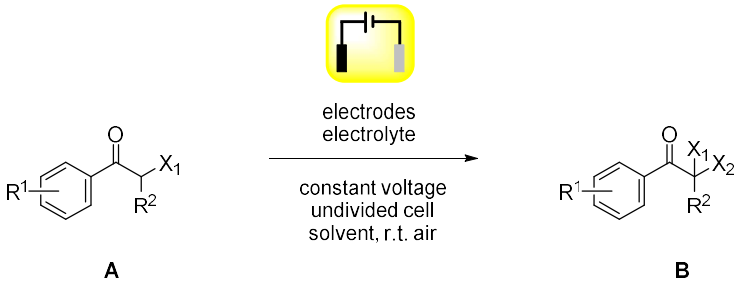
Mahorone (R=H)
5-Bromomahorone (R=Br)
antibacterial activity



Voxilaprevir
protease inhibitor for Hepatitis C

Scheme S1. *α,α-Gem*-dihalide monoterpenes among marine bio-active natural products.

2. Reaction conditions optimization

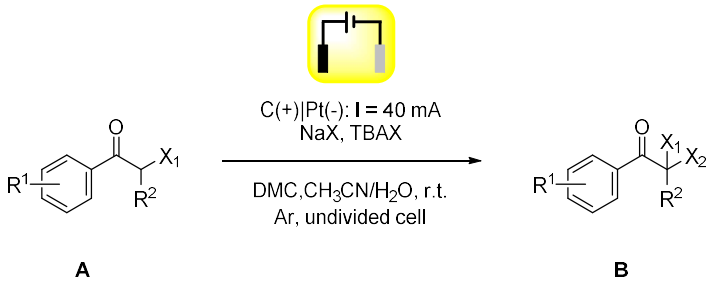


Entry	Variations of standard conditions	Yield (%) [a]
1	none	82
2	no CH_3CN	13
3	toluene, THF, or dioxane replace CH_3CN	13-25
4	H_2O (0.5 or 2.0 mol·L^{-1})	35-35
5	no DMC	57
6	without TBAC	37
7	$^{n}Bu_4NBF_4$ or $^{n}Bu_4NPF_6$ replace TBAC	35-38
8	TBAF	16
9	Nickel as cathode	18
10	5 mA or 100 mA current	12-35
11	Ar or O_2 atmosphere	81-80
12	6h reaction time	20
13	without electric current	0
14	K_2CO_3 (0.2 mol·L^{-1})	12
15	AcOH (0.2 mol·L^{-1})	11
16	NaOH (1.0 mol·L^{-1})	dimer [b]

Table S1. Typical electro halogenation. Standard reaction conditions: glassy carbon plate (10 mm × 10 mm × 2 mm) as anode, Pt plate (10 mm × 10 mm × 0.2 mm) as cathode, constant current = 40 mA, reactant **A** (200 mg, 1.0 mmol), TBAC (55.6 mg, 0.2 mmol), NaCl (725 mg, 1.0 mol·L^{-1}), CH_3CN (5.0 mL), H_2O (5.0 mL), DMC (2.5 mL), room temperature, ambient atmosphere, 30 min, undivided cell. [a] Isolated yield by silica gel column chromatography, the same for other yields. [b] A dimer condensation product.

3. General electrocatalysis reactions

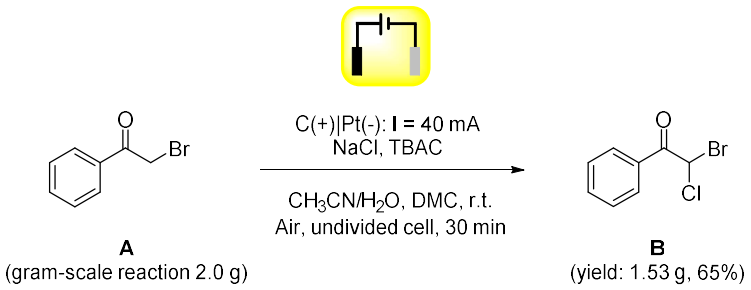
3.1 Typical electro-halogenation



Scheme S2. Electrocatalytic halogenation

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, *2*-halide acetophenone (200 mg, 1.0 mmol), tetrabutylammonium halides (TBAC or TBAB, 50 mg, 0.2 mmol), brine (e.g., NaCl, KCl, NaBr, KBr, or NaF, 1.0 mol·L^{-1}, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were added. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathode and a carbon plate (10 mm × 10 mm × 2 mm) as the anode. The reaction was conducted under an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA at room temperature for 30 min. The reaction was monitored by TLC, using UV light as a visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. When the material no longer decreased, the solution was extracted with ethyl acetate (EtOAc) (3 × 10 mL) and H_2O (3 × 10 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on silica gel using EtOAc and petroleum ether as the eluent. The products were further identified by FTIR spectroscopy, NMR spectroscopy, and HRMS analysis.

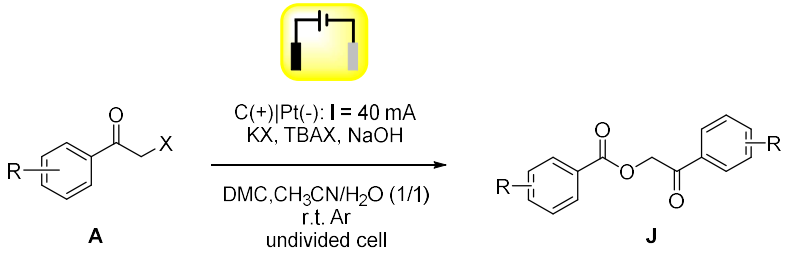
3.2 Gram-scale electro-halogenation



Scheme S3. Gram-scale electro-halogenation

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar, *2*-bromo-acetophenone (2.0 g, 1.0 mmol), TBAC (564.3 mg, 0.2 mmol), NaCl (3.8 g, 6.5 mmol), CH_3CN (50.0 mL), H_2O (50.0 mL), and DMC (25.0 mL) were combined and added. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathode and a carbon plate (10 mm × 10 mm × 2 mm) as the anode. The reaction was conducted under an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA at room temperature for 30 min. The reaction was monitored by TLC, using UV light as a visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. When the material no longer decreased, the solution was extracted with ethyl acetate (EtOAc) (3 × 10 mL) and H_2O (3 × 10 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on silica gel using EtOAc and petroleum ether as the eluent. Product α-bromo-α-chloro-acetophenone was obtained with a yield of 1.53 g, 65%.

3.3 Electrocatalytic dimer condensation



Scheme S4. Electrocatalysis for dimer condensation

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, 2-halo-acetophenone (200 mg, 1.0 mmol), tetrabutylammonium halide (TBAC or TBAB, ~ 50 mg, 0.2 mmol), brine (e.g., NaCl, KCl, NaBr, KBr, or NaF, 1.0 mol·L^{-1}, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were added. NaOH (500 mg, 1.0 mol·L^{-1}) was added to the reaction solutions. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathode and a carbon plate (10 mm × 10 mm × 2.0 mm) as the anode. The reaction was conducted under an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA at room temperature for 30 min. The reaction was monitored by TLC, using UV light as visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. When the material no longer decreased, the solution was extracted with EtOAc (3 × 10 mL) and H_2O (3 × 10 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on silica gel using EtOAc and petroleum ether as the eluent. The products were further identified by FTIR spectroscopy, NMR spectroscopy, and HRMS analysis.

3.4 X-ray of the dimer condensation product

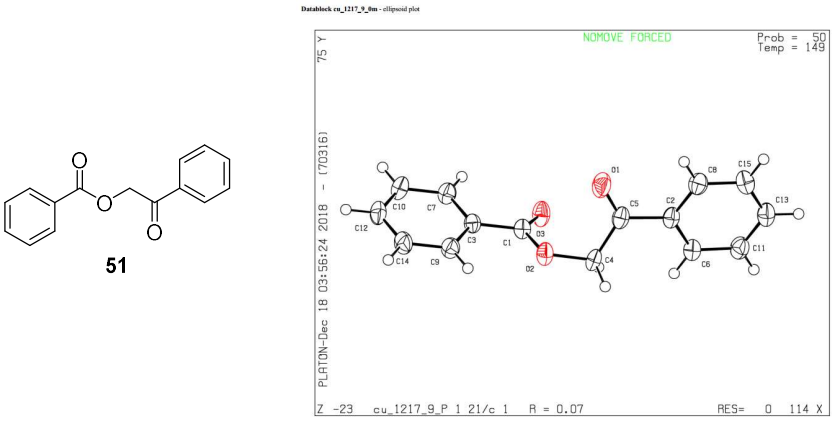


Figure S2. X-ray of dime condensation product **51** (CCDC *No.* 2106444)

Table 1. Crystal data and structure refinement for C:_1217_9.

Identification code	cu_1217_9_0m	
Empirical formula	C15 H12 O3	
Formula weight	240.25	
Temperature	149.44 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 8.9535(3) Å	α= 90°.
	b = 14.0575(5) Å	β= 90.799(2)°.
	c = 9.4542(3) Å	γ = 90°.
Volume	1189.83(7) Å^3	
Z	4	
Density (calculated)	1.341 Mg/m^3	
Absorption coefficient	0.763 mm^{-1}	
F(000)	504	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	4.940 to 72.084°.	
Index ranges	-11<=h<=11, -17<=k<=16, -11<=l<=11	
Reflections collected	19949	
Independent reflections	2335 [R(int) = 0.1052]	
Completeness to theta = 67.679°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7538 and 0.3884
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2335 / 0 / 164
Goodness-of-fit on F^2	1.097
Final R indices [I>2sigma(I)]	R1 = 0.0669, wR2 = 0.1616
R indices (all data)	R1 = 0.0826, wR2 = 0.1745
Extinction coefficient	0.0119(18)
Largest diff. peak and hole	0.316 and -0.333 e.Å^{-3}

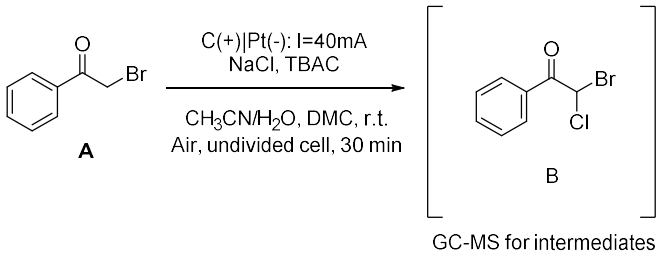
Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for C:_1217_9. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8939(2)	4904(1)	7079(2)	48(1)
O(2)	7566(2)	3929(1)	5032(2)	35(1)
O(3)	5606(2)	4143(1)	6457(2)	38(1)
C(1)	6470(2)	3614(2)	5884(2)	27(1)
C(2)	8489(2)	6454(2)	6204(2)	28(1)
C(3)	6425(2)	2564(2)	6000(2)	27(1)
C(4)	7644(2)	4951(2)	4893(2)	31(1)
C(5)	8393(2)	5399(2)	6151(2)	31(1)
C(6)	7624(2)	7036(2)	5318(2)	32(1)
C(7)	5478(2)	2164(2)	6991(2)	32(1)
C(8)	9473(2)	6866(2)	7176(2)	35(1)
C(9)	7266(3)	1976(2)	5133(2)	34(1)
C(10)	5376(3)	1183(2)	7111(3)	37(1)
C(11)	7748(3)	8020(2)	5424(3)	38(1)
C(12)	6198(3)	602(2)	6236(3)	37(1)
C(13)	8745(3)	8423(2)	6382(3)	37(1)
C(14)	7147(3)	996(2)	5247(3)	38(1)
C(15)	9599(3)	7845(2)	7265(3)	37(1)

3.5 Control experiments

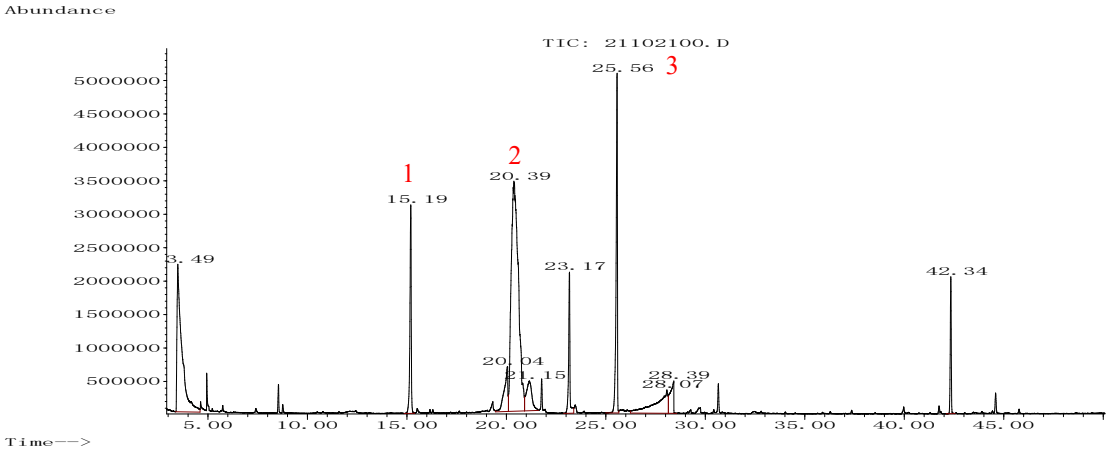
GC–MS analysis of menthyl and isomenthyl acetates was also performed on a Hewlett-Packard 6890 N gas chromatograph (equipped with the same HP-5MS capillary column) under identical operating conditions used in Mass Spectral Library by R. P. Adams (Adams, 2007). In this experiment, the GC was operated under the following conditions: injector and interface temperatures were 220 and 240 ◦C, respectively; oven temperature was raised from 60 ℃ to 246 ℃ at a heating rate of 3 ℃/min; the flow of helium carrier gas was 1.0 mL/min.

3.5.1 GC–MS for electrocatalytic halogenation



Scheme S5. Electrocatalysis for halogenation

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar, *2*-bromo-acetophenone (200 mg, 1.0 mmol), TBAC (56.4 mg, 0.2 mmol), NaCl (380 mg, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The flask was equipped with a platinum plate (50 mm×50 mm×0.2 mm) as the cathodic electrode and a carbon plate (50 mm×50 mm×2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 30 min.



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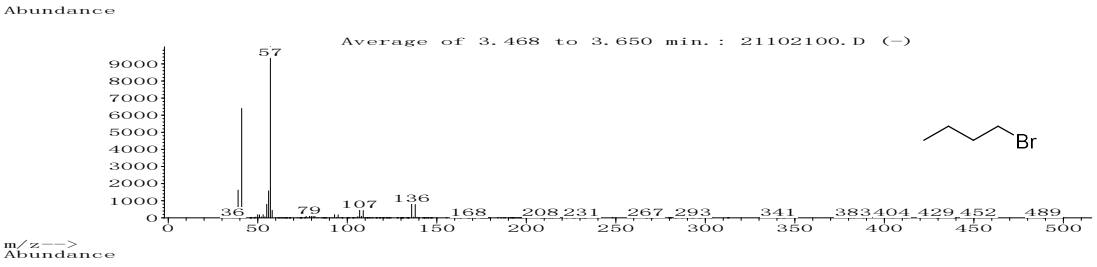
Abundance
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57
136
107
79
36
Br
m/z-->
Abundance
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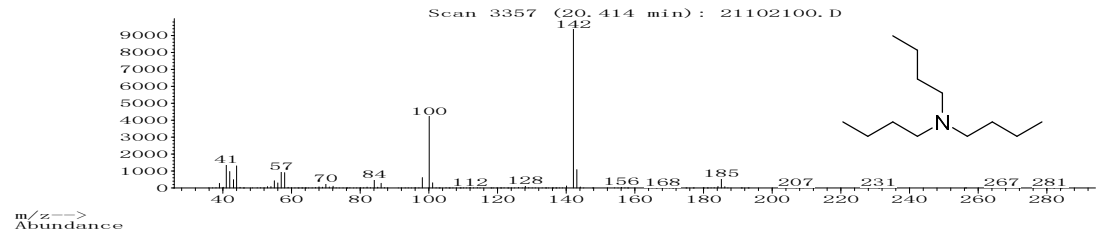
57
29
136
107
80
m/z-->

2


Abundance
Scan 3357 (20.414 min): 21102100.D
142
100
41
57
70
84
185
N
m/z-->
Abundance
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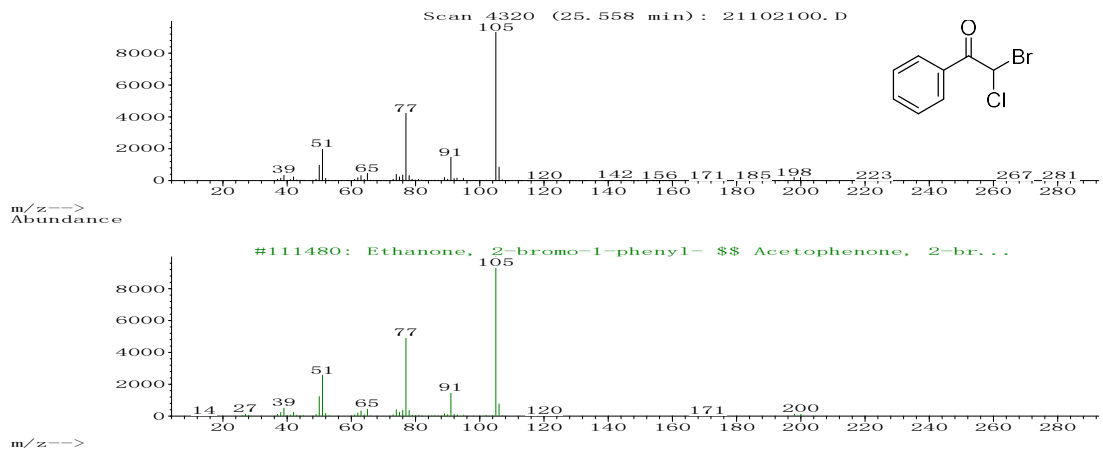
142
100
41
58
70
84
185
m/z-->

3


Abundance
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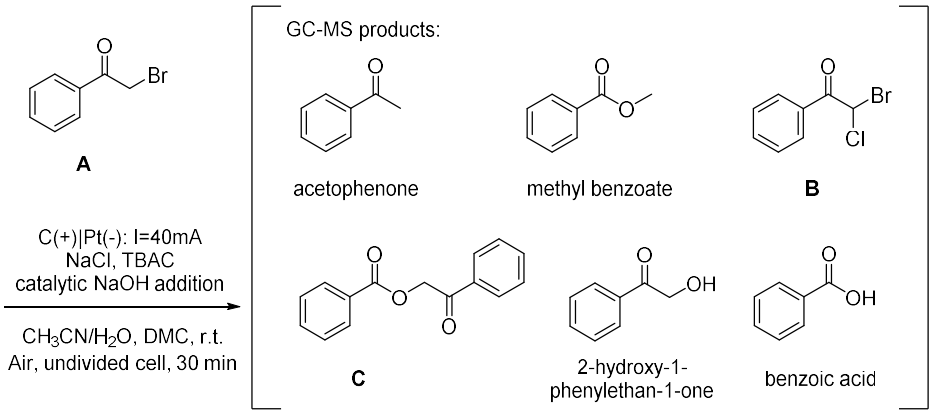
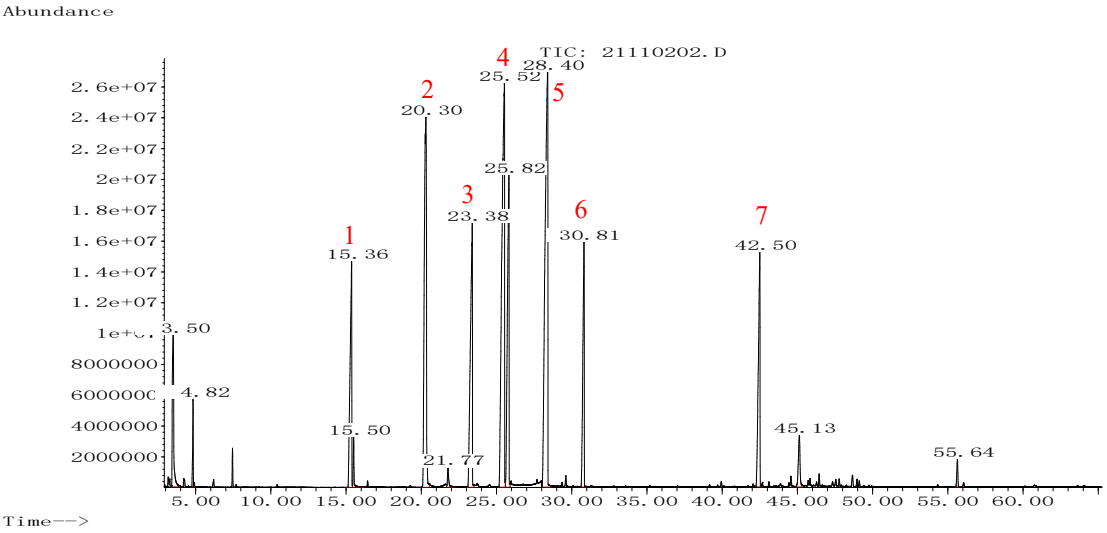
105
77
51
91
39
65
O
Br
Cl
m/z-->
Abundance
#111480: Ethanone, 2-bromo-1-phenyl- $$ Acetophenone, 2-br...
105
77
51
91
39
65
14
27
m/z-->

3.5.2 GC–MS for electrocatalytic dimer condensation



Scheme S6. Electrocatalysis for dimer condensation

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, 2-halo-acetophenone (~ 200 mg, 1.0 mmol), tetrabutylammonium halide (TBAC or TBAB, ~ 50 mg, 0.2 mmol), brine (eg: NaCl, KBr, NaF, 1.0 mol·L^{-1}, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. NaOH (1.0 mmol(L-1, 500 mg)) was added to the reaction solutions. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathodic electrode and a carbon plate (10 mm × 10 mm × 2.0 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under room temperature for 10 min.


Abundance
TIC: 21110202.D
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2
3
4
5
6
7
15.36
20.30
23.38
25.52
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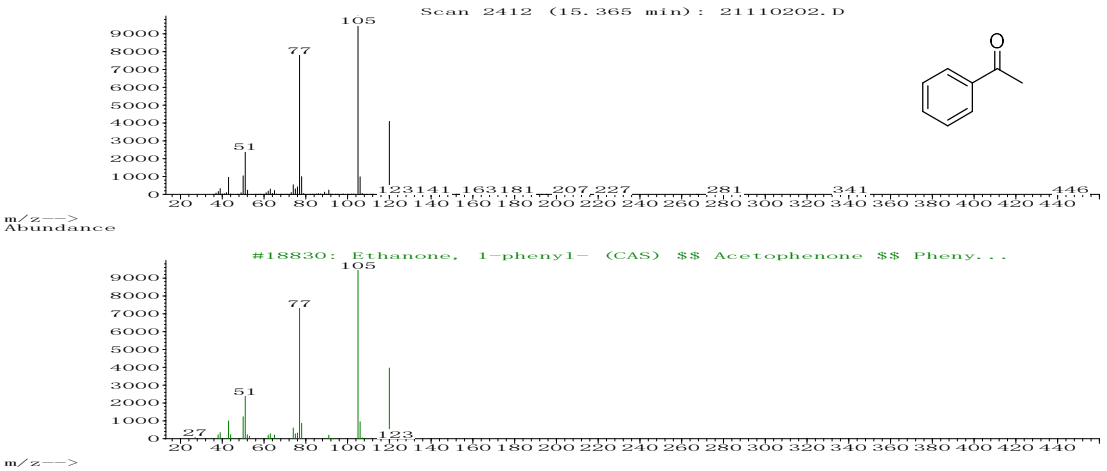
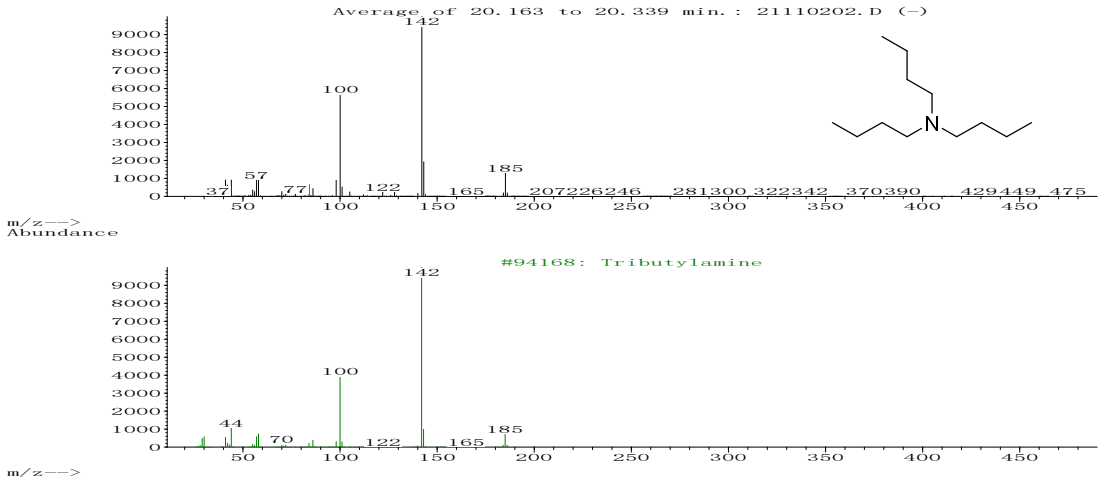
4.82
15.50
21.77
45.13
55.64
Time-->

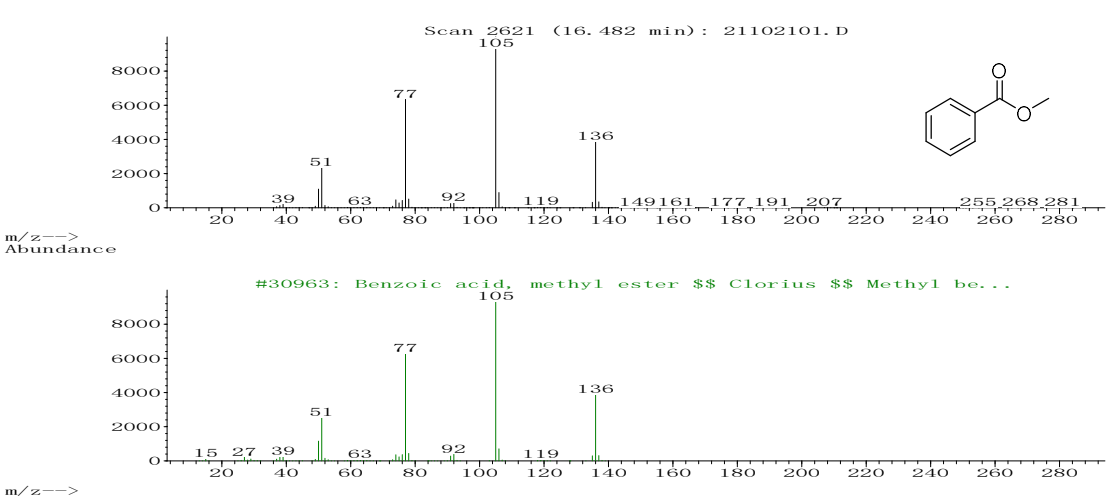
1


Abundance
Scan 2412 (15.365 min): 21110202.D
105
77
51
m/z-->
Abundance
#18830: Ethanone, 1-phenyl- (CAS) $$ Acetophenone $$ Pheny...
105
77
51
27
123
m/z-->

2


Abundance
Average of 20.163 to 20.339 min.: 21110202.D (-)
142
100
185
57
37
77
122
165
m/z-->
Abundance
#94168: Tributylamine
142
100
44
70
122
165
185
m/z-->

3


Abundance
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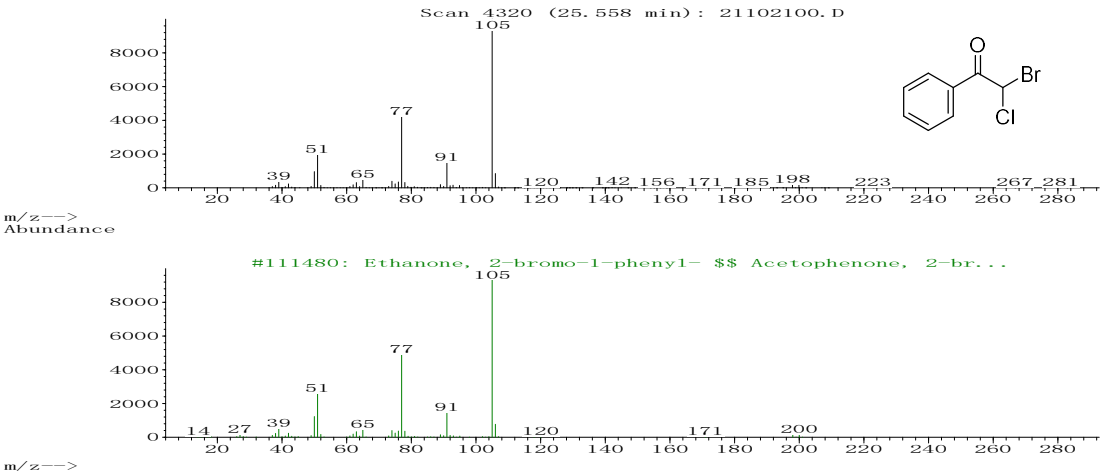
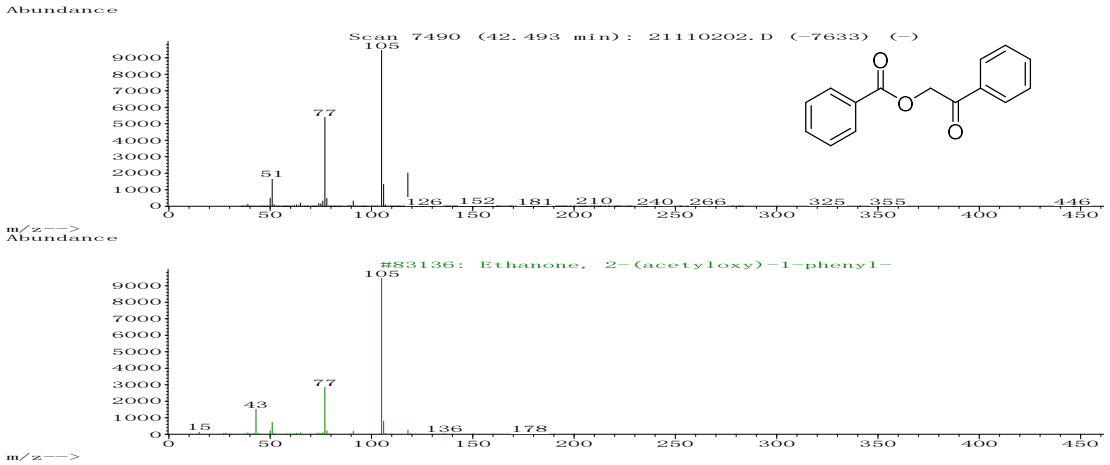
105
77
136
51
39
63
92
119
149 161 177 191 207
255 268 281
m/z-->
Abundance
#30963: Benzoic acid, methyl ester $$ Clorius $$ Methyl be...
105
77
136
51
15 27 39
63
92
119
m/z-->

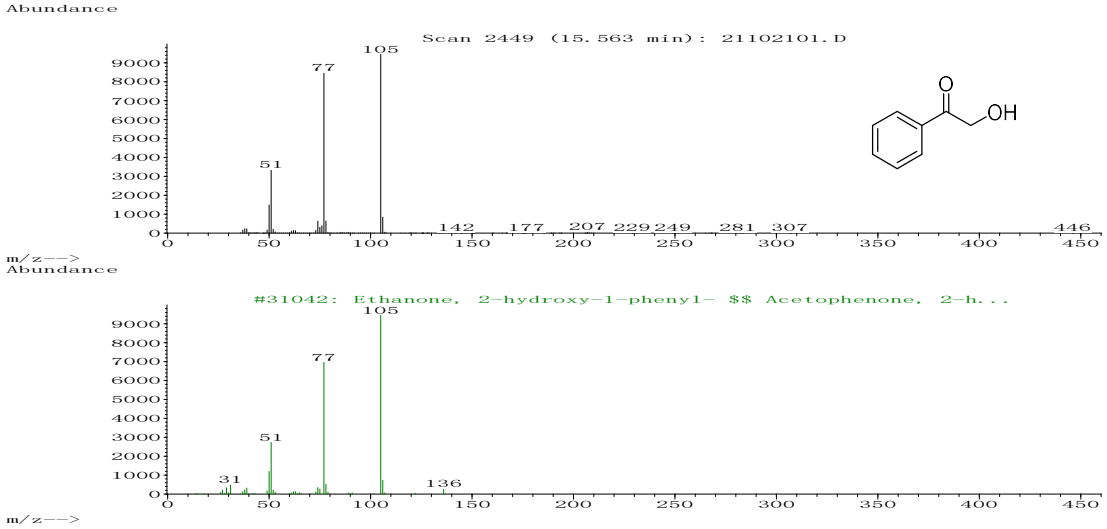
4


Abundance
Scan 4320 (25.558 min): 21102100.D
105
77
51
91
39
65
120
142 156 171 185 198
223
267 281
Br
Cl
m/z-->
Abundance
#111480: Ethanone, 2-bromo-1-phenyl- $$ Acetophenone, 2-br...
105
77
51
91
14 27 39
65
120
171
200
m/z-->

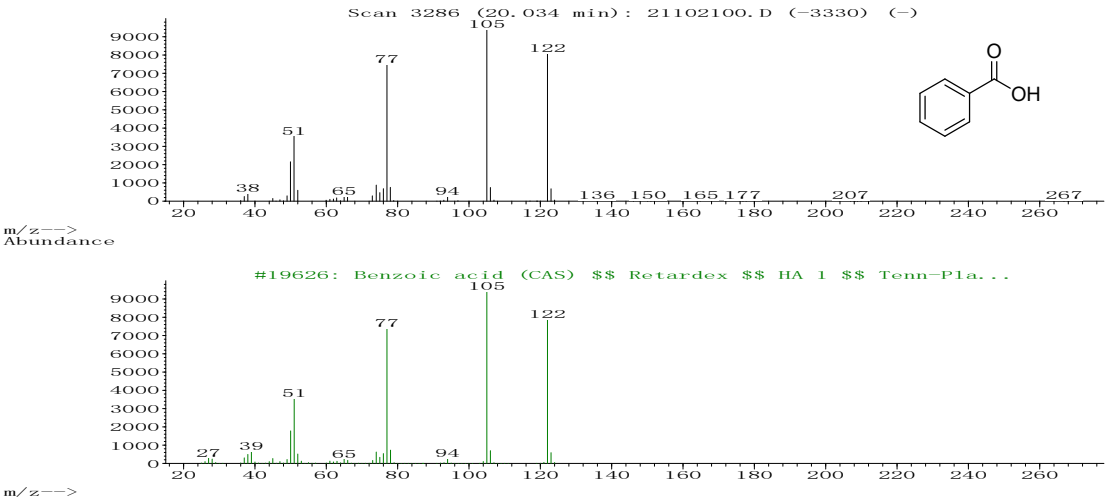
5


Abundance
Scan 7490 (42.493 min): 21110202.D (-7633) (-)
105
77
51
126 152 181 210 240 266
325 355
446
m/z-->
Abundance
#83136: Ethanone, 2-(acetyloxy)-1-phenyl-
105
77
43
15
136
178
m/z-->

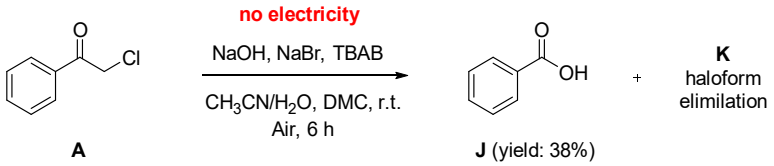
6


Abundance
Scan 2449 (15.563 min): 21102101.D
105
77
51
142
177
207
229
249
281
307
446
O
OH
m/z-->
Abundance
#31042: Ethanone, 2-hydroxy-1-phenyl- $$ Acetophenone, 2-h...
105
77
51
31
136
m/z-->

7

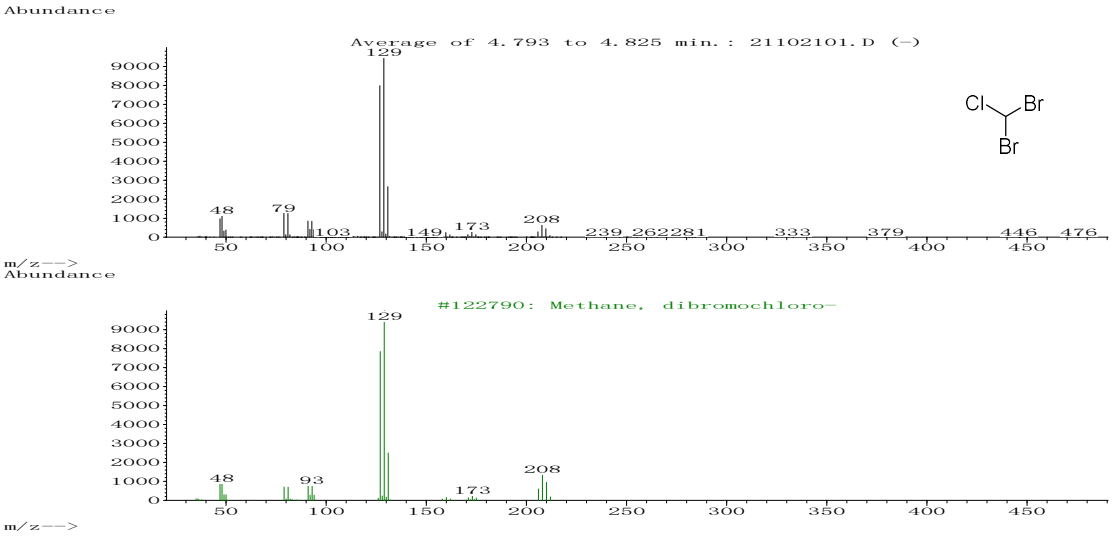

Abundance
Scan 3286 (20.034 min): 21102100.D (-3330) (-)
105
122
77
51
38
65
94
136
150
165
177
207
267
O
OH
m/z-->
Abundance
#19626: Benzoic acid (CAS) $$ Retardex $$ HA 1 $$ Tenn-Pla...
105
122
77
51
27
39
65
94
m/z-->

3.5.3 NaOH addition experiment without electricity

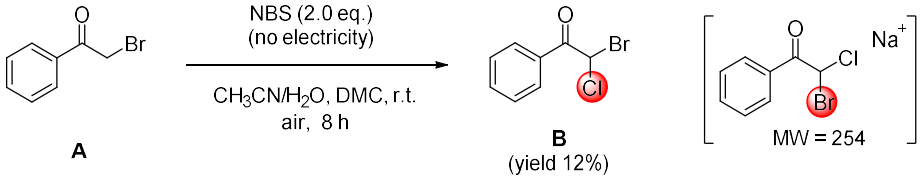


Scheme S7. NaOH addition experiment without electricity

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, 2-halo-acetophenone (200 mg, 1.0 mmol), TBAB(0.2 mmol, 55.6 mg), NaBr (1.0 mol·L^{-1}, 725 mg), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. NaOH (1.0 mol(L-1, 500 mg) was added to the reaction solutions. No electricity was used. The reaction was in an ambient atmosphere. The reaction mixture was stirred at room temperature for 6 h. TLC, UV light as a visualizing agent, the reaction was monitored, and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. When the material was no longer decreased, the solution was extracted with EtOAc (3 × 10 mL) and H_2O (3 × 10 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on silica gel using EtOAc and petroleum ether as the eluent solvents. Then benzoic acid was isolated with a yield of 46.4 mg, 38%.



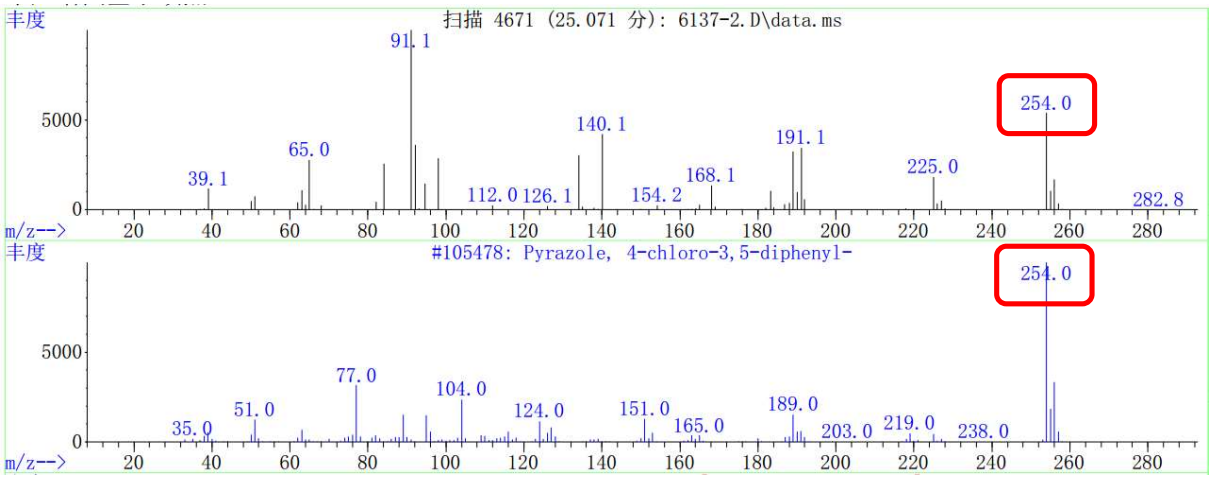
3.5.4 NBS experiment



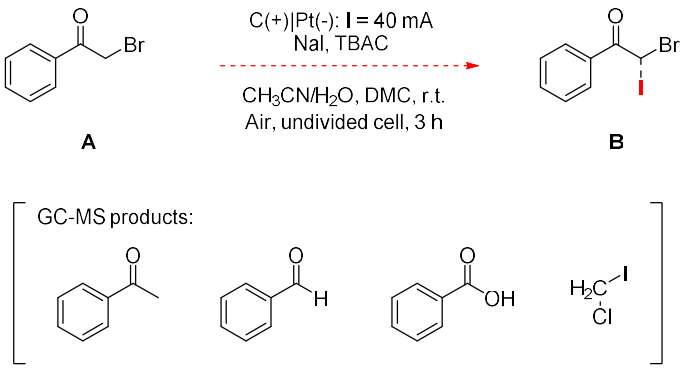
Scheme S8. NBS experiment

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar, *2*-bromo-acetophenone (200 mg, 1.0 mmol), TBAC (56.4 mg, 0.2 mmol), NaCl (380 mg, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The reaction was in an ambient atmosphere, without electricity for 8 h.

GC-MS result for NBS experiment.



3..5.5 NaI experiment

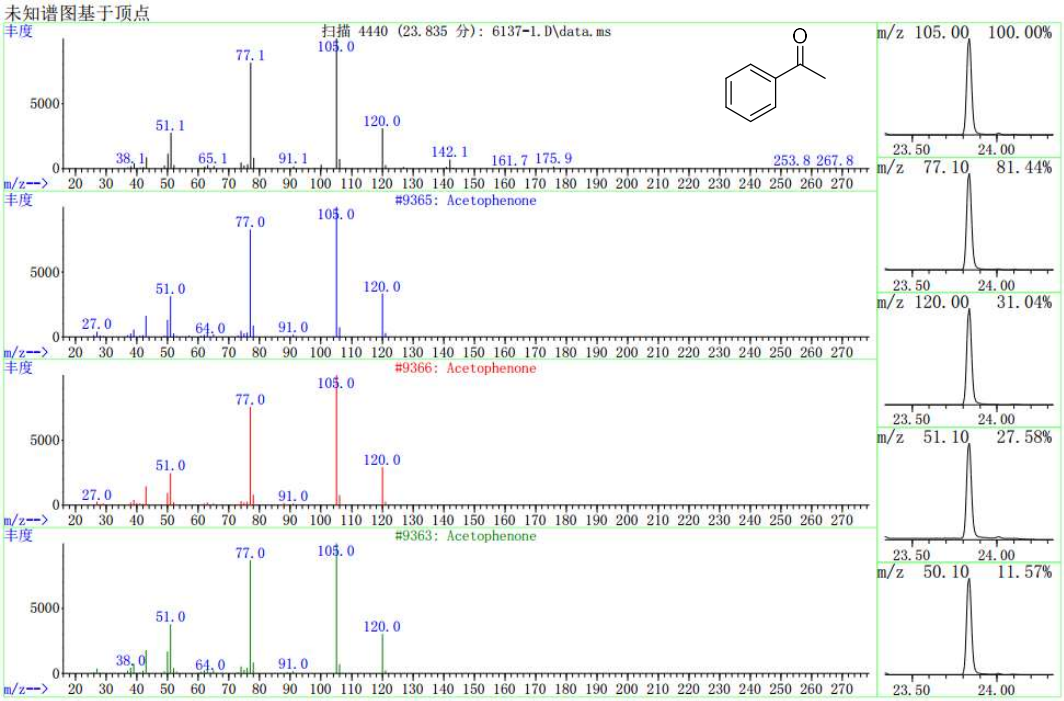


Scheme S9. NaI experiment

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar, *2*-bromo-acetophenone (200 mg, 1.0 mmol), TBAC (56.4 mg, 0.2 mmol), NaI (715 mg, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The flask was equipped with a platinum plate (50 mm×50 mm×0.2 mm) as the cathodic electrode and a carbon plate (50 mm×50 mm×2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 3 h.

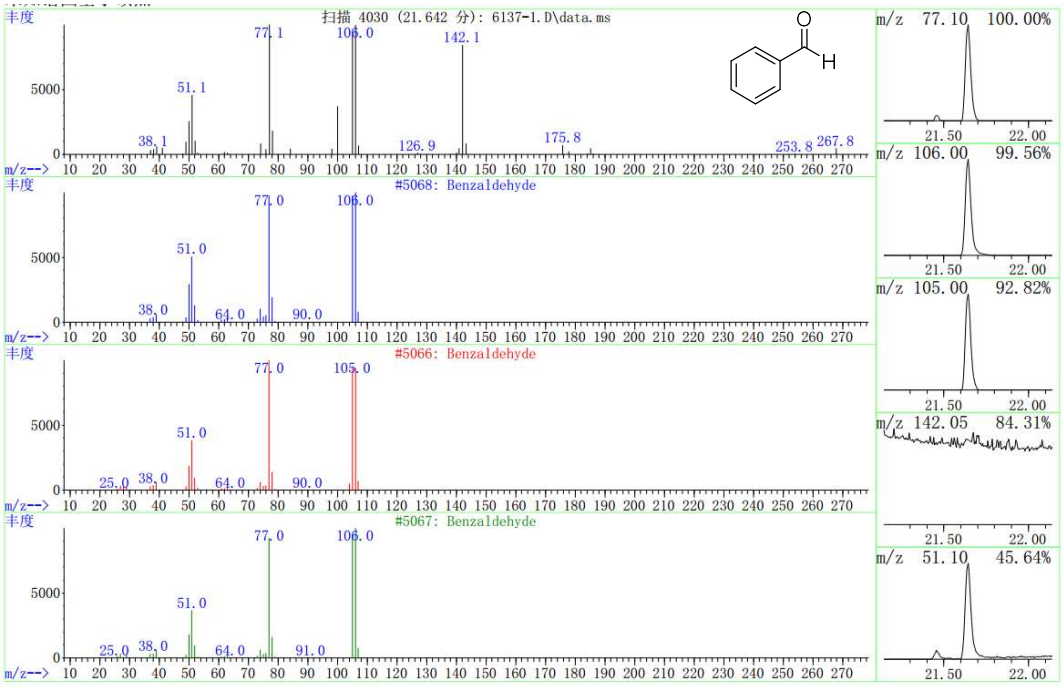
GC-MS result for NaI experiment.

1) acetophenone



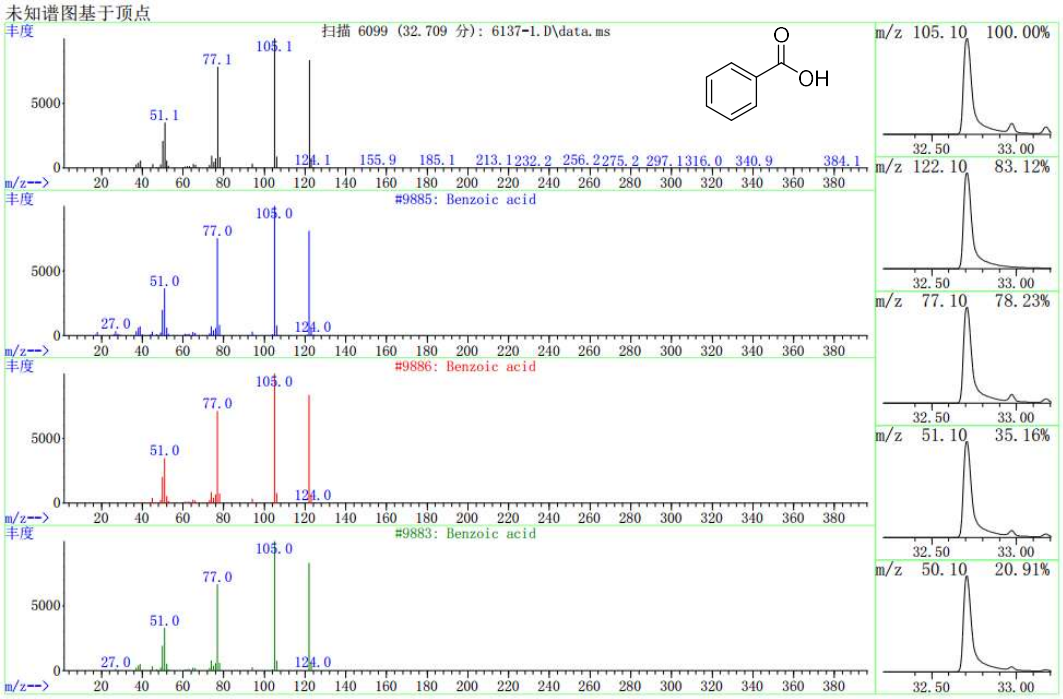
每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Acetophenone	9365	000098-86-2	94
2 Acetophenone	9366	000098-86-2	91
3 Acetophenone	9363	000098-86-2	91

2) benzaldehyde



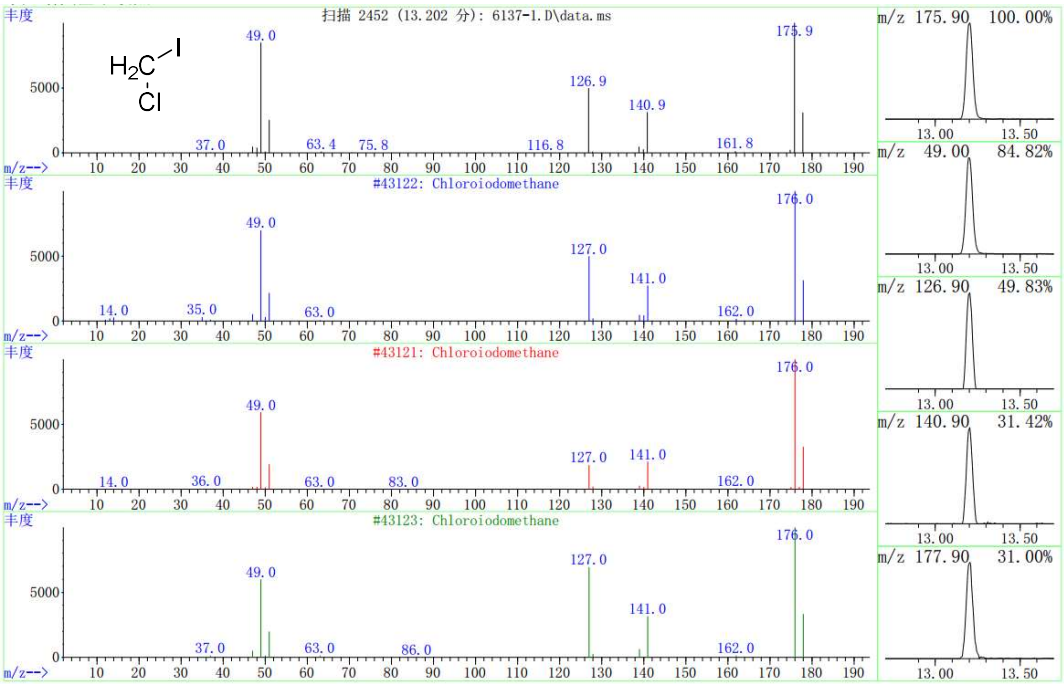
每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Benzaldehyde	5068	000100-52-7	91
2 Benzaldehyde	5066	000100-52-7	91
3 Benzaldehyde	5067	000100-52-7	64

3) benzoic acid



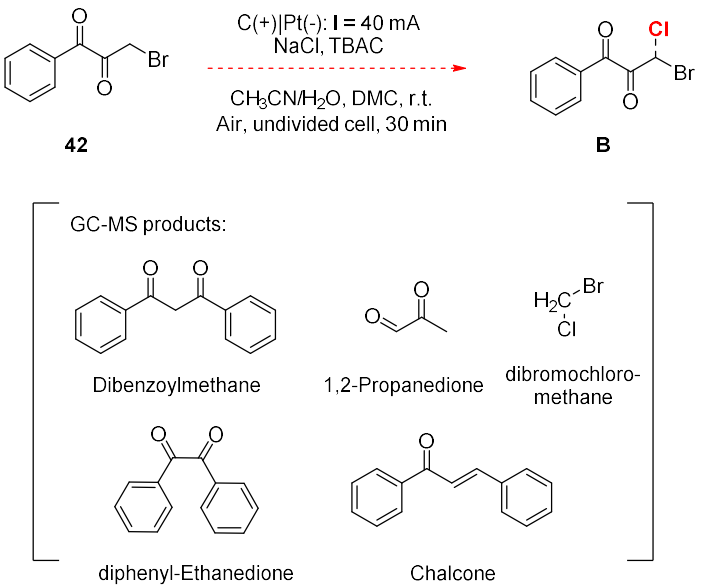
每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Benzoic acid	9885	000065-85-0	97
2 Benzoic acid	9886	000065-85-0	96
3 Benzoic acid	9883	000065-85-0	94

4) chloroiodomethane



每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Chloroiodomethane	43122	000593-71-5	91
2 Chloroiodomethane	43121	000593-71-5	49
3 Chloroiodomethane	43123	000593-71-5	43

3.5.6 1,2-dione experiment

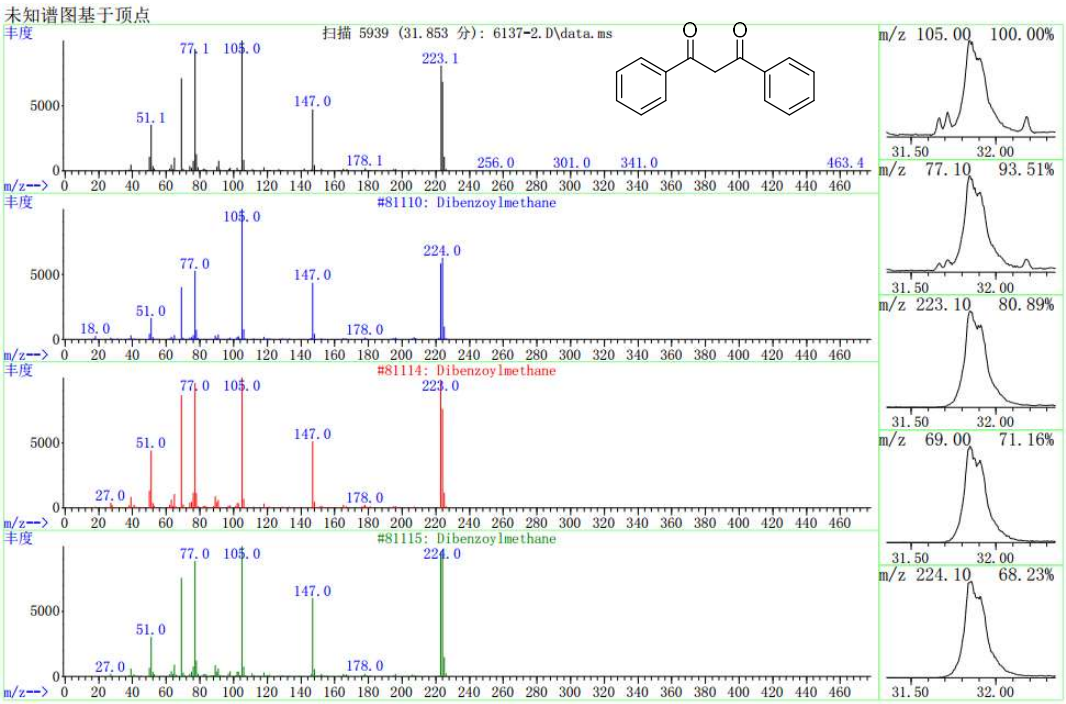


Scheme S10. 3-bromo-1-phenylpropane-1,2-dione experiment

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar, 3-bromo-1-phenylpropane-1,2-dione (227 mg, 1.0 mmol), TBAC (56.4 mg, 0.2 mmol), NaI (715 mg, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The flask was equipped with a platinum plate (50 mm×50 mm×0.2 mm) as the cathodic electrode and a carbon plate (50 mm×50 mm×2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 30 min.

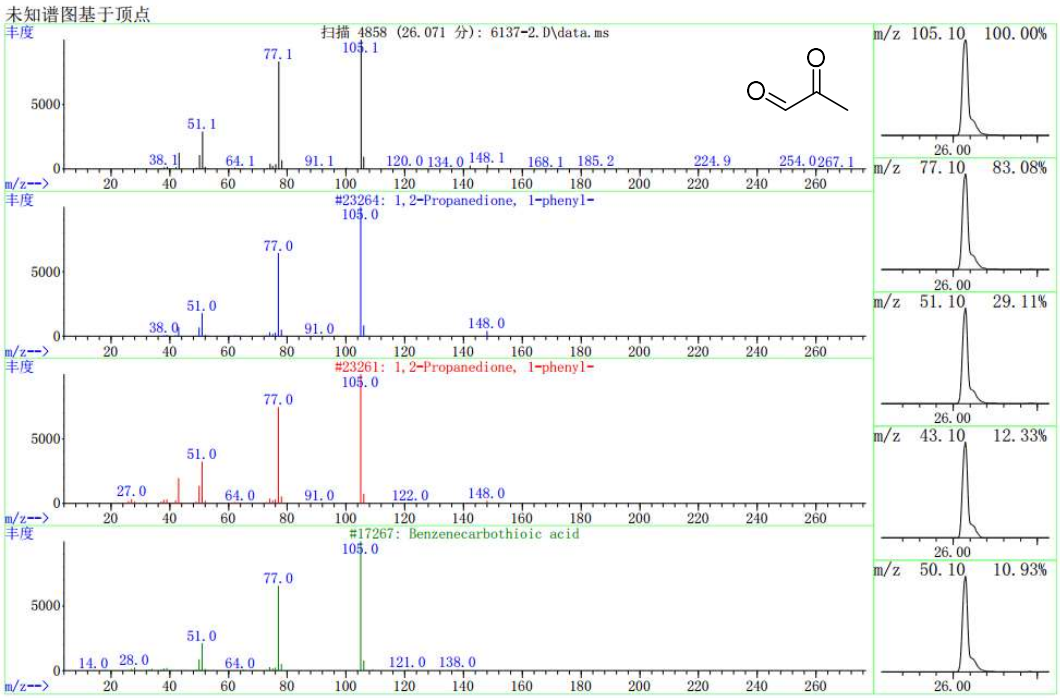
GC-MS result for 1,2-dione experiment.

1) Dibenzoylmethane



每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Dibenzoylmethane	81110	000120-46-7	94
2 Dibenzoylmethane	81114	000120-46-7	94
3 Dibenzoylmethane	81115	000120-46-7	94

2) 1,2-Propanedione

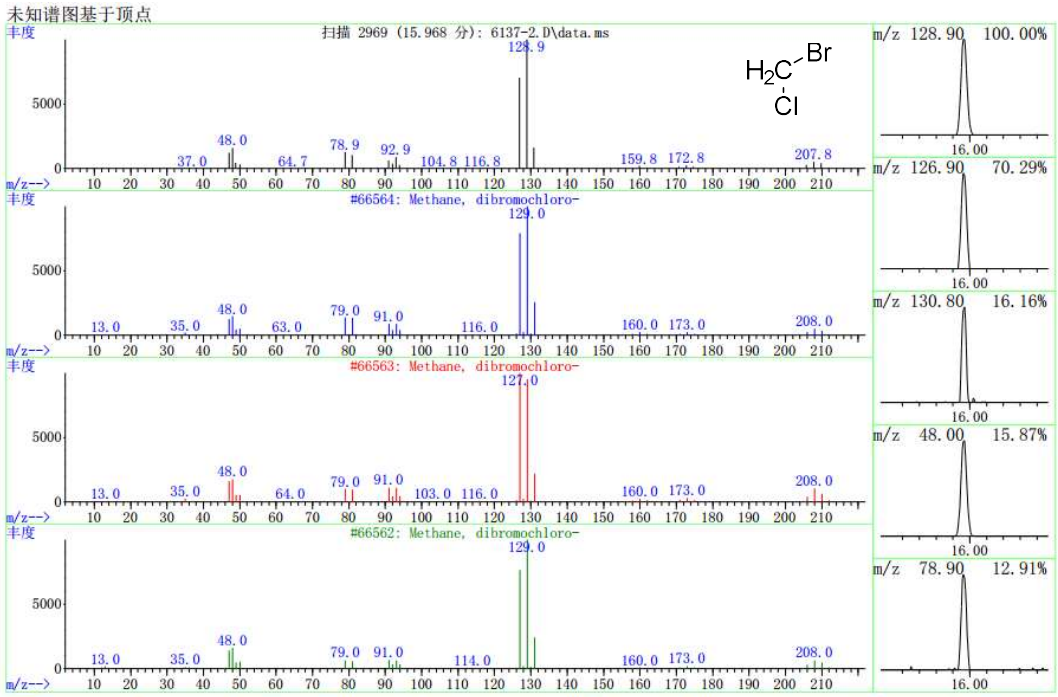


每个谱库中 3 个最匹配的记录。 Ref\# CAS\# 匹配度

C:\Database\NIST11.L

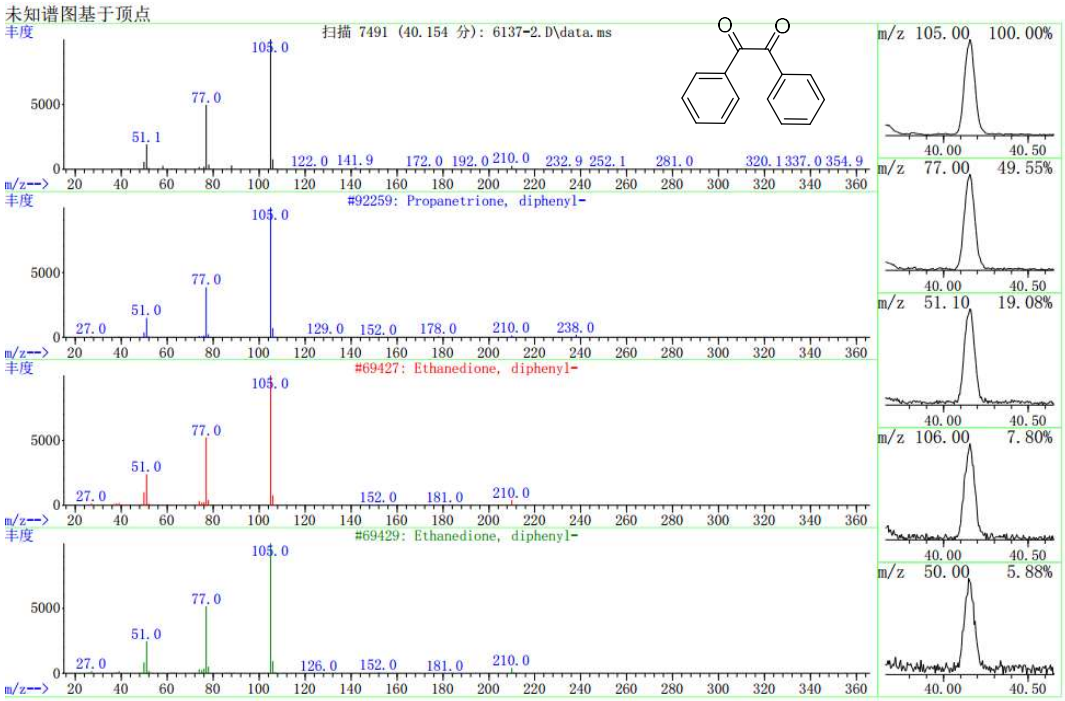
1	1,2-Propanedione, 1-phenyl-	23264	000579-07-7	91
2	1,2-Propanedione, 1-phenyl-	23261	000579-07-7	91
3	Benzenecarbothioic acid	17267	000098-91-9	90

3) dibromochloro-methane



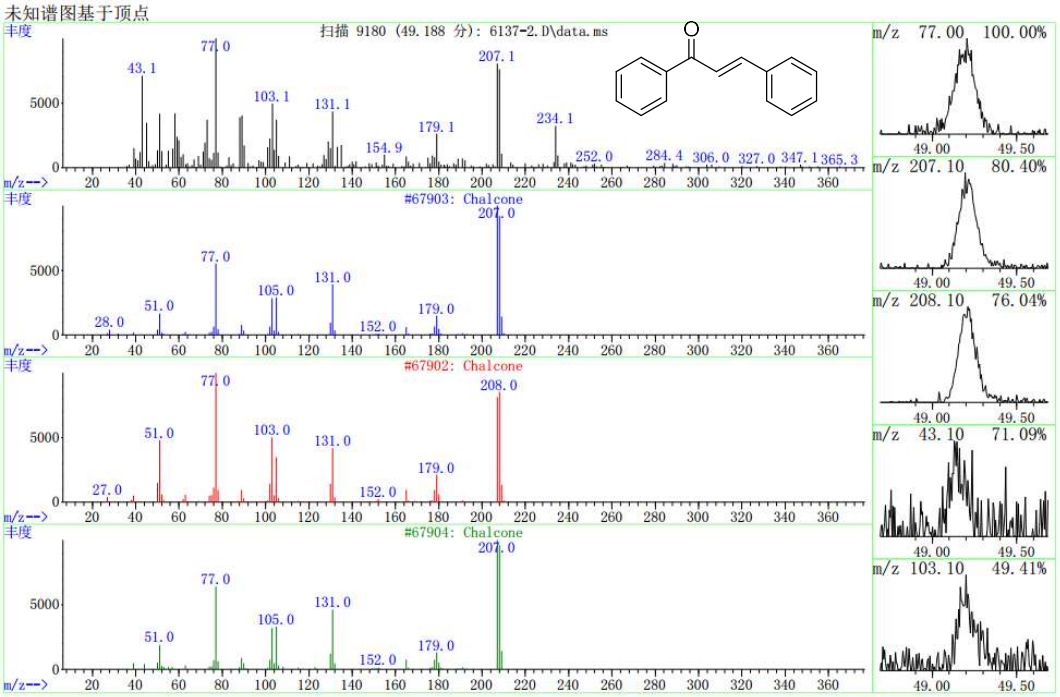
每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Methane, dibromochloro-	66564	000124-48-1	95
2 Methane, dibromochloro-	66563	000124-48-1	89
3 Methane, dibromochloro-	66562	000124-48-1	76

4) diphenyl-Ethanedione



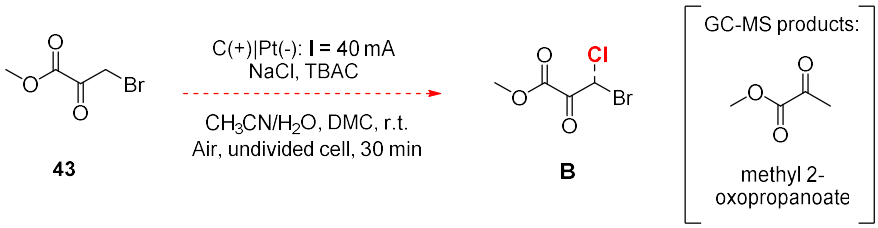
每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Propanetrione, diphenyl-	92259	000643-75-4	78
2 Ethanedione, diphenyl-	69427	000134-81-6	78
3 Ethanedione, diphenyl-	69429	000134-81-6	74

5) Chalcone



每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Chalcone	67903	000094-41-7	93
2 Chalcone	67902	000094-41-7	93
3 Chalcone	67904	000094-41-7	86

3.5.7 α-keto ester experiment

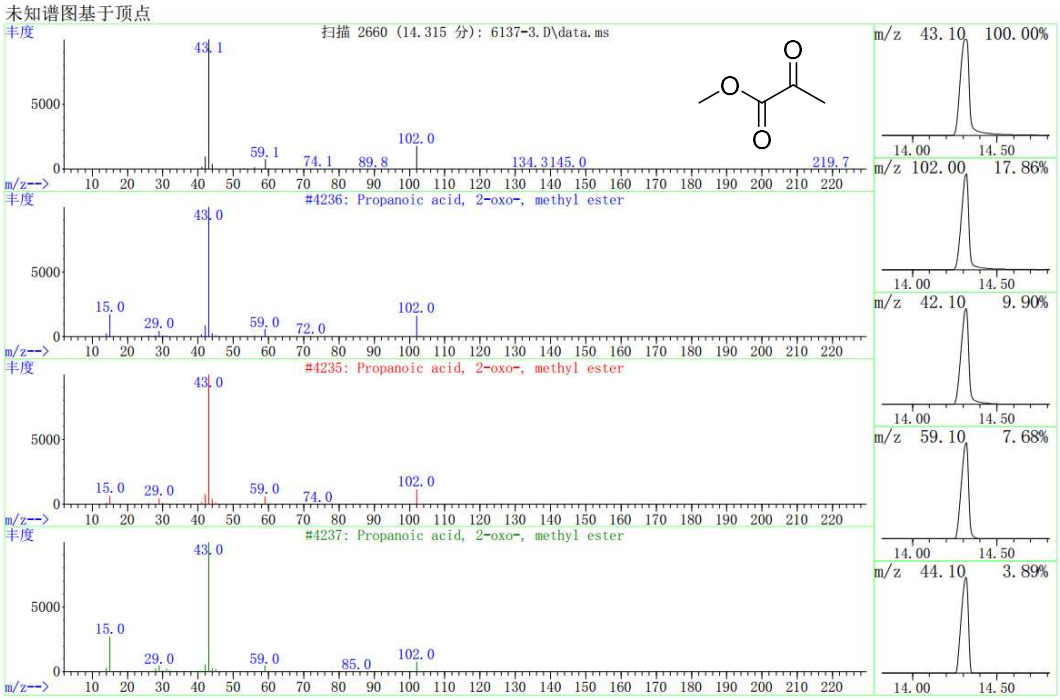


Scheme S11. methyl 3-bromo-2-oxopropanoate experiment

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar, methyl 3-bromo-2-oxopropanoate (181 mg, 1.0 mmol), TBAC (56.4 mg, 0.2 mmol), NaI (715 mg, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The flask was equipped with a platinum plate (50 mm×50 mm×0.2 mm) as the cathodic electrode and a carbon plate (50 mm×50 mm×2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 30 min.

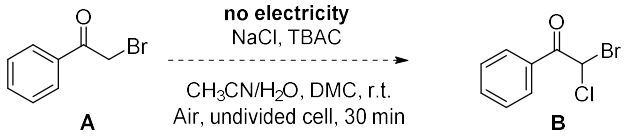
GC-MS result for α-keto ester experiment.

1) Methyl pyruvate



每个谱库中 3 个最匹配的记录。	Ref\#	CAS\#	匹配度
C:\Database\NIST11.L			
1 Propanoic acid, 2-oxo-, methyl e...	4236	000600-22-6	80
2 Propanoic acid, 2-oxo-, methyl e...	4235	000600-22-6	72
3 Propanoic acid, 2-oxo-, methyl e...	4237	000600-22-6	7

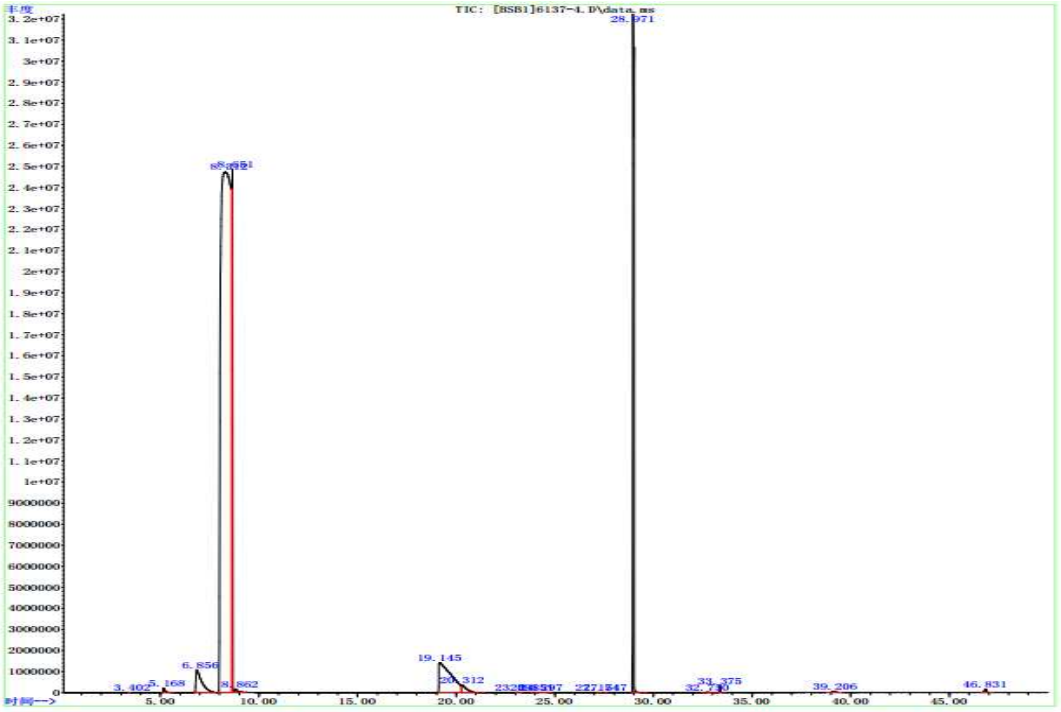
3.5.8 NaCl, TBAC (without electricity) experiment



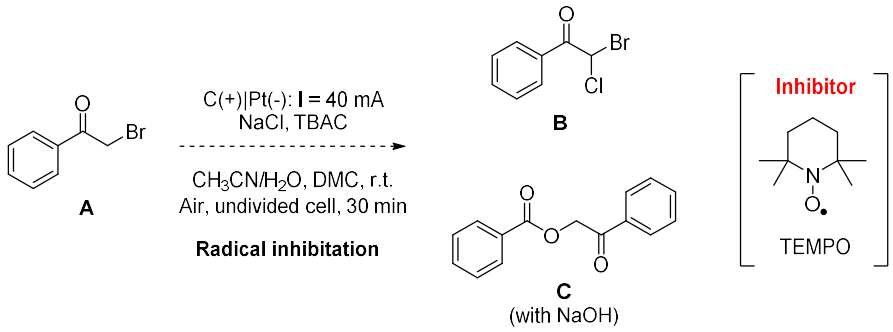
Scheme S12. NaOH addition experiment without electricity.

In an oven-dried undivided two-necked flask (250 mL) equipped with a stir bar，*2*-bromo-acetophenone (200 mg, 1.0 mmol), TBAC (56.4 mg, 0.2 mmol), NaCl (380 mg, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The reaction was in an ambient atmosphere, without electricity for 30 min.

GC-MS map for NaCl, TBAC (without electricity) experiment



3.6 Radical inhibition experiment



Scheme S13. Radical inhibition experiments.

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, 2-halo-acetophenone (200 mg, 1.0 mmol), TBAC (0.2 mmol, 55.6 mg), NaCl (1.0 mol·L^{-1}, 725 mg), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. To test the radical inhabitation of this electrocatalysis experiment, a chemical equivalent of TEMPOwas added to the reaction solutions. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathodic electrode and a carbon plate (10 mm × 10 mm × 2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 30 min. TLC, UV light as a visualizing agent, the reaction was monitored, and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. Another experiment with an addition of a buffer of NaOH (1.0 mol·L^{-1}, 500 mg) was also conducted for the radical inhibition experiment, and no dimer condensation product was observed.

3.7 EPR experiments

EPR spectra were recorded at room temperature on a Bruker EMX micro A300 spectrometer operated at 9.8543 GHz. Typical spectrometer parameters are shown as follows, sweep width: 6000 G; center field set: 3000 G; time constant: 81.92 ms; sweep time: 327.68 s modulation amplitude: 1.00 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^3; microwave power: 18.53 mW.

EPR experiment for halogenation:

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, *2*-halo-acetophenone (200 mg, 1.0 mmol), TBAC (0.2 mmol, 55.6 mg), NaCl (1.0 mol·L^{-1}, 725 mg), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathodic electrode and a carbon plate (10 mm × 10 mm × 2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 10 min.

EPR experiments were performed to detect the radical intermediates with the addition of free radical spin trapping agent 5,5-dimethyl-1-pyrroline N-oxide (DMPO). The control experiment was conducted without electricity. Results showed that no distinct free radical signal was detected under reaction conditions without electricity with any substrates; however, EPR signals were identified after the electrocatalysis. DMPO could quickly trap the free radicals to form a relatively stable radical (DMPO·R, R represents alkoxy radical) (g=2.00662, aN=14.28, aH^{β}=13.27).

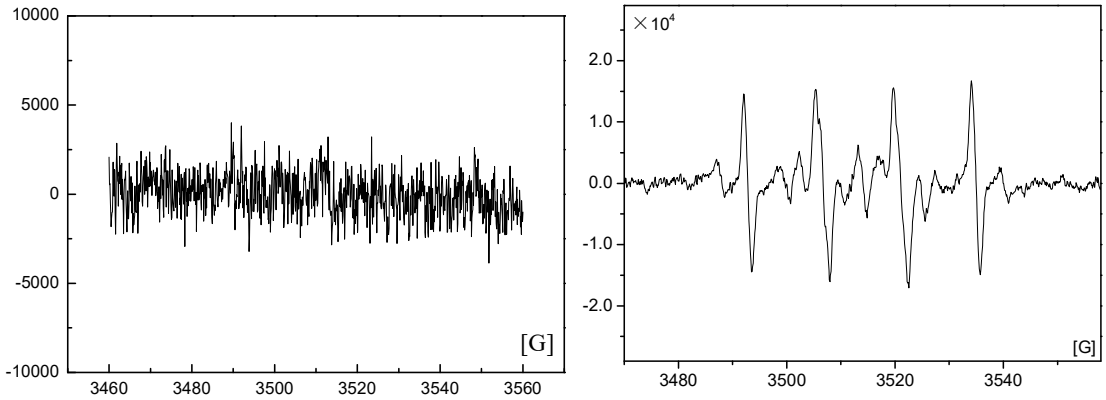


Figure S3. EPR of reactant **A** for electrohalogenation

EPR experiment for dimer condensation:

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, *2*-halo-acetophenone (200 mg, 1.0 mmol), TBAC (0.2 mmol, 55.6 mg), NaCl (1.0 mol·L^{-1}, 725 mg), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. NaOH (1.0 mol(L-1, 500 mg) was added to the reaction solutions. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathodic electrode and a carbon plate (10 mm × 10 mm × 2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 10 min.

EPR experiments were performed to detect the radical intermediates with the addition of free radical spin trapping agent 5,5-dimethyl-1-pyrroline N-oxide (DMPO). The control experiment was conducted without electricity. Results stated that no distinct free radical signal was detected under reaction conditions without electricity with any substrates; however, EPR signals were identified after the electrocatalysis. DMPO can quickly trap the free radicals to form a typical hydroxyl radical (DMPO·OH, g=2.00634, aN=14.98 G, aH^{β}=14.86 G).

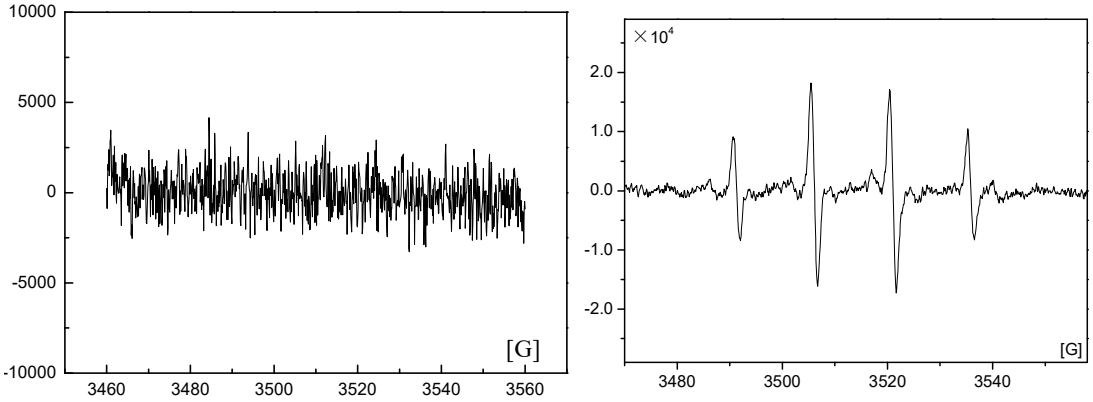


Figure S4. EPR of reactant **A** for dimer condensation

3.8 Microcoulometric experiments

Microcoulometric experiments was conducted to investigate the electro-catalysis reversibility and electron transfer number (n-value). For the halogenation experiments, Q_{exp} = it = 40 x 0.001 x 30 x 60 = 72 C, Q_{theor} = 0.001 x 1 x 96500 = 96.5 C. The Columbic yield (current efficiency) is 96.5/72 x 0.8 x 100 = 107% ≅ 1. This means that the reaction involves in conversion of one haloketone molecule with one electron.

CV experiments for oxidation peak of A:

Using CH_3CN (20 mL), and H_2O (20 mL) as co-solvent. Without NaOH, cyclic voltammetry (CVs) experiments of reactant *2*-bromo-acetophenone (**A**, 199.4 mg) were conducted at different scan rates. At a scan rate of 0.010 V/s, from – 0.5 V to 2.0 V, the oxidation peak of **A** was reversible (i_{pa1} = 0.32 mA, i_{pc1} = 0.28 mA, i_{pa1}/i_{pc1} = 1.1 ≈ 1). The relationship of E_{pa} and i_{pa} at different scan rate are E_{pa} = 0.0728 Log i_{pa1} + 0.094 (R^2 = 0.8397). Results indicated that, in the electrohalogenation process the transferred electrons for the oxidation peak of **A** is one (n = 0.0712/0.0728 = 0.98 ≈ 1).

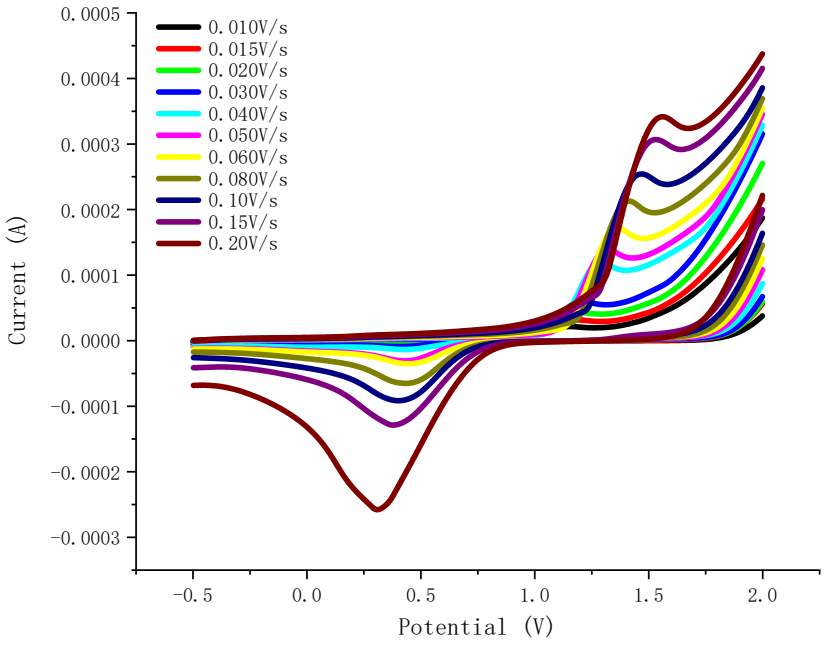


Figure S5. CVs of **A** at different scan rates

E_{pa1}	i_{pa1}	Lg i_{pa1}
0.50	$-2.04*10^{-6}$	-5.69
0.496	$-4.07*10^{-6}$	-5.39
0.473	$-4.49*10^{-6}$	-5.35
0.44	$-8.78*10^{-6}$	-5.06
0.447	$-1.36*10^{-5}$	-4.87
0.43	$-3.10*10^{-5}$	-4.51
0.447	$-3.50*10^{-5}$	-4.46
0.429	$-6.46*10^{-5}$	-4.19
0.40	$-9.12*10^{-5}$	-4.04
0.38	$-1.29*10^{-4}$	-3.89
0.31	$-2.58*10^{-4}$	-3.59

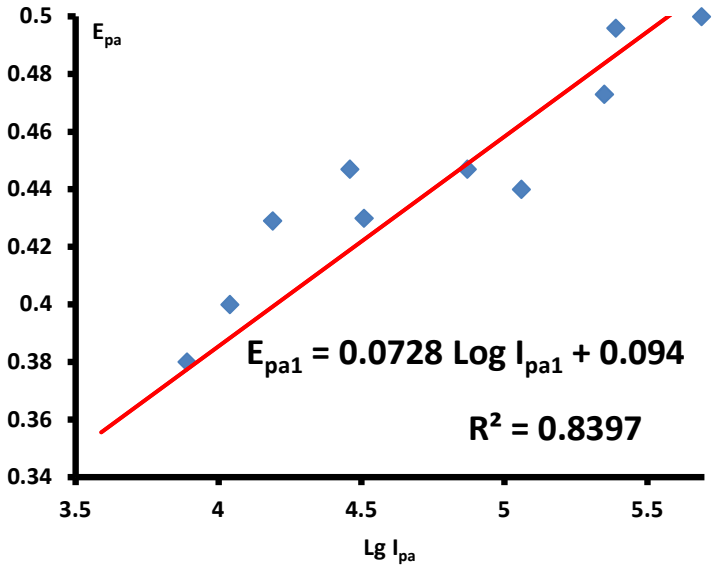


Figure S6. Line fitting of E_{pa1} and log_{ipa1} for the oxidation peak of **A**

CV experiments for oxidation peak of A, with NaOH addition:

CH_3CN (20 mL) and H_2O (20 mL) as co-solvent. NaOH (200 mg) was added to the reaction solution, cyclic voltammetry (CVs) experiments of reactant *2*-bromo-acetophenone (**A**, 199.4 mg) were conducted at different scan rates. At a scan rate of 0.010 V/s, from – 0.5 V to 2.5 V, the oxidation peak of **A** was irreversible. The relationship of E_{pa} and i_{pa} at different scan rate are E_{pc} = -0.6491 Log i_{pc} + 3.6361 (R^2 = 0.808).

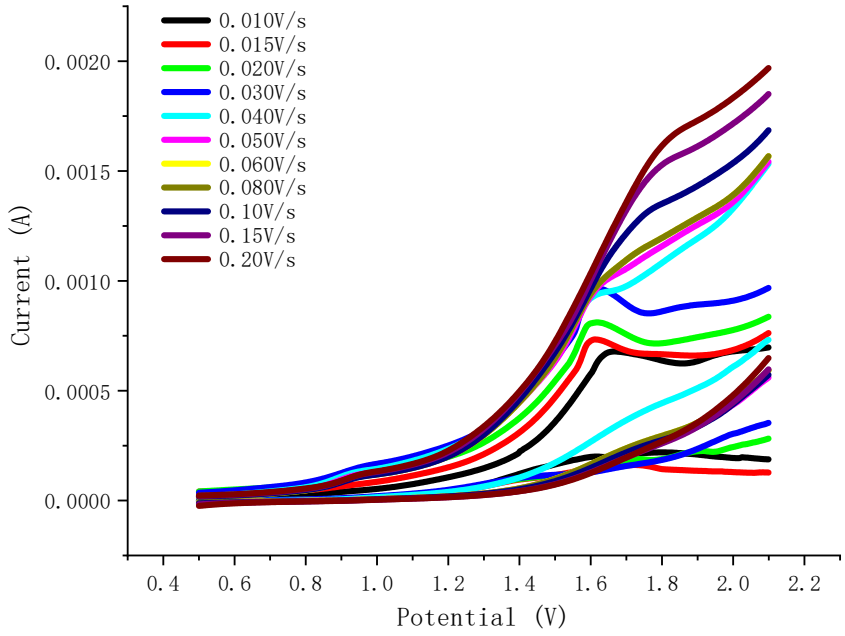


Figure S7. CVs of A at different scan rates with NaOH

E_{pc}	i_{pc}	Lg i_{pc}
1.66	$6.78*10^{-4}$	-3.17
1.61	$7.33*10^{-4}$	-3.13
1.62	$8.11*10^{-4}$	-3.09
1.622	$9.64*10^{-4}$	-3.02
1.622	$9.44*10^{-4}$	-3.025
1.64	$9.93*10^{-4}$	-3.003
1.71	$1.10*10^{-3}$	-2.96
1.75	$1.16*10^{-3}$	-2.94
1.80	$1.35*10^{-3}$	-2.87
1.82	$1.55*10^{-3}$	-2.81
1.86	$1.70*10^{-3}$	-`2.77

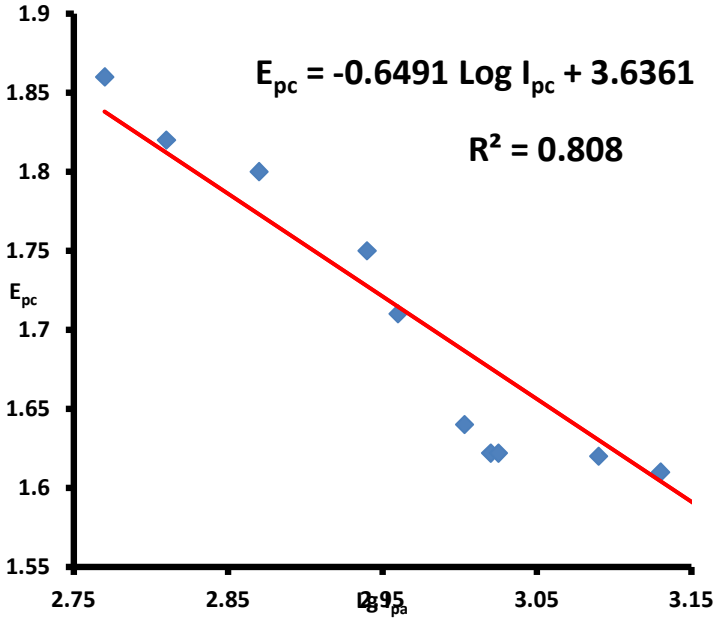


Figure S8. Line fitting of E_{pa1} and log_{ipa1} for the oxidation peak of **A** (with NaOH addition)

CV experiments for oxidation peak of Ferrocene:

Using CH_3CN (20 mL) and H_2O (20 mL) as co-solvent. Cyclic voltammetry (CVs) experiments of Ferrocene (186.0 mg) were conducted at different scan rates. At a scan rate of 0.010 V/s, from 0 V to 0.8 V, the oxidation peak of Ferrocene was irreversible. The relationship of E_{pa} and i_{pa} at different scan rate are E_{pc} = 0.0712 Log i_{pa} – 0.1033 (R^2 = 0.9599).

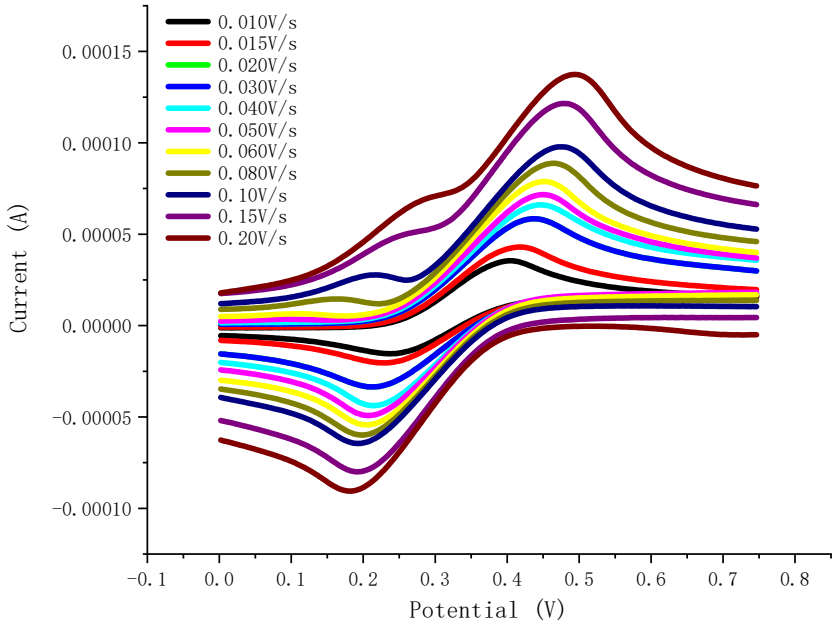


Figure S9. CVs of Ferrocene at different scan rates

E_{pa}	i_{pa}	Lg i_{pa}
0.24	$-1.54*10^{-5}$	-4.81
0.23	$-2.02*10^{-5}$	-4.69
0.211	$-3.342*10^{-5}$	-4.475
0.212	$-3.339*10^{-5}$	-4.476
0.213	$-4.37*10^{-5}$	-4.36
0.206	$-4.92*10^{-5}$	-4.31
0.204	$-5.43*10^{-5}$	-4.27
0.20	$-5.97*10^{-5}$	-4.22
0.192	$-6.44*10^{-5}$	-4.19
0.19	$-7.99*10^{-5}$	-4.10
0.18	$-9.07*10^{-5}$	-4.04

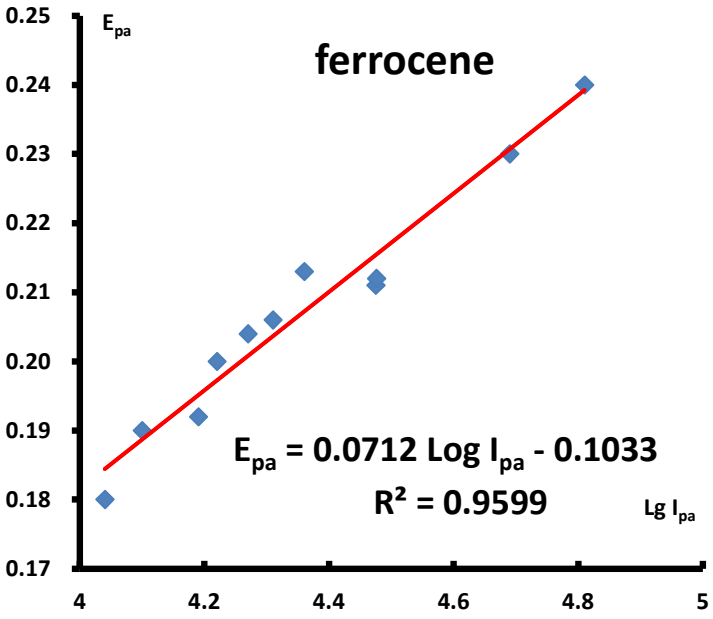


Figure S10. Line fitting of E_{pa1} and log_{ipa1} for the oxidation peak of Ferrocene

3.9 Cyclic voltammetry experiments

Cyclic voltammograms were conducted on a Metrohm PGSTAT302N potentiostat and performed in a three-electrode cell connected to a Schlenk line under nitrogen at room temperature. The working electrode was a carbon plate electrode. The counter electrode was a platinum wire. The reference was a Hg/Hg_2Cl_2 electrode submerged in saturated aqueous KBr solution and separated from the reaction by a salt bridge.

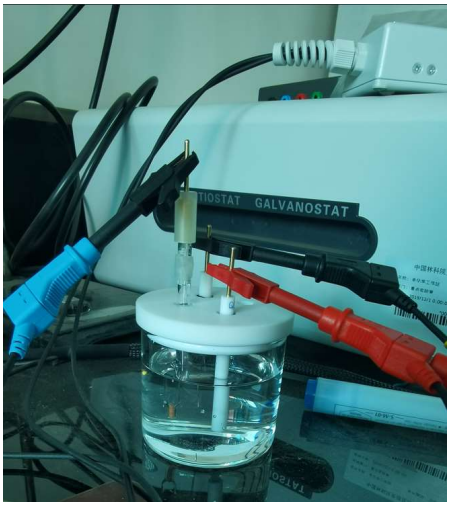


Figure S11. Cyclic voltammograms experiments

(A) CV Procedure for NaCl. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaCl (1.19g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s, ranging from -2.0 V to 3.0 V.

(B) CV Procedure for NaCl and 2-bromo-acetophenone. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaCl (1.19g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent) and 2-bromo-acetophenone (1.5459g, 0.01 $mol \cdot L^{-1}$, 1.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s, ranging from -2.0 V to 3.0 V.

(C) CV Procedure for NaBr. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaBr (0.52 g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s,

ranging from -2.0 V to 3.0 V.

(D) CV Procedure for NaF. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaF (0.21 g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s, ranging from -1.5 V to 2.5 V.

(E) CV Procedure for NaOH. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaOH (0.20g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s, ranging from -2.0 V to 2.5 V.

(F) CV Procedure for NaOH and 2-bromo-acetophenone. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaOH (0.20g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent) and 2-bromo-acetophenone (1.5459g, 0.01 $mol \cdot L^{-1}$, 1.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 10 mA. The scan rate was 0.10 V/s, ranging from -2.0 V to 2.5 V.

(G) CV Procedure for NaCl, NaOH and 2-bromo-acetophenone. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing NaCl (1.19g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent), NaOH (0.20g, 0.01 $mol \cdot L^{-1}$, 5.0 chemical equivalent) and 2-bromo-acetophenone (1.5459g, 0.01 $mol \cdot L^{-1}$, 1.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s, ranging from -1.0 V to 3.0 V.

(H) CV Procedure for TBAC. A mixed solvent (CH_3CN/H_2O = 15 mL /15 mL) containing TBAC (0.3230g, 0.01 $mol \cdot L^{-1}$, 1.0 chemical equivalent), was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 1 mA. The scan rate was 0.10 V/s, ranging from -0.7 V to 2.5 V.

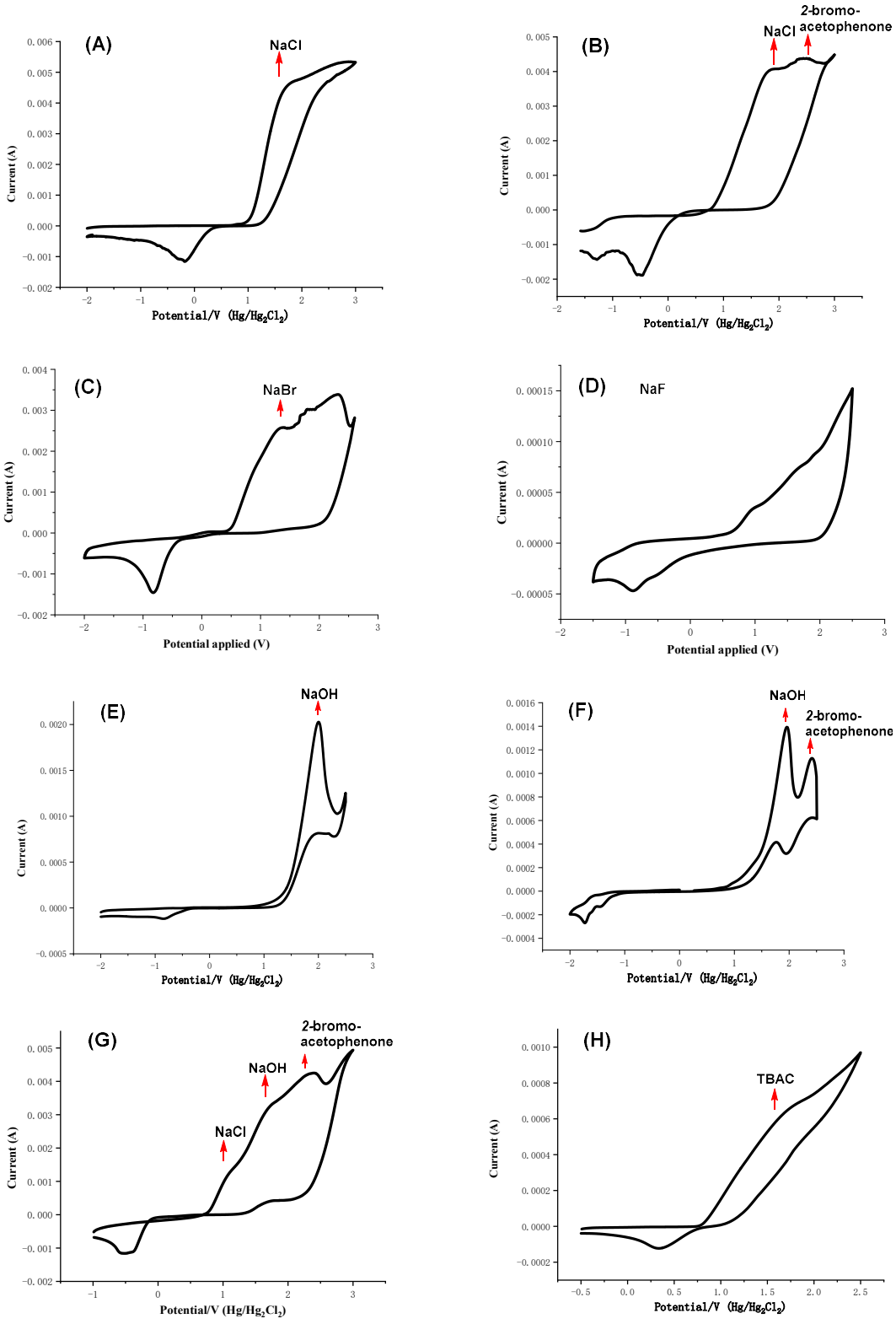
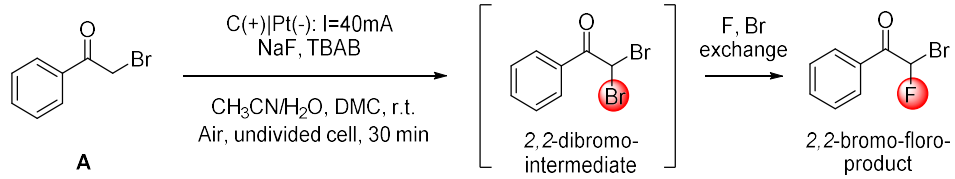
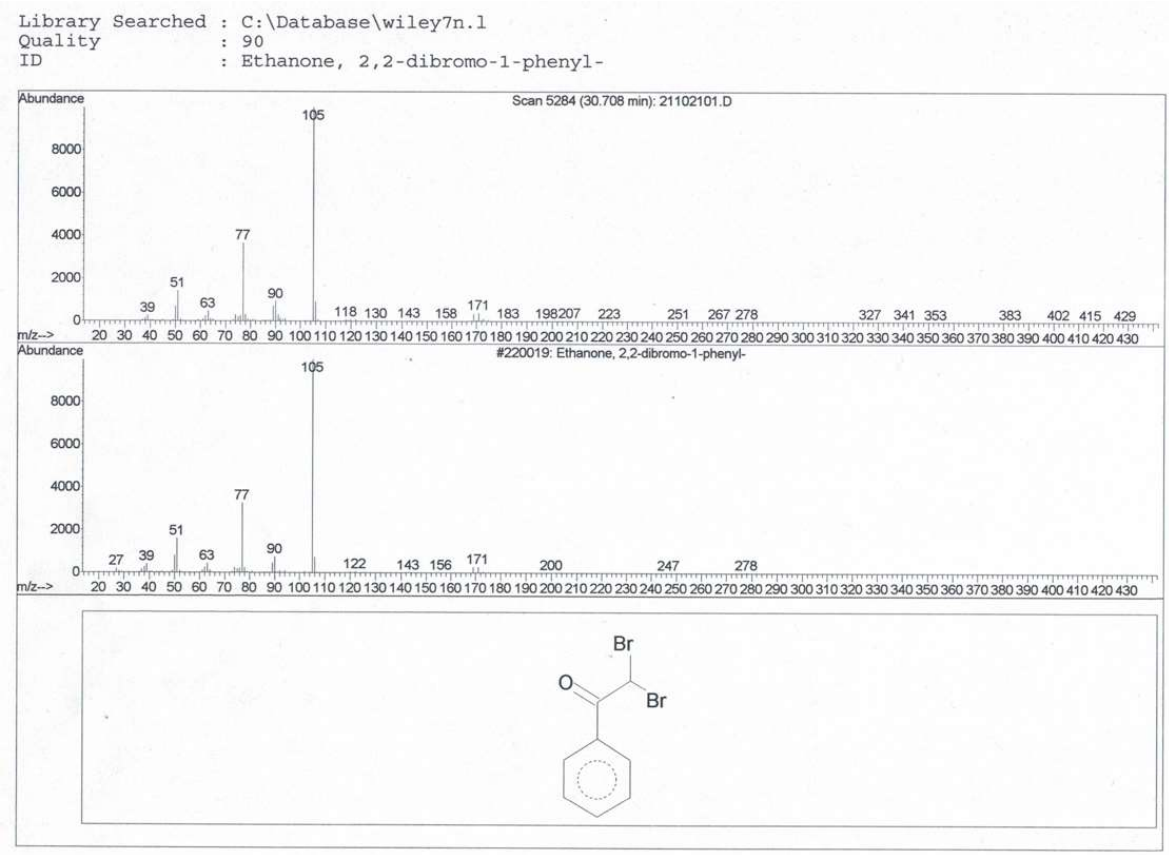


Figure S12. Cyclic voltammograms maps

3.10 GC-MS experiment for electro-fluorination

In an oven-dried undivided two-necked flask (50 mL) equipped with a stir bar, *2*-bromo-acetophenone (200 mg, 1.0 mmol), TBAB (50 mg, 0.2 mmol), KBr (1.0 mol·L^{-1}, 6.5 mmol), CH_3CN (5.0 mL), H_2O (5.0 mL), and DMC (2.5 mL) were combined and added. The flask was equipped with a platinum plate (10 mm × 10 mm × 0.2 mm) as the cathodic electrode and a carbon plate (10 mm × 10 mm × 2 mm) as the anodic electrode. The reaction was in an ambient atmosphere. The reaction mixture was stirred and electrolyzed at a constant current of 40 mA under room temperature for 30 min. The reaction was conducted with the GC-MS.

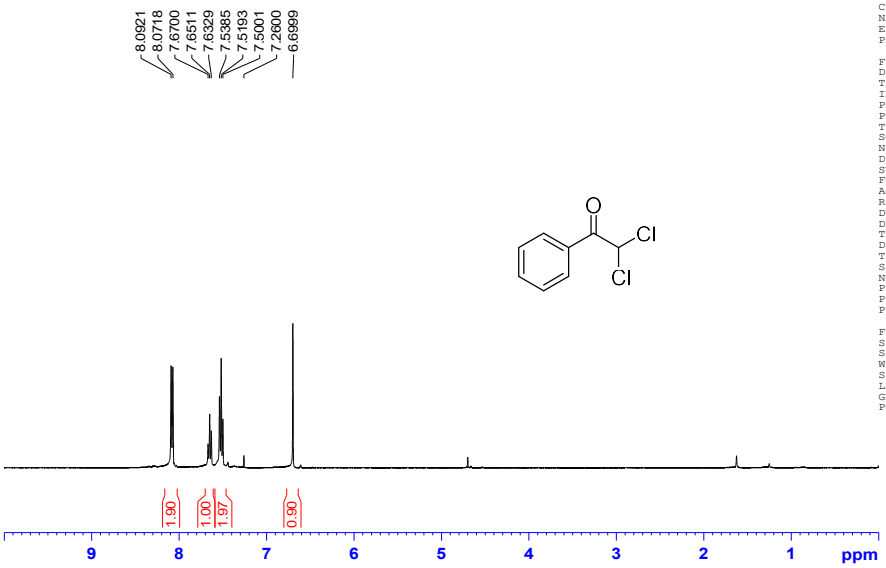




Scheme S14. GC-MS analysis of *2,2*-dibromo-intermediate in TBAB involved fluorination

4. ^{1}H-NMR ^{13}C-NMR, and ^{19}F-NMR spectra

^{1}H-NMR (400 MHz, $CDCl_3$)

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PROCNO                  1

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SOLVENT              CDCl3
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DS                       0
SWH               5555.556 Hz
FIDRES            0.169542 Hz
AQ                5.8982401 sec
RG                     101
DW                 90.000 usec
DE                  9.42 usec
TE                  295.9 K
D1              1.00000000 sec
TD0                      1
SFO1           400.1321847 MHz
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P1                  10.75 usec
PLW1           16.71999931 W

F2 - Processing parameters
SI                   65536
SF              400.1300096 MHz
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SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
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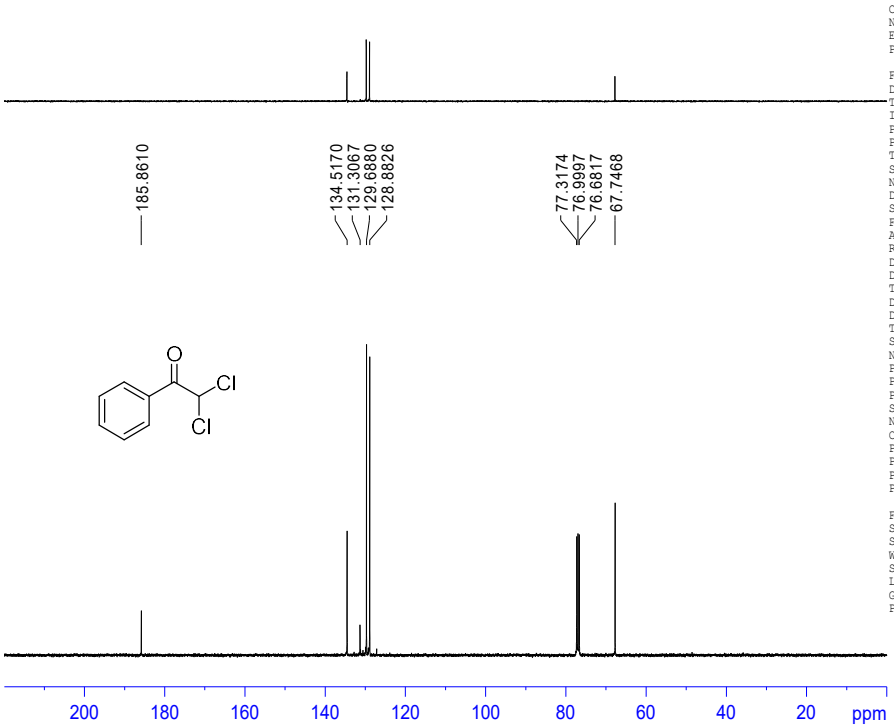
^{13}C-NMR (100 MHz, $CDCl_3$)

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PROCNO                  1

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DS                       0
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FIDRES            0.762939 Hz
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RG                     101
DW                 20.000 usec
DE                  6.50 usec
TE                  296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           100.6238359 MHz
NUC1                   13C
P0                   3.33 usec
P1                  10.00 usec
PLW1           75.41799927 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz65
PCPD2               80.00 usec
PLW2           16.71999931 W
PLW12           0.37619999 W
PLW13           0.18892001 W

F2 - Processing parameters
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GB        0
PC                   1.40
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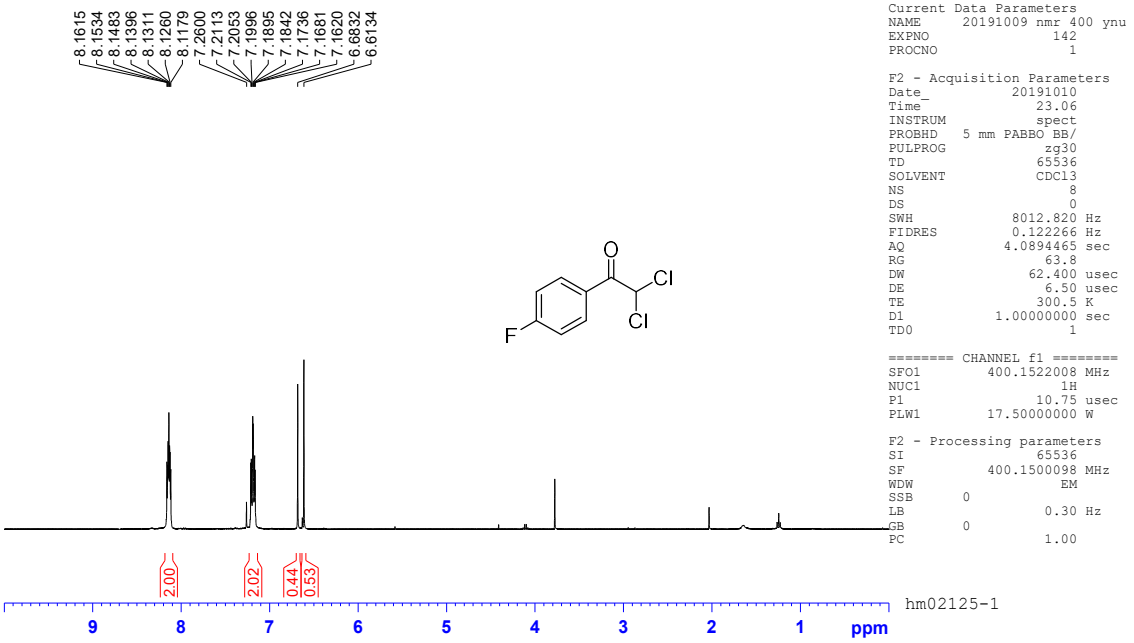
^{1}H-NMR (400 MHz, $CDCl_3$)

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PROCNO                   1

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PULPROG           zg30
TD               65536
SOLVENT          CDCl3
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DS                   0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                63.8
DW              62.400 usec
DE               6.50 usec
TE              300.5 K
D1           1.00000000 sec
TD0                  1

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NUC1               1H
P1              10.75 usec
PLW1        17.50000000 W

F2 - Processing parameters
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SSB       0
LB              0.30 Hz
GB        0
PC              1.00
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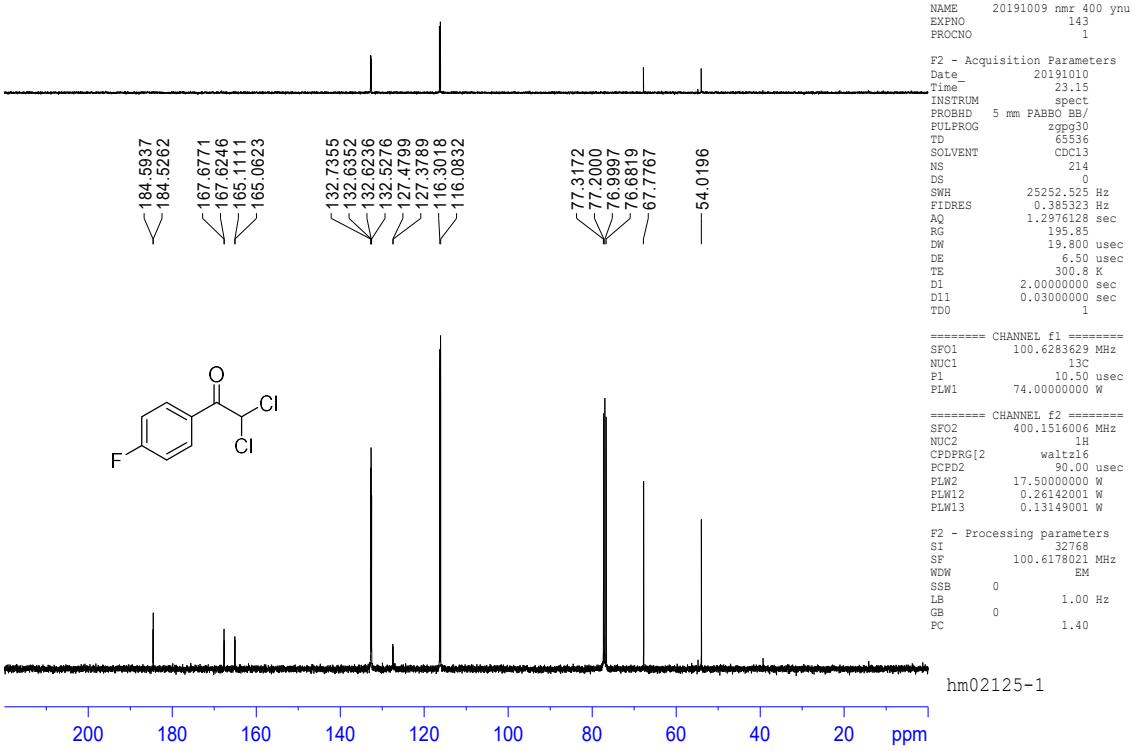
^{13}C-NMR (100 MHz, $CDCl_3$)

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PROCNO                   1

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PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 214
DS                   0
SWH          25252.525 Hz
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AQ            1.2976128 sec
RG               195.85
DW              19.800 usec
DE               6.50 usec
TE              300.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6283629 MHz
NUC1               13C
P1              10.50 usec
PLW1        74.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2           90.00 usec
PLW2        17.50000000 W
PLW12        0.26142001 W
PLW13        0.13149001 W

F2 - Processing parameters
SI               32768
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SSB       0
LB              1.00 Hz
GB        0
PC              1.40
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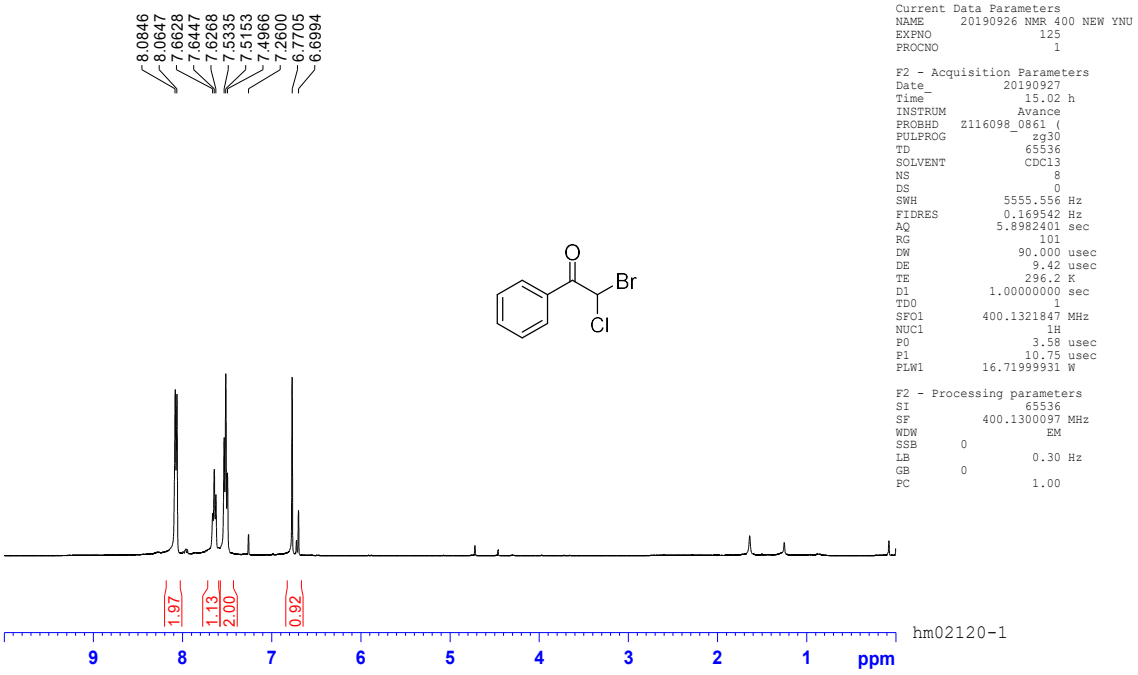
^{1}H-NMR (400 MHz, $CDCl_3$)

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PROCNO               1

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PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           5555.556 Hz
FIDRES        0.169542 Hz
AQ            5.8982401 sec
RG                 101
DW              90.000 usec
DE               9.42 usec
TE              296.2 K
D1           1.00000000 sec
TD0                  1
SFO1        400.1321847 MHz
NUC1                1H
P0                3.58 usec
P1               10.75 usec
PLW1        16.71999931 W

F2 - Processing parameters
SI               65536
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SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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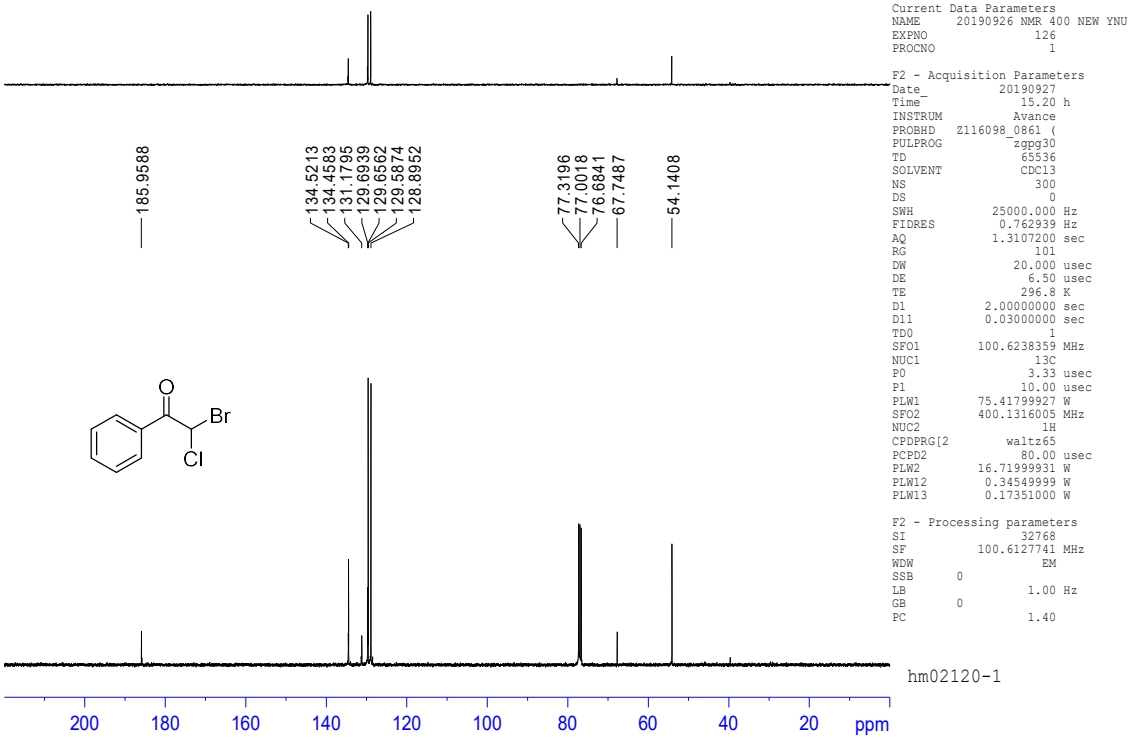
^{13}C-NMR (100 MHz, $CDCl_3$)

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PROCNO               1

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PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 300
DS                   0
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FIDRES        0.762939 Hz
AQ            1.3107200 sec
RG                 101
DW              20.000 usec
DE               6.50 usec
TE              296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        100.6238359 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        75.41799927 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        16.71999931 W
PLW12        0.34549999 W
PLW13        0.17351000 W

F2 - Processing parameters
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GB        0
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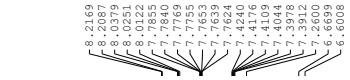
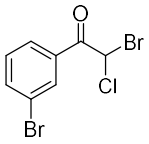
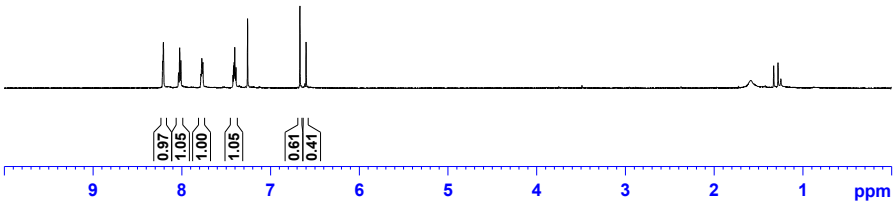
^{1}H-NMR (400 MHz, $CDCl_3$)





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PROCNO                 1

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DS                      2
RG                 121.23
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DS                      2
NS                      2
TD0                     1
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NUC1                   1H
P1                 10.00 usec
PLW1         26.09399986 W

F2 - Processing parameters
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PC                  1.00
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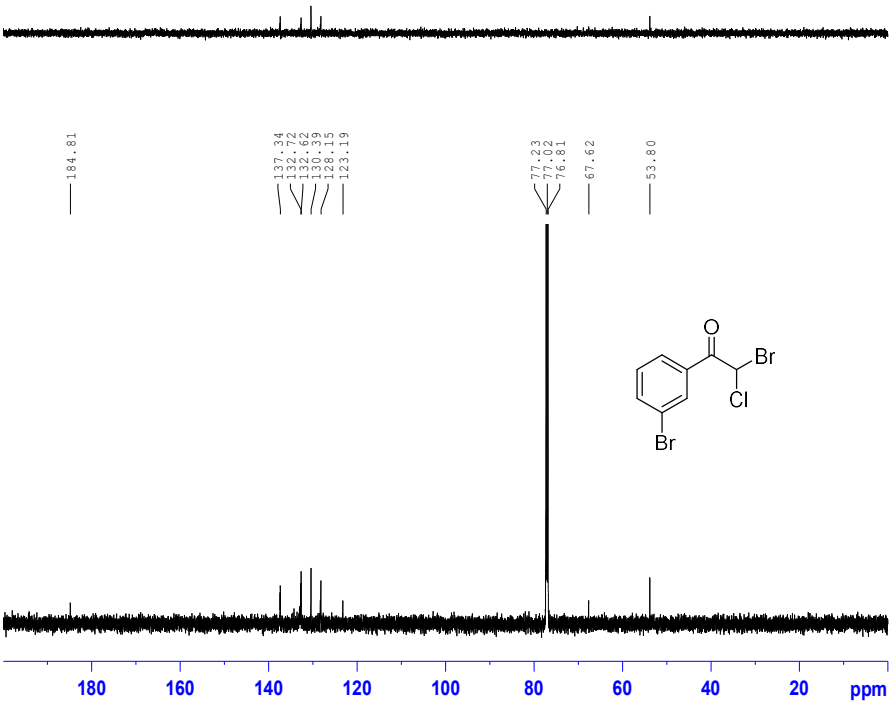
HM02212

^{13}C-NMR (150 MHz, $CDCl_3$)

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EXPNO                 61
PROCNO                 1

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DS                      4
RG                 188.35
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DS                      4
NS                    256
TD0                     1
SFO1         150.9279578 MHz
NUC1                   13C
P1                 12.00 usec
PLW1         97.67099762 W
SFO2         600.1724007 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
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PLW12         0.40399119 W
PLW13         0.20248041 W

F2 - Processing parameters
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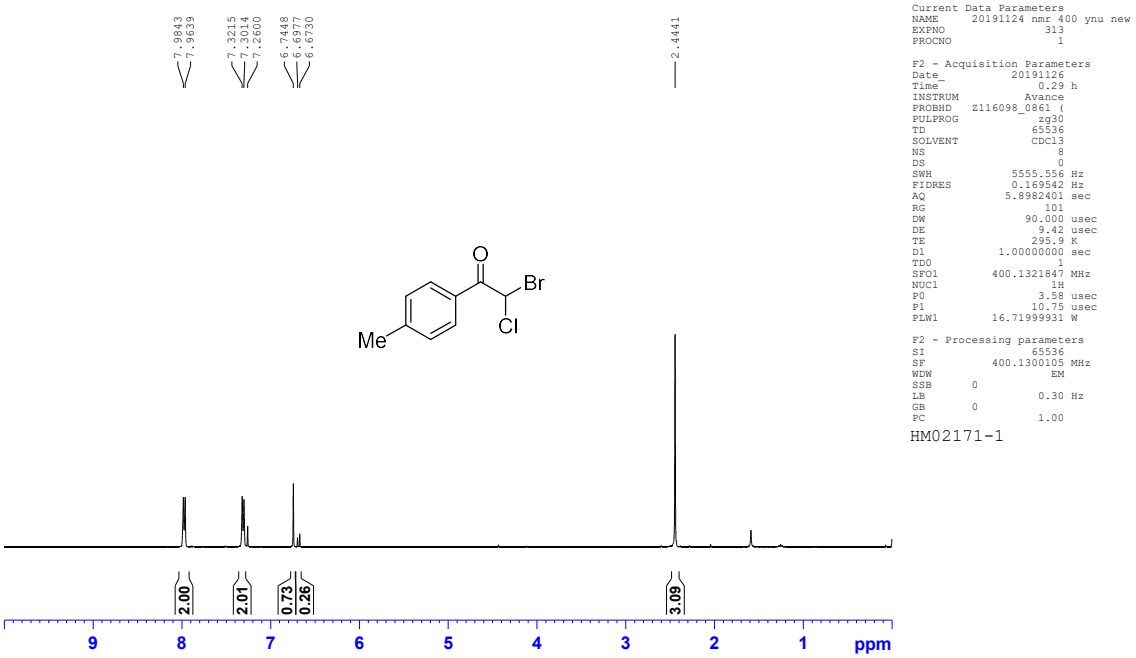
HM02212

^{1}H-NMR (400 MHz, $CDCl_3$)

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PROCNO                 1

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TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
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FIDRES          0.169542 Hz
AQ              5.8982401 sec
RG                   101
DW                90.000 usec
DE                 9.42 usec
TE                295.9 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1321847 MHz
NUC1                  1H
P0                 3.58 usec
P1                10.75 usec
PLW1          16.71999931 W

F2 - Processing parameters
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PC                 1.00
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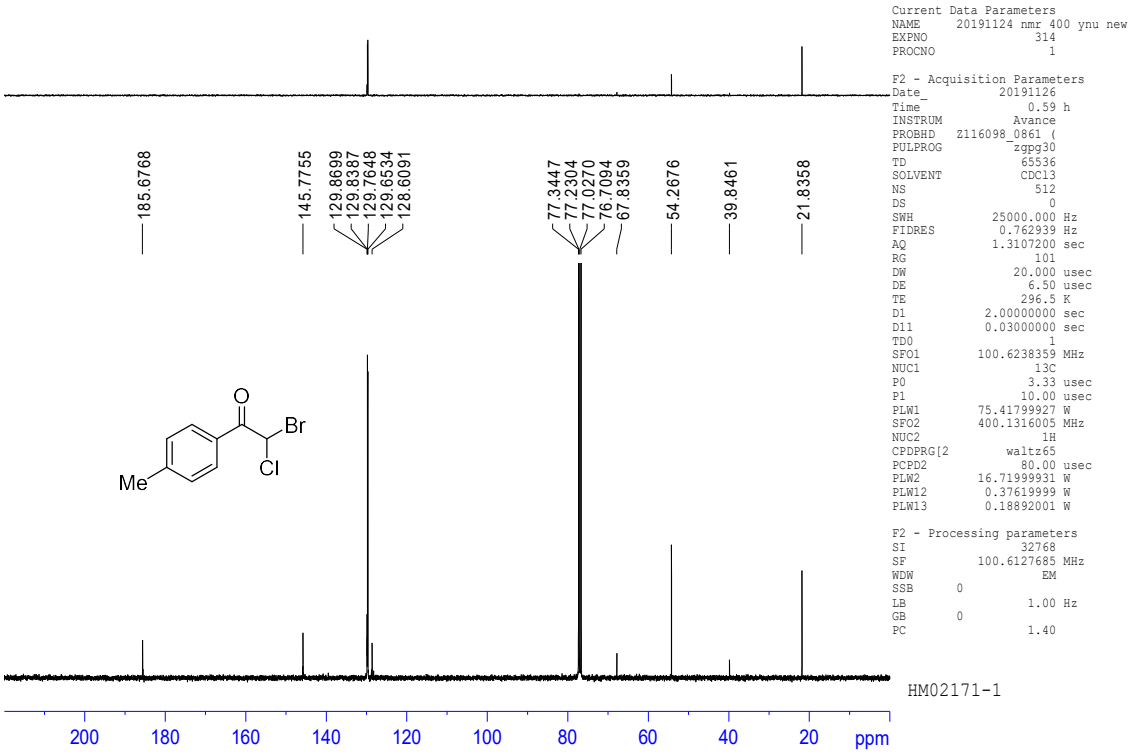
HM02171-1

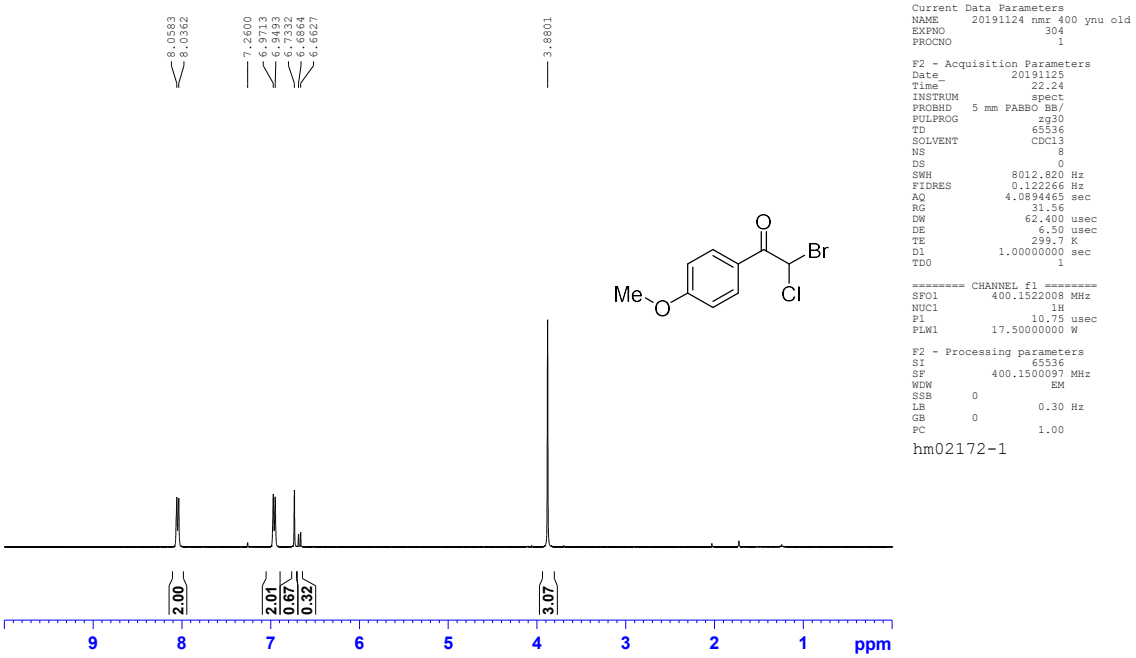
^{13}C-NMR (100 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20191124 nmr 400 ynu new
EXPNO                314
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time                0.59 h
INSTRUM           Avance
PROBHD   Z116098_0861 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            25000.000 Hz
FIDRES          0.762939 Hz
AQ              1.3107200 sec
RG                   101
DW                20.000 usec
DE                 6.50 usec
TE                296.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6238359 MHz
NUC1                  13C
P0                 3.33 usec
P1                10.00 usec
PLW1          75.41799927 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2             80.00 usec
PLW2          16.71999931 W
PLW12          0.37619999 W
PLW13          0.18892001 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

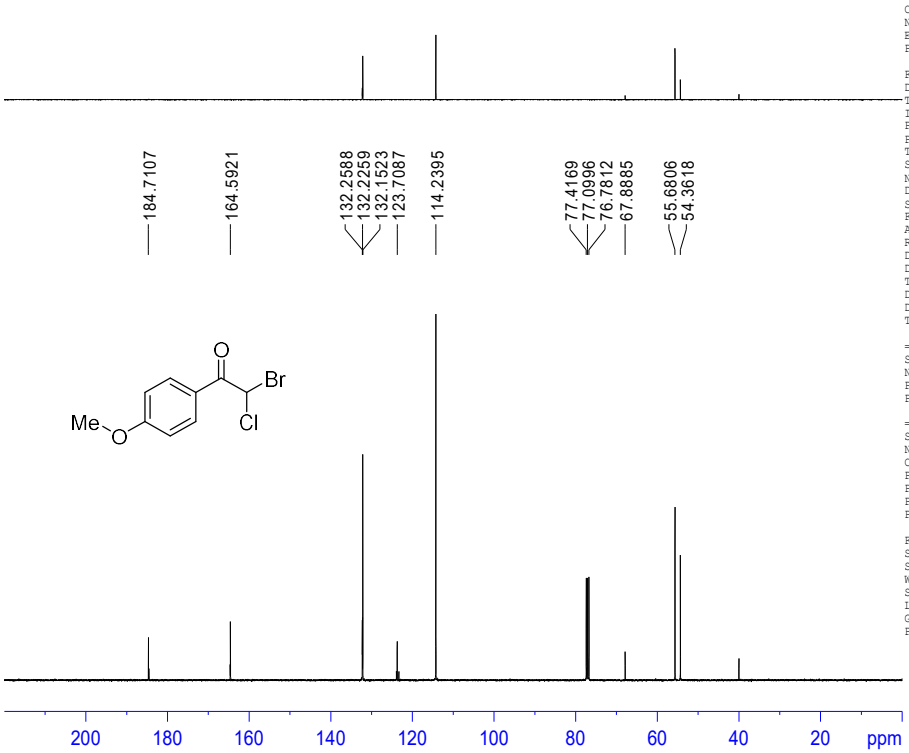
HM02171-1

^{1}H-NMR (400 MHz, $CDCl_3$)



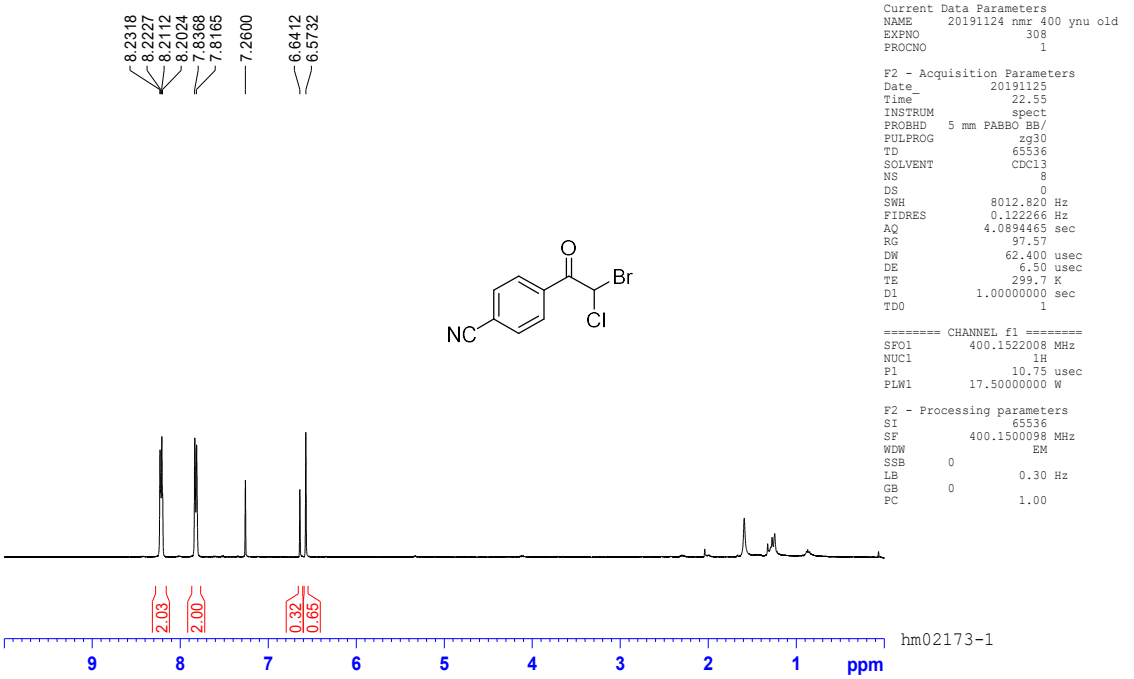

```
Current Data Parameters
NAME      20191124 nmr 400 ynu old
EXPNO                304
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time_              22.24
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                  31.56
DW                62.400 usec
DE                 6.50 usec
TE                299.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1522008 MHz
NUC1                   1H
P1                 10.75 usec
PLW1          17.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1500097 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
hm02172-1
```

^{13}C-NMR (100 MHz, $CDCl_3$)



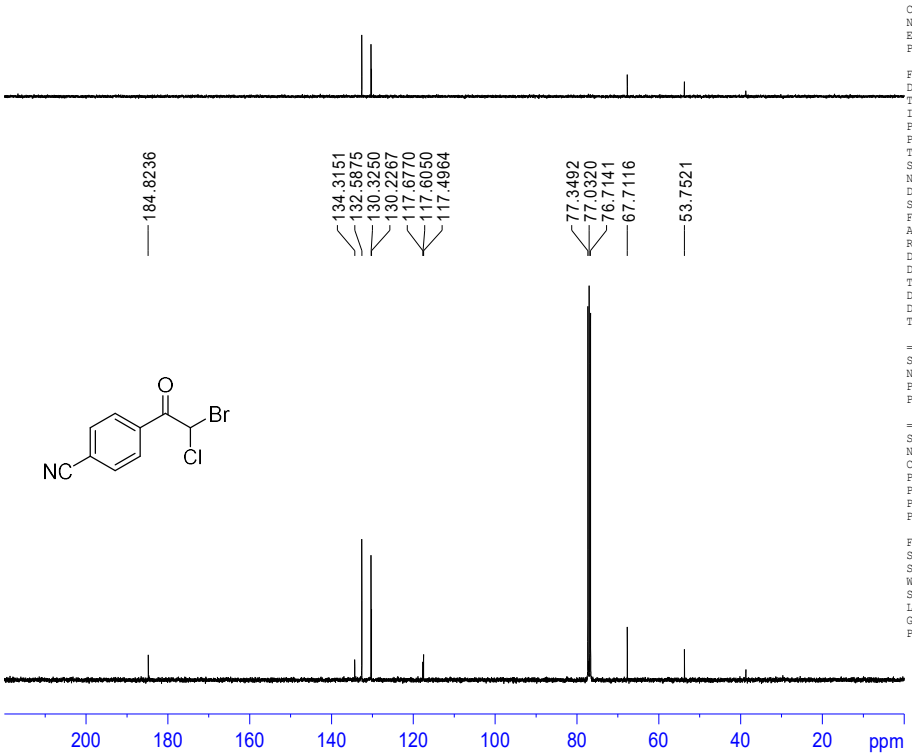

```
Current Data Parameters
NAME      20191124 nmr 400 ynu old
EXPNO                305
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time_              22.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   245
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                 195.85
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6283629 MHz
NUC1                   13C
P1                 10.50 usec
PLW1          74.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          17.50000000 W
PLW12          0.26142001 W
PLW13          0.13149001 W

F2 - Processing parameters
SI                 32768
SF            100.6177980 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
hm02172-1
```

^{1}H-NMR (400 MHz, $CDCl_3$)



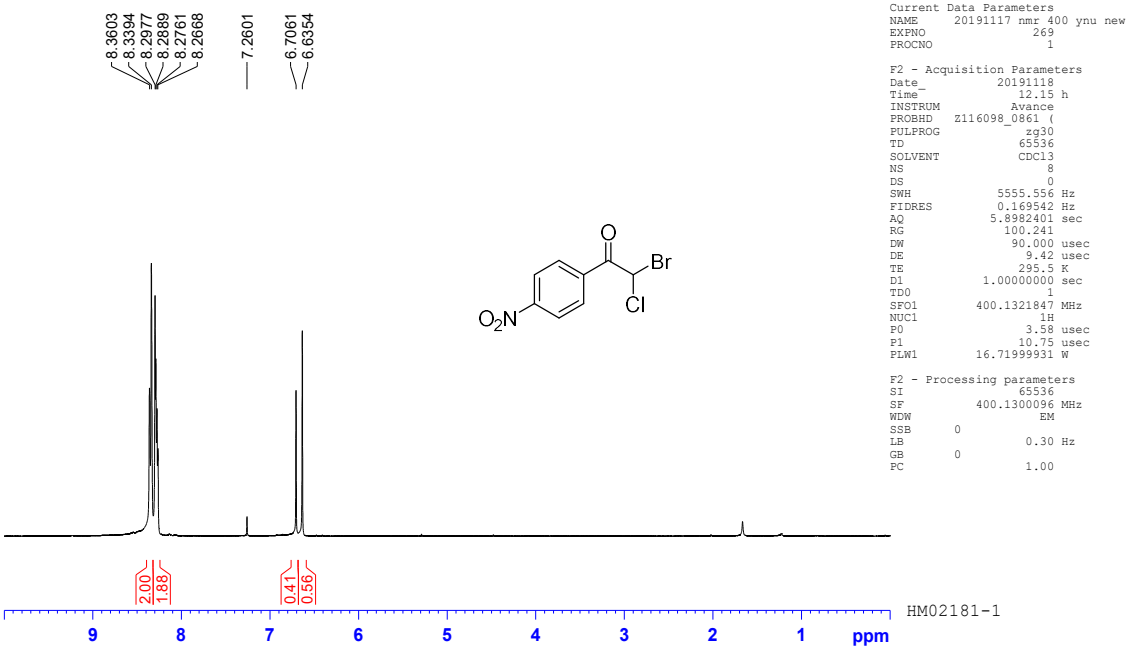

```
Current Data Parameters
NAME      20191124 nmr 400 ynu old
EXPNO                308
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time              22.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                97.57
DW               62.400 usec
DE                6.50 usec
TE               299.7 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1522008 MHz
NUC1                 1H
P1                10.75 usec
PLW1         17.50000000 W

F2 - Processing parameters
SI                65536
SF           400.1500098 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)



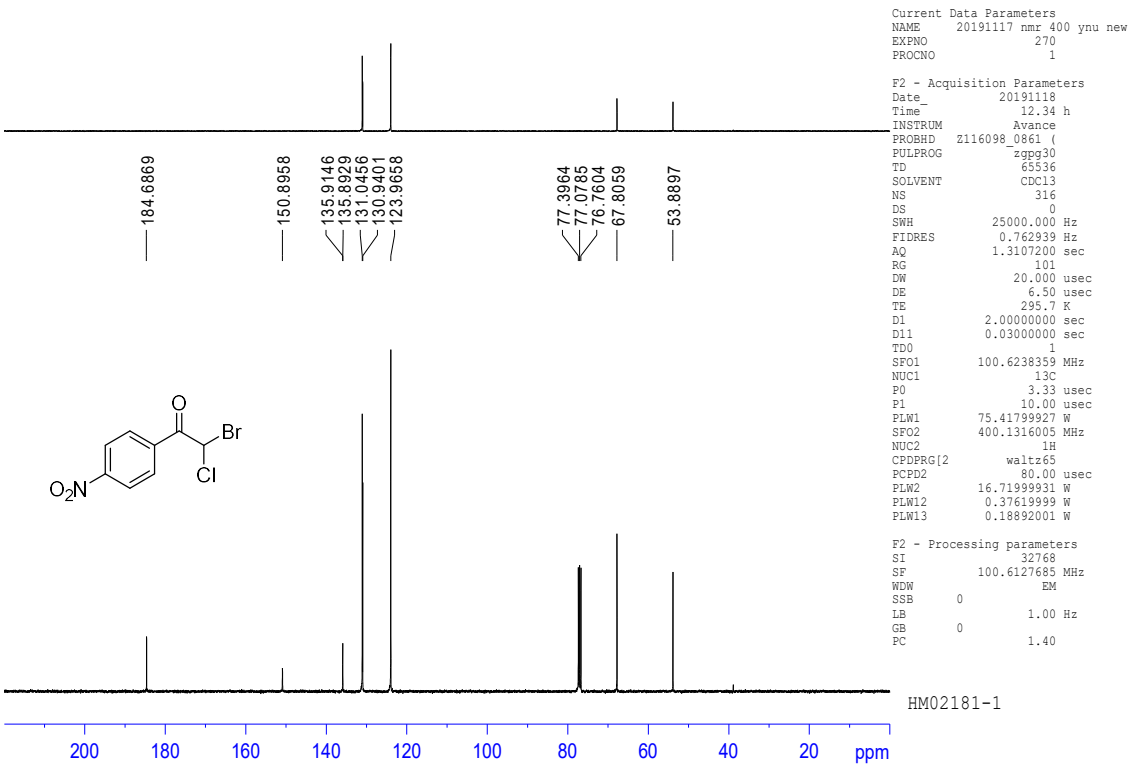

```
Current Data Parameters
NAME      20191124 nmr 400 ynu old
EXPNO                309
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191125
Time              23.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                175.44
DW               19.800 usec
DE                6.50 usec
TE               300.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6283629 MHz
NUC1                13C
P1                10.50 usec
PLW1         74.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         17.50000000 W
PLW12         0.26142001 W
PLW13         0.13149001 W

F2 - Processing parameters
SI                32768
SF           100.6177980 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H-NMR (400 MHz, $CDCl_3$)



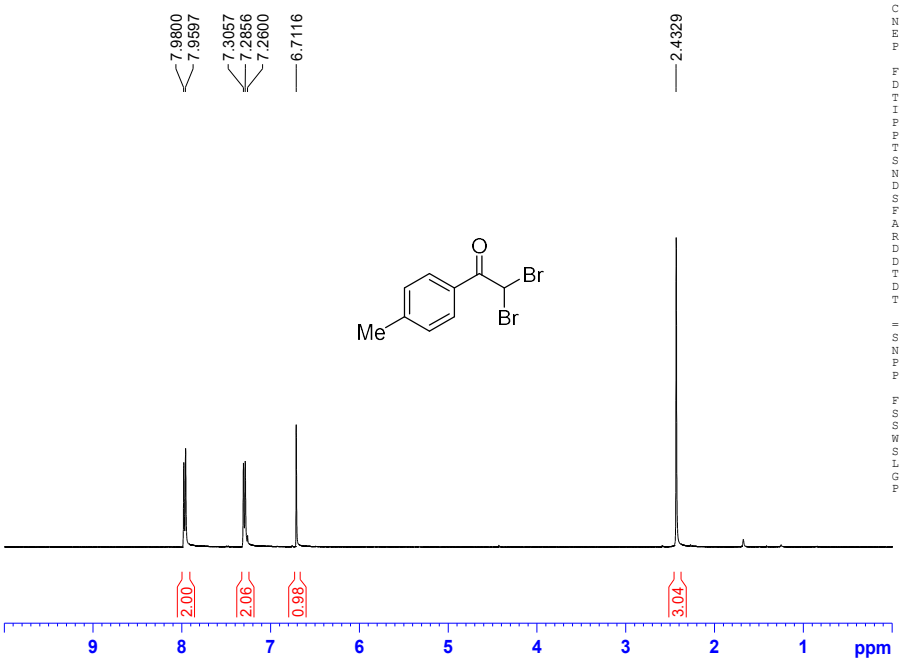

```
Current Data Parameters
NAME      20191117 nmr 400 ynu new
EXPNO                 269
PROCNO                  1

F2 - Acquisition Parameters
Date_           20191118
Time              12.15 h
INSTRUM           Avance
PROBHD    Z116098_0861 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             5555.556 Hz
FIDRES          0.169542 Hz
AQ              5.8982401 sec
RG                100.241
DW                 90.000 usec
DE                  9.42 usec
TE                 295.5 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1321847 MHz
NUC1                  1H
P0                  3.58 usec
P1                 10.75 usec
PLW1         16.71999931 W

F2 - Processing parameters
SI                 65536
SF            400.1300096 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)



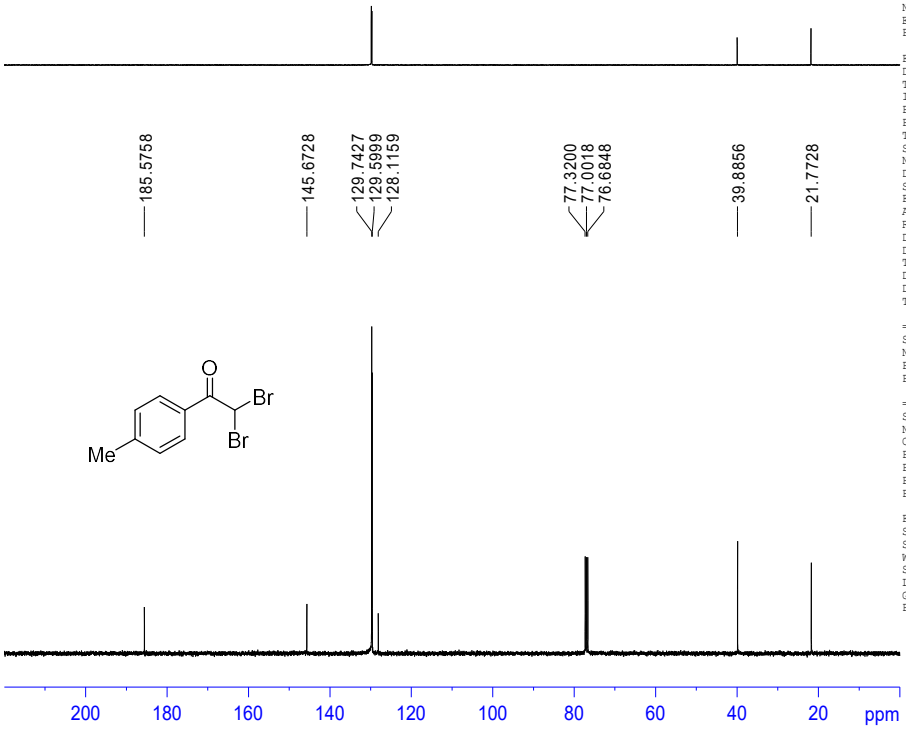

```
Current Data Parameters
NAME      20191117 nmr 400 ynu new
EXPNO                 270
PROCNO                  1

F2 - Acquisition Parameters
Date_           20191118
Time              12.34 h
INSTRUM           Avance
PROBHD    Z116098_0861 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   316
DS                     0
SWH            25000.000 Hz
FIDRES          0.762939 Hz
AQ              1.3107200 sec
RG                   101
DW                20.000 usec
DE                 6.50 usec
TE                 295.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6238359 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1         75.41799927 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2              80.00 usec
PLW2         16.71999931 W
PLW12         0.37619999 W
PLW13         0.18892001 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

^{1}H-NMR (400 MHz, $CDCl_3$)



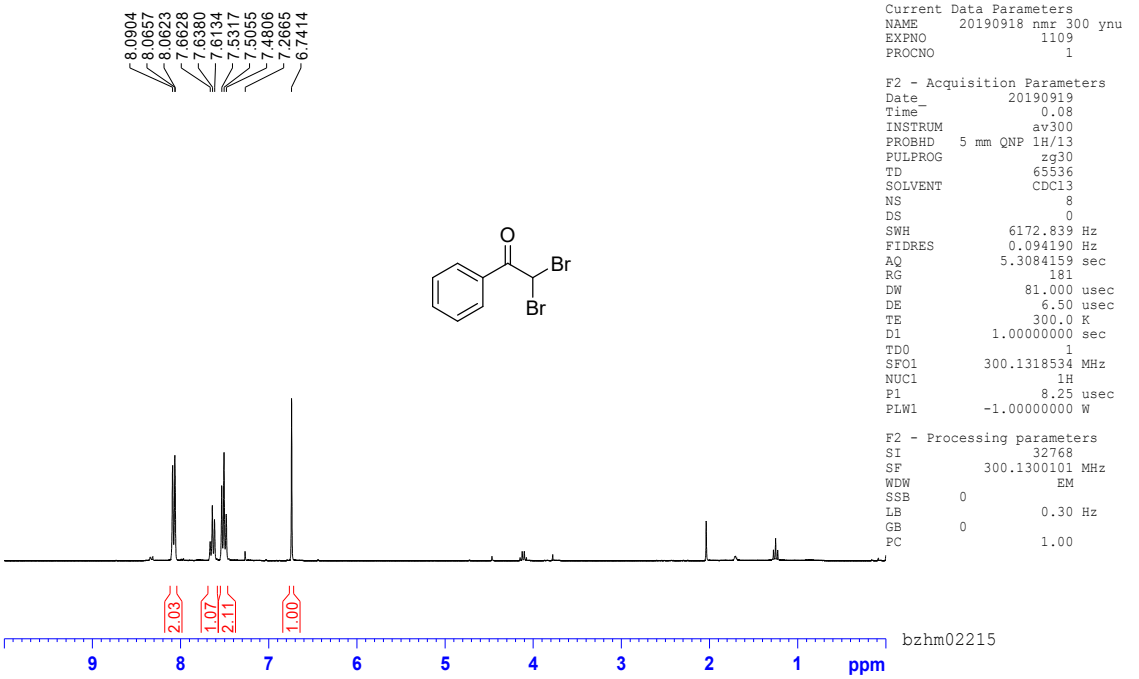

```
Current Data Parameters
NAME      20191013 nmr 400 ynu old
EXPNO                190
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191014
Time                17.41
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.56
DW                62.400 usec
DE                 6.50 usec
TE                300.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1522008 MHz
NUC1                   1H
P1                 10.75 usec
PLW1         17.50000000 W

F2 - Processing parameters
SI                 65536
SF          400.1500103 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)



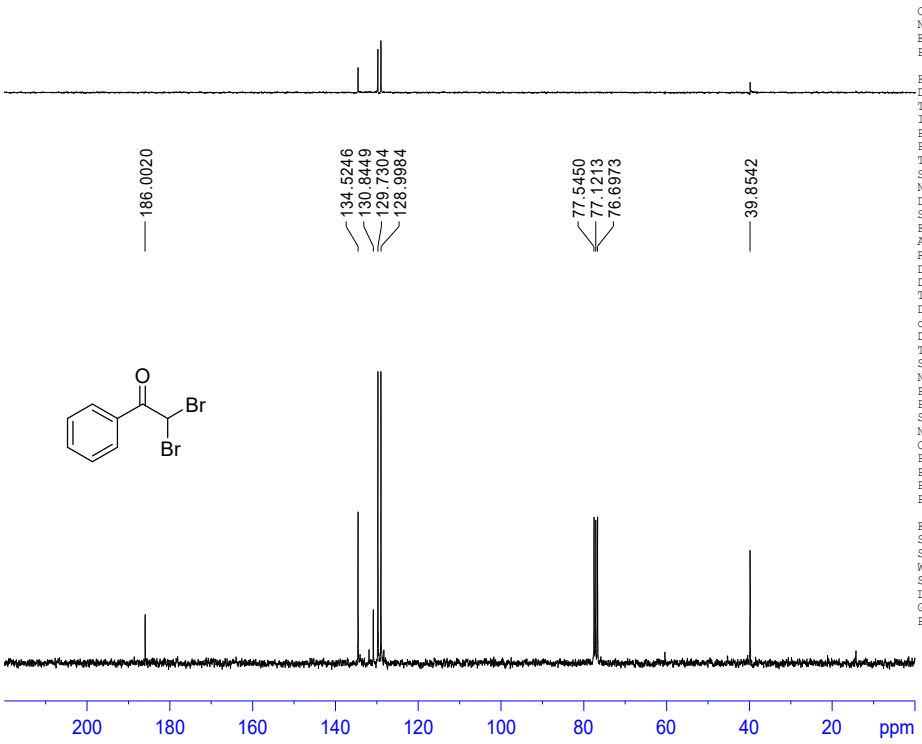

```
Current Data Parameters
NAME      20191013 nmr 400 ynu old
EXPNO                191
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191014
Time                17.45
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   129
DS                     0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                195.85
DW                19.800 usec
DE                 6.50 usec
TE                300.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6283629 MHz
NUC1                  13C
P1                 10.50 usec
PLW1         74.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         17.50000000 W
PLW12         0.26142001 W
PLW13         0.13149001 W

F2 - Processing parameters
SI                 32768
SF          100.6178067 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{1}H-NMR (300 MHz, $CDCl_3$)



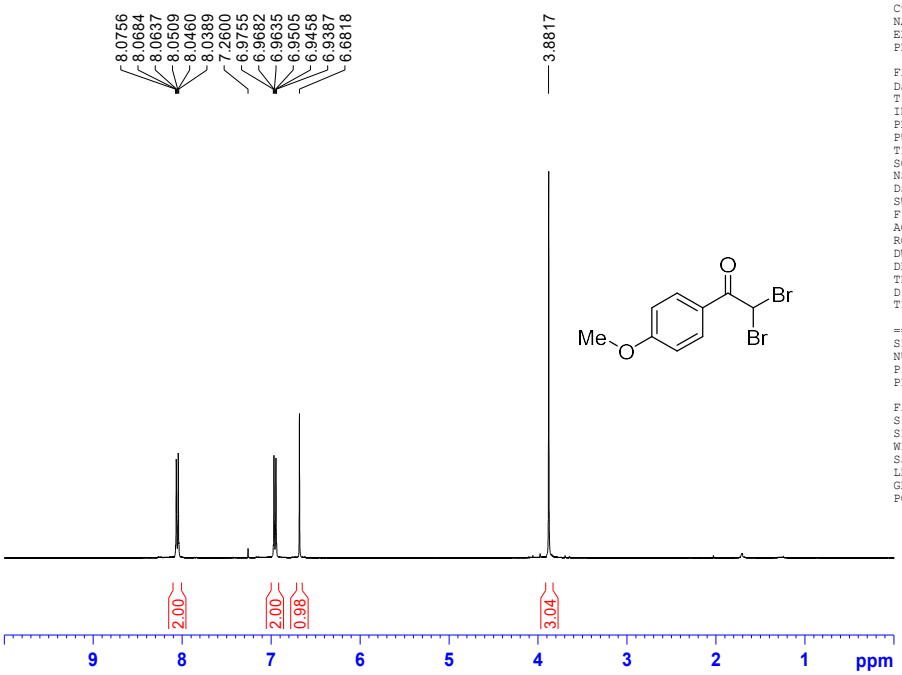

```
Current Data Parameters
NAME      20190918 nmr 300 ynu
EXPNO                 1109
PROCNO                   1

F2 - Acquisition Parameters
Date_              20190919
Time                  0.08
INSTRUM             av300
PROBHD    5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6172.839 Hz
FIDRES           0.094190 Hz
AQ                5.3084159 sec
RG                     181
DW                  81.000 usec
DE                   6.50 usec
TE                  300.0 K
D1             1.00000000 sec
TD0                      1
SFO1          300.1318534 MHz
NUC1                    1H
P1                   8.25 usec
PLW1          -1.00000000 W

F2 - Processing parameters
SI                   32768
SF            300.1300101 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

^{13}C-NMR (75 MHz, $CDCl_3$)



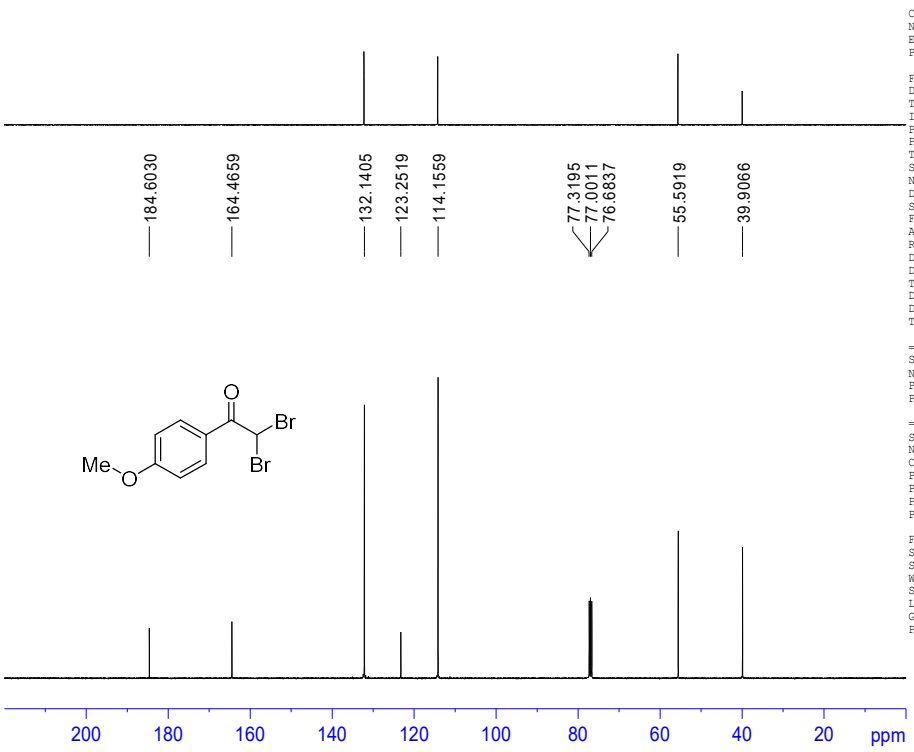

```
Current Data Parameters
NAME      20190918 nmr 300 ynu
EXPNO                 1113
PROCNO                   1

F2 - Acquisition Parameters
Date_              20190919
Time                  0.36
INSTRUM             av300
PROBHD    5 mm QNP 1H/13
PULPROG           zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     103
DS                       0
SWH              20325.203 Hz
FIDRES           0.310138 Hz
AQ                1.6121856 sec
RG                   16384
DW                  24.600 usec
DE                   6.50 usec
TE                  300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1
SFO1          75.4752953 MHz
NUC1                   13C
P1                  28.00 usec
PLW1          -1.00000000 W
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          -1.00000000 W
PLW12         -1.00000000 W
PLW13         -1.00000000 W

F2 - Processing parameters
SI                   32768
SF            75.4677490 MHz
WDW                     EM
SSB       0
LB                   3.00 Hz
GB        0
PC                   1.40
```

^{1}H-NMR (400 MHz, $CDCl_3$)



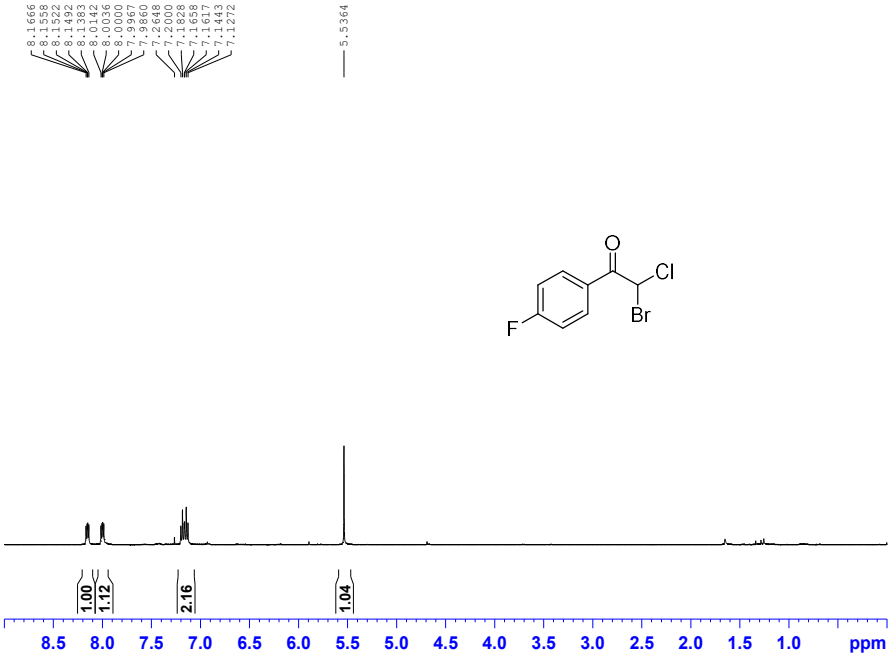

```
Current Data Parameters
NAME      20191013 nmr 400 ynu old
EXPNO              186
PROCNO               1

F2 - Acquisition Parameters
Date_          20191014
Time              16.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                31.56
DW               62.400 usec
DE                6.50 usec
TE               300.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1522008 MHz
NUC1              1H
P1               10.75 usec
PLW1        17.50000000 W

F2 - Processing parameters
SI                65536
SF          400.1500099 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)



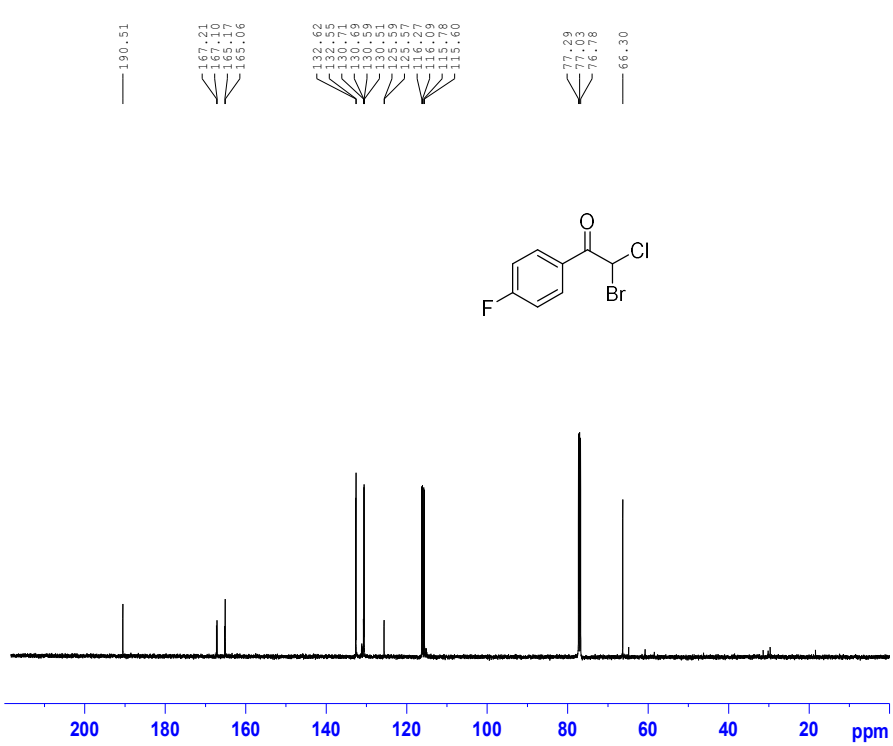

```
Current Data Parameters
NAME      20191013 nmr 400 ynu old
EXPNO              187
PROCNO               1

F2 - Acquisition Parameters
Date_          20191014
Time              17.27
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   0
SWH          25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976128 sec
RG               195.85
DW               19.800 usec
DE                6.50 usec
TE               300.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6283629 MHz
NUC1              13C
P1               10.50 usec
PLW1        74.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        17.50000000 W
PLW12        0.26142001 W
PLW13        0.13149001 W

F2 - Processing parameters
SI                32768
SF          100.6178067 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H-NMR (400 MHz, $CDCl_3$)



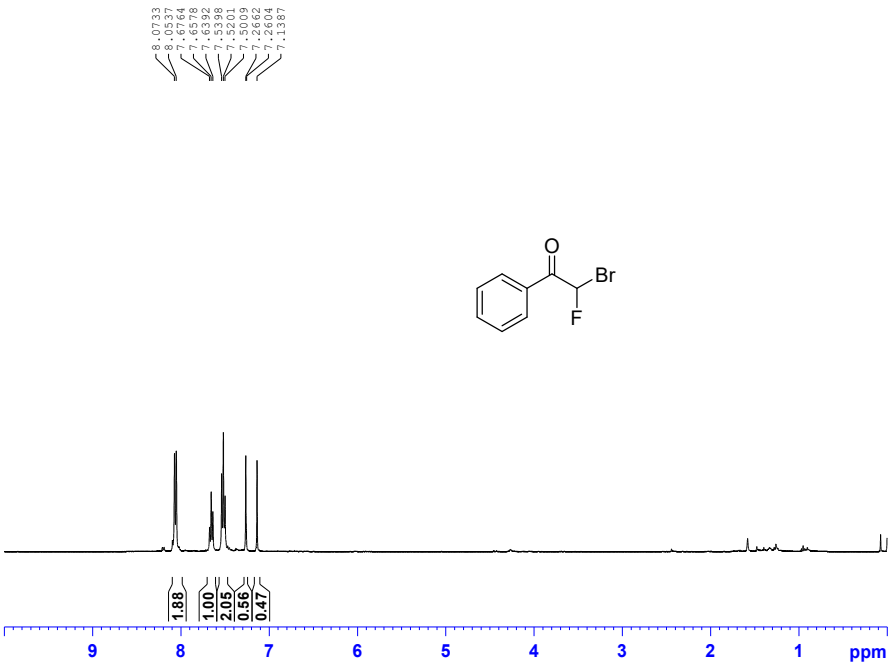

```
Current Data Parameters
NAME      20210820 nmr h
EXPNO               90
PROCNO               1

F2 - Acquisition Parameters
Date_          20210820
Time_             11.14 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH          10000.000 Hz
FIDRES         0.305176 Hz
AQ           3.2767999 sec
RG               86.69
DW              50.000 usec
DE               6.50 usec
TE              296.5 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1                9.60 usec
PLW1       22.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300095 MHz
WDW                 EM
SSB      0
LB              0.30 Hz
GB       0
PC              1.00

HM02123-2
```

^{13}C-NMR (100 MHz, $CDCl_3$)



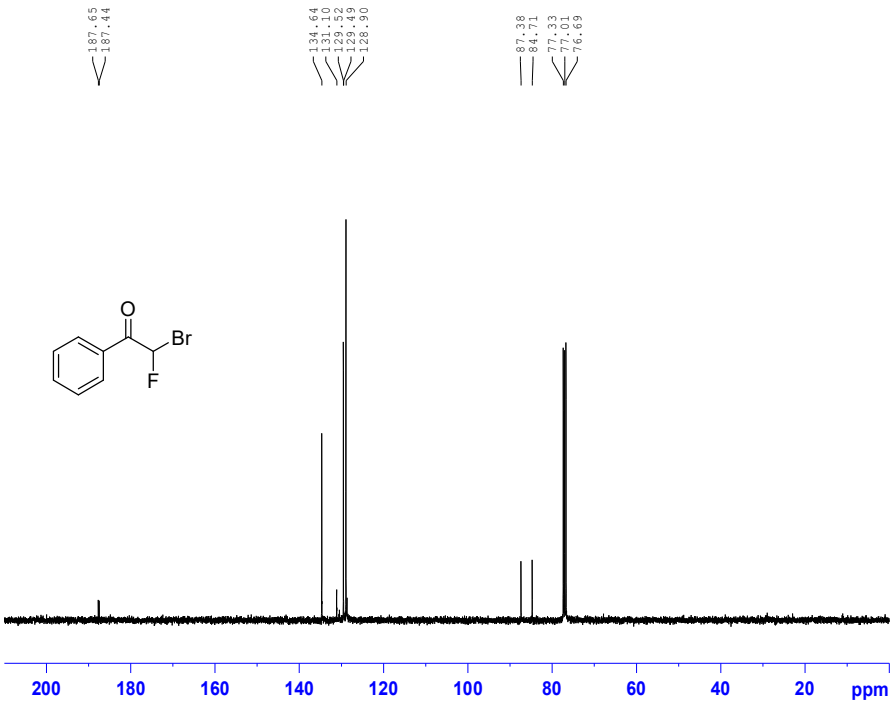

```
Current Data Parameters
NAME      20210820 nmr c
EXPNO               92
PROCNO               1

F2 - Acquisition Parameters
Date_          20210820
Time_             23.08 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 350
DS                   4
SWH          29761.904 Hz
FIDRES         0.908261 Hz
AQ           1.1010048 sec
RG              190.79
DW              16.800 usec
DE               6.50 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1               13C
P1               12.00 usec
PLW1       90.00000000 W
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2       22.00000000 W
PLW12       0.34720001 W
PLW13       0.17464000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB              1.00 Hz
GB       0
PC              1.40

HM02123-2
```

^{1}H-NMR (400 MHz, $CDCl_3$)



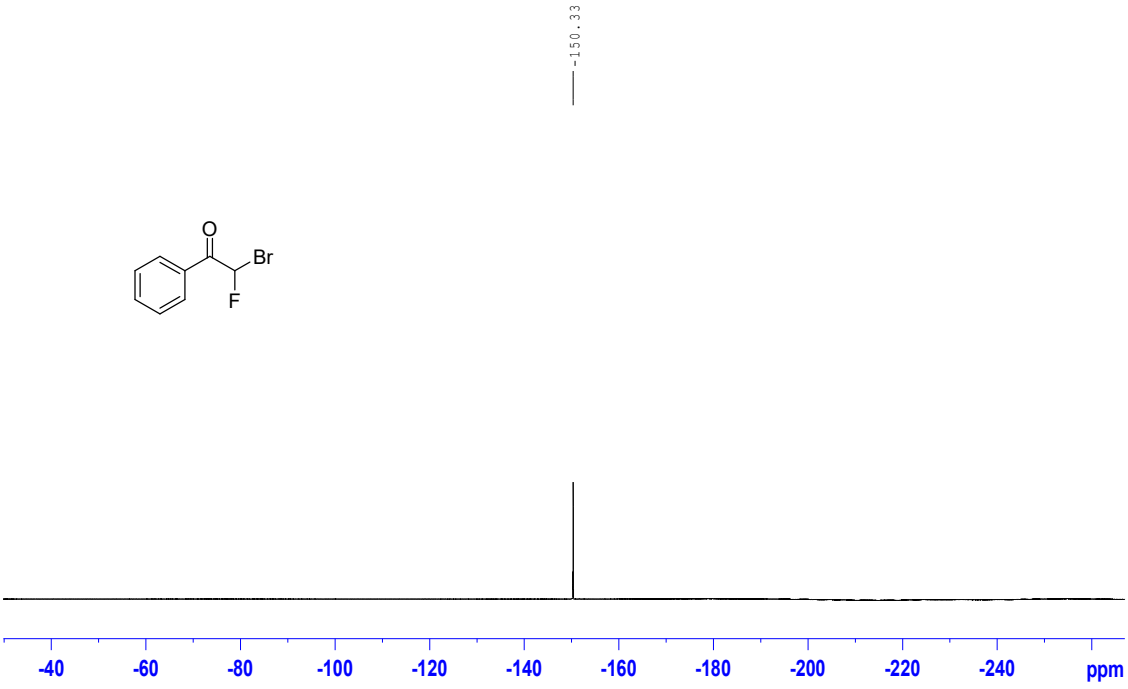

```
Current Data Parameters
NAME          tyf04072-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220126
Time_              22.16
INSTRUM            spect
PROBHD   5 mm QNP 1H/15
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                120.71
DW                62.400 usec
DE                 6.50 usec
TE                297.6 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1318812 MHz
NUC1                   1H
P1                  16.50 usec
PLW1          8.30000019 W

F2 - Processing parameters
SI                    65536
SF           400.1300097 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.00
tyf04072-1
```

^{13}C-NMR (100 MHz, $CDCl_3$)

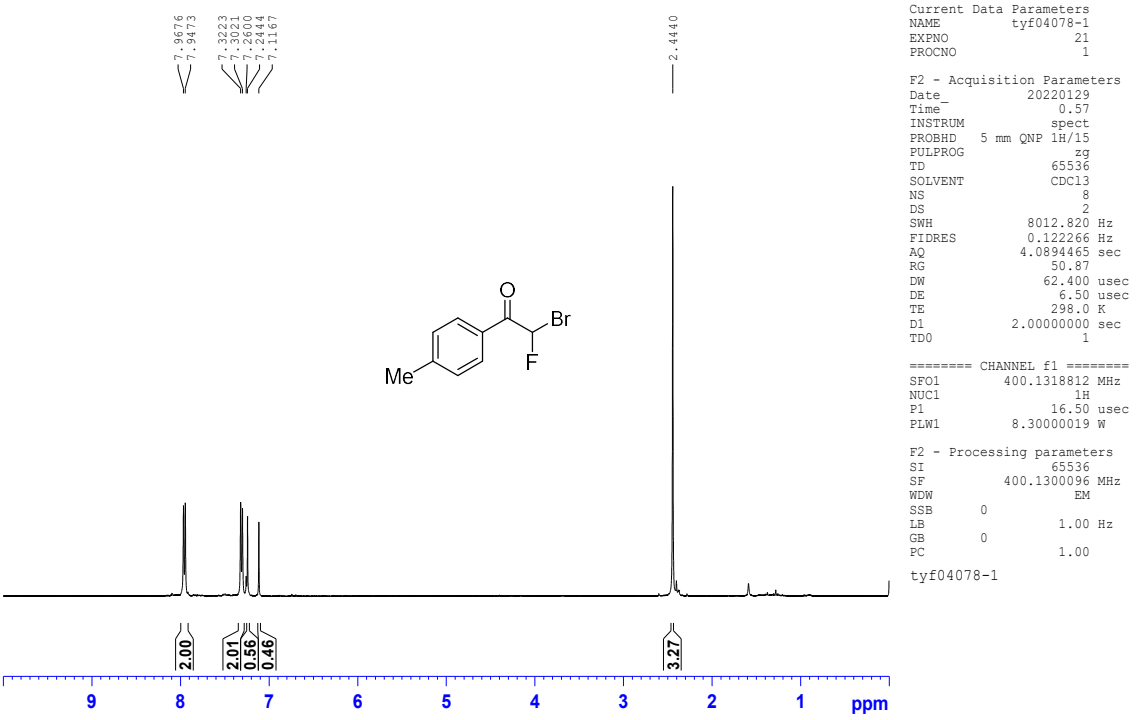



```
Current Data Parameters
NAME          tyf04072-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220126
Time_              22.18
INSTRUM            spect
PROBHD   5 mm QNP 1H/15
PULPROG             zgdc
TD                65536
SOLVENT           CDCl3
NS                  255
DS                    4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                214.83
DW                20.800 usec
DE                 6.50 usec
TE                298.4 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6241382 MHz
NUC1                  13C
P1                  10.00 usec
PLW1         45.97900009 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          2.08929992 W
PLW12         0.39991000 W

F2 - Processing parameters
SI                    32768
SF           100.6127690 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
tyf04072-1
```

^{19}F NMR (376 MHz, $CDCl_3$)

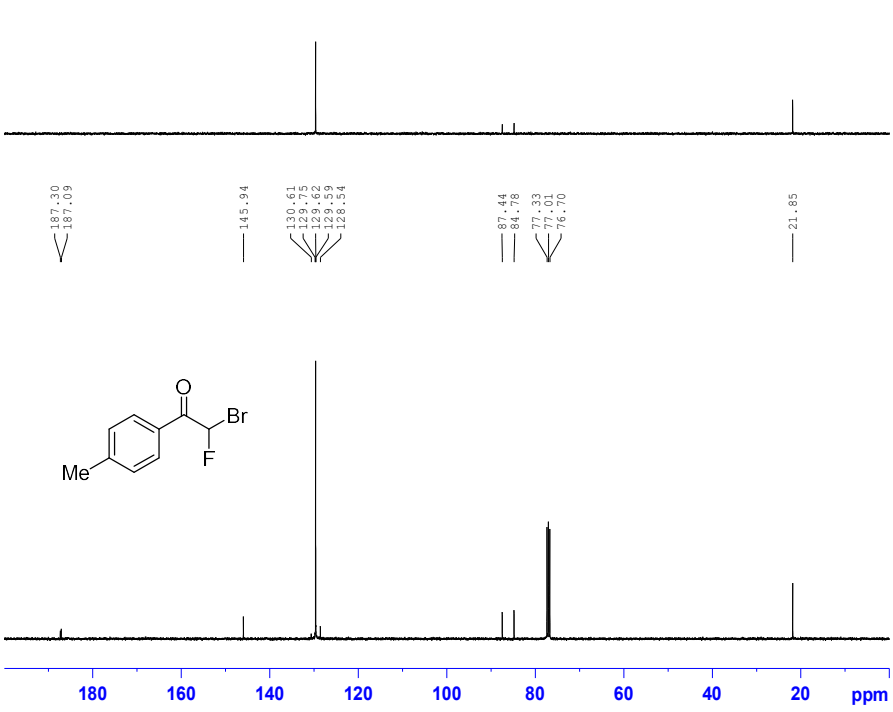


^{1}H-NMR (400 MHz, $CDCl_3$)



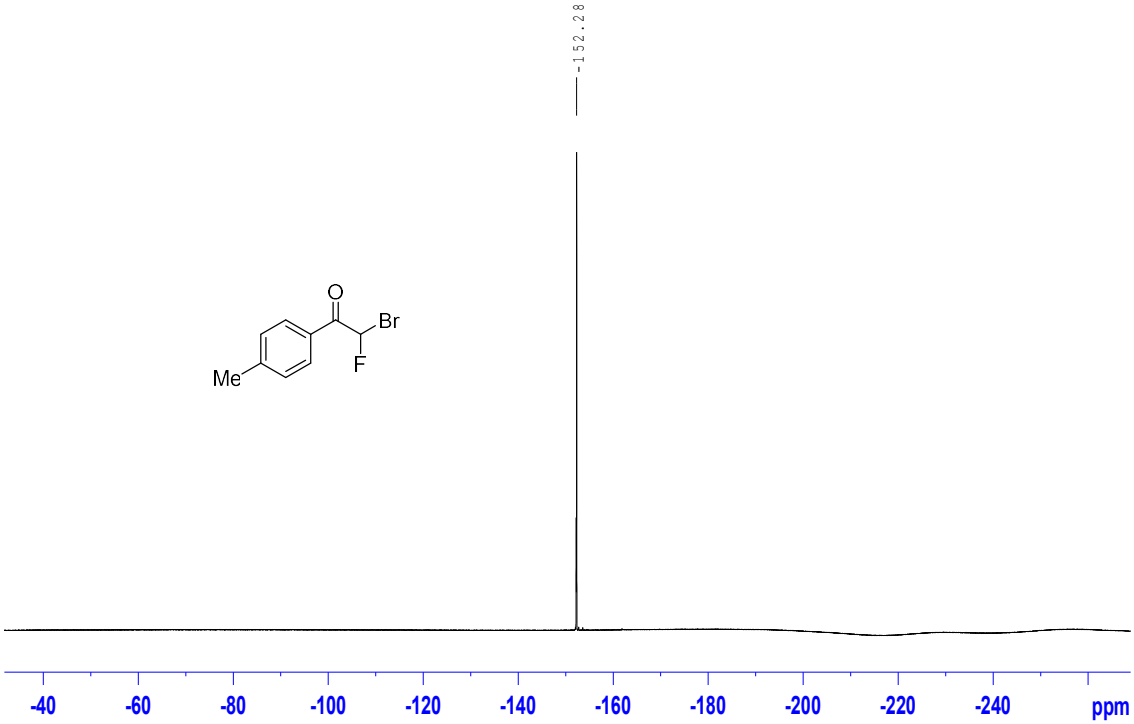

```
Current Data Parameters
NAME          tyf04078-1
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220129
Time                0.57
INSTRUM            spect
PROBHD   5 mm QNP 1H/15
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 50.87
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1318812 MHz
NUC1                   1H
P1                 16.50 usec
PLW1          8.30000019 W

F2 - Processing parameters
SI                 65536
SF           400.1300096 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00

tyf04078-1
```

^{13}C-NMR (100 MHz, $CDCl_3$)

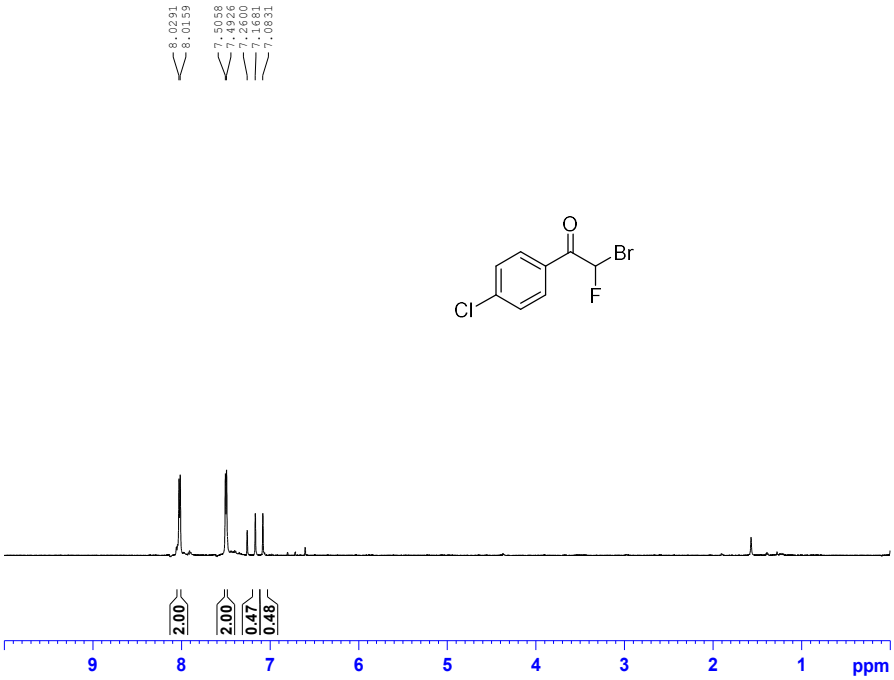



```
Current Data Parameters
NAME          tyf04078-1
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220129
Time                0.59
INSTRUM            spect
PROBHD   5 mm QNP 1H/15
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                   280
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                214.83
DW                20.800 usec
DE                 6.50 usec
TE                299.0 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6241382 MHz
NUC1                13C
P1                10.00 usec
PLW1         45.97900009 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          2.08929992 W
PLW12         0.39991000 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
tyf04078-1
```

^{19}F NMR (376 MHz, $CDCl_3$)

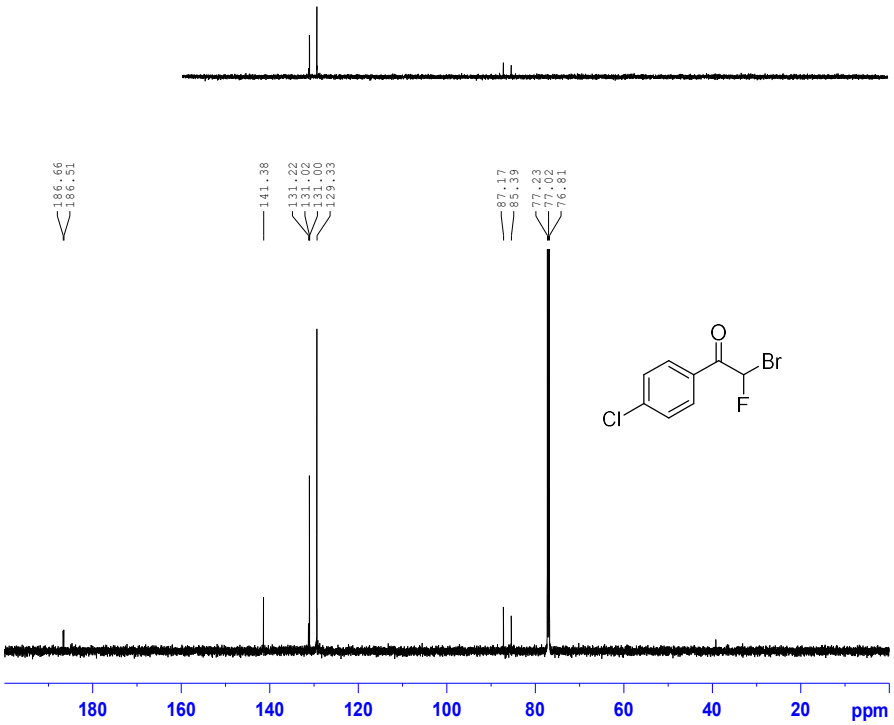


^{1}H-NMR (600 MHz, $CDCl_3$)



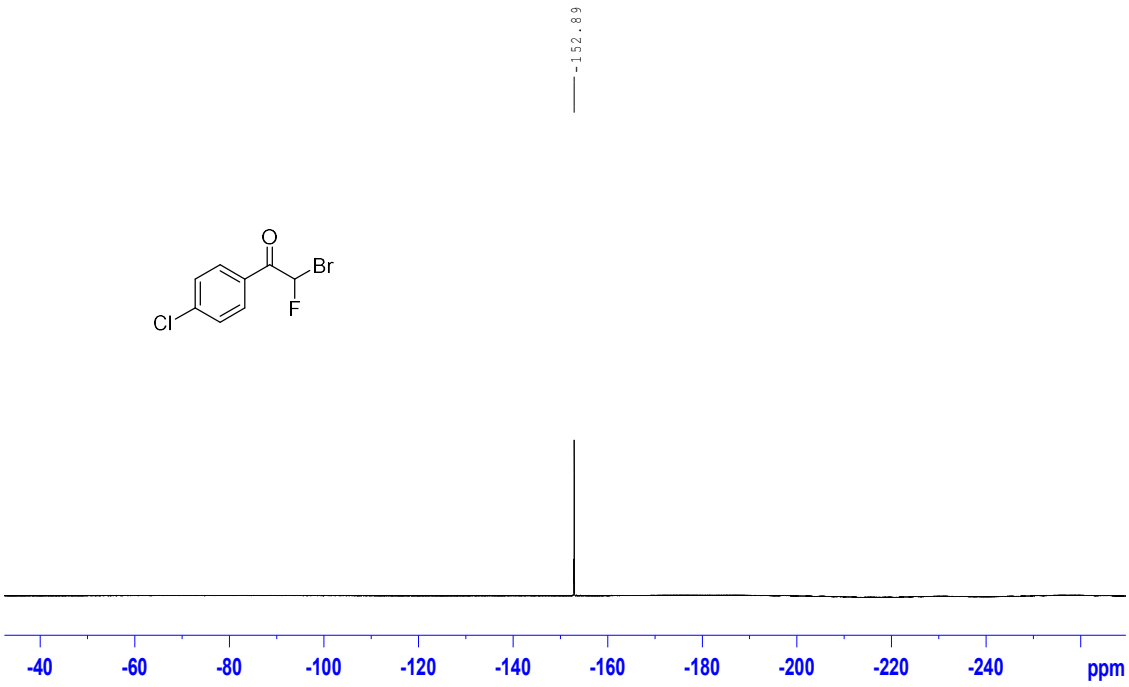

```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220212
Time              16.53 h
INSTRUM             spect
PROBHD   Z114607_0222 (
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                     2
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              2.7262976 sec
RG                121.23
DW               41.600 usec
DE               11.27 usec
TE                291.5 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1737060 MHz
NUC1                  1H
P0                 3.33 usec
P1                10.00 usec
PLW1         26.09399986 W

F2 - Processing parameters
SI                 65536
SF            600.1700163 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
TYF04076-1
```

^{13}C-NMR (150 MHz, $CDCl_3$)

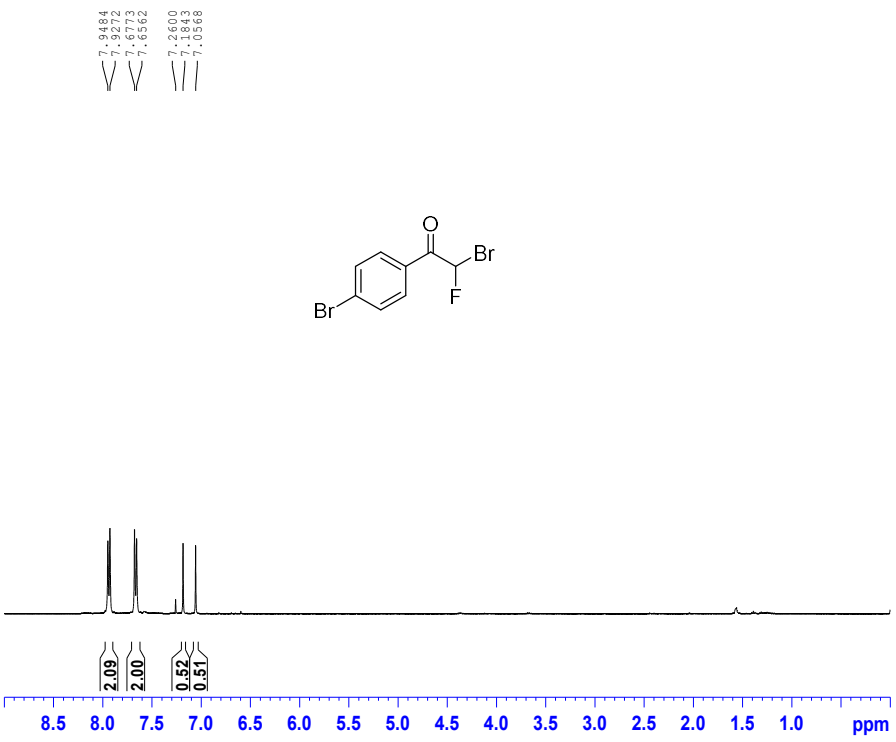



```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220212
Time              17.08 h
INSTRUM             spect
PROBHD   Z114607_0222 (
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   285
DS                     4
SWH            36231.883 Hz
FIDRES          1.105709 Hz
AQ              0.9043968 sec
RG                188.35
DW               13.800 usec
DE                6.50 usec
TE                292.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         150.9279578 MHz
NUC1                  13C
P0                 4.00 usec
P1                12.00 usec
PLW1         97.67099762 W
SFO2         600.1724007 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2         27.73900032 W
PLW12         0.56610000 W
PLW13         0.28475001 W

F2 - Processing parameters
SI                 32768
SF            150.9128665 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
TYF04076-1
```

^{19}F NMR (376 MHz, $CDCl_3$)

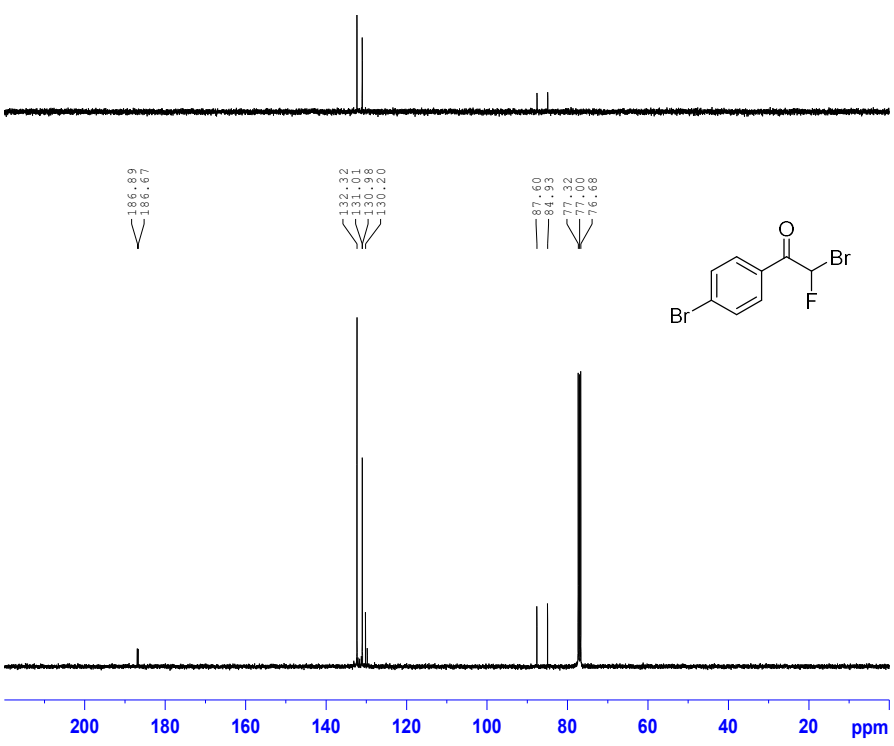


^{1}H-NMR (400 MHz, $CDCl_3$)



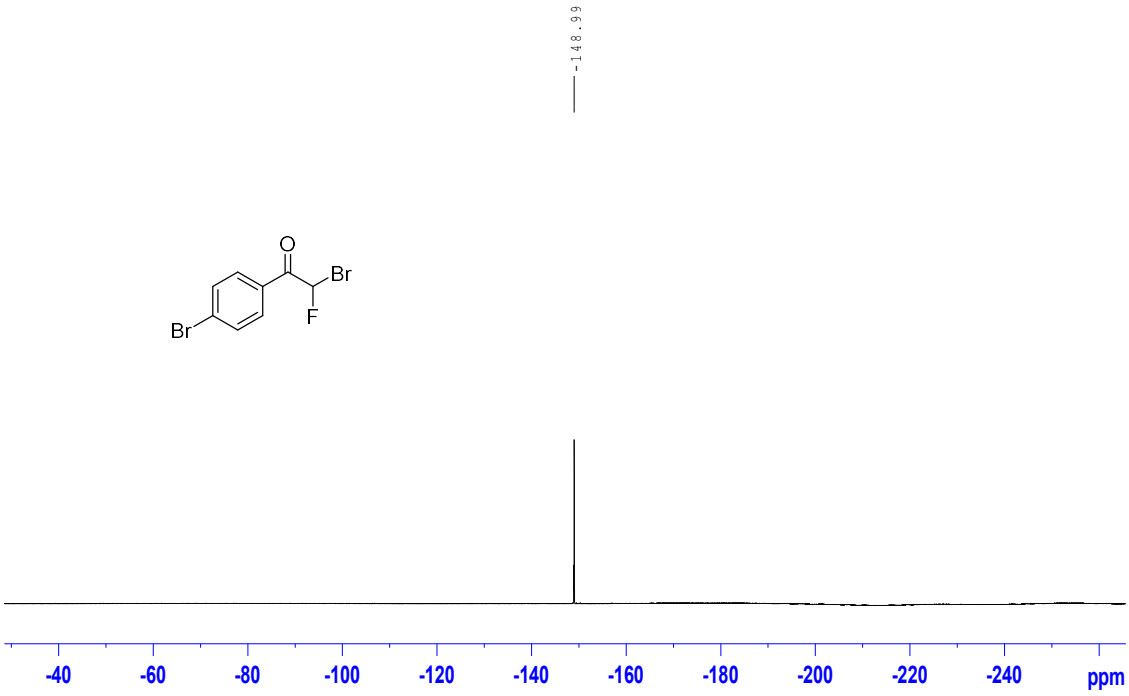

```
Current Data Parameters
NAME          tyf04083-3
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220228
Time                0.08
INSTRUM            spect
PROBHD   5 mm QNP 1H/15
PULPROG                zg
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                159.21
DW                62.400 usec
DE                 6.50 usec
TE                297.8 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1318812 MHz
NUC1                   1H
P1                16.50 usec
PLW1          8.30000019 W

F2 - Processing parameters
SI                 65536
SF           400.1300102 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
tyf04083-3
PROTON CDCl3
```

^{13}C-NMR (100 MHz, $CDCl_3$)

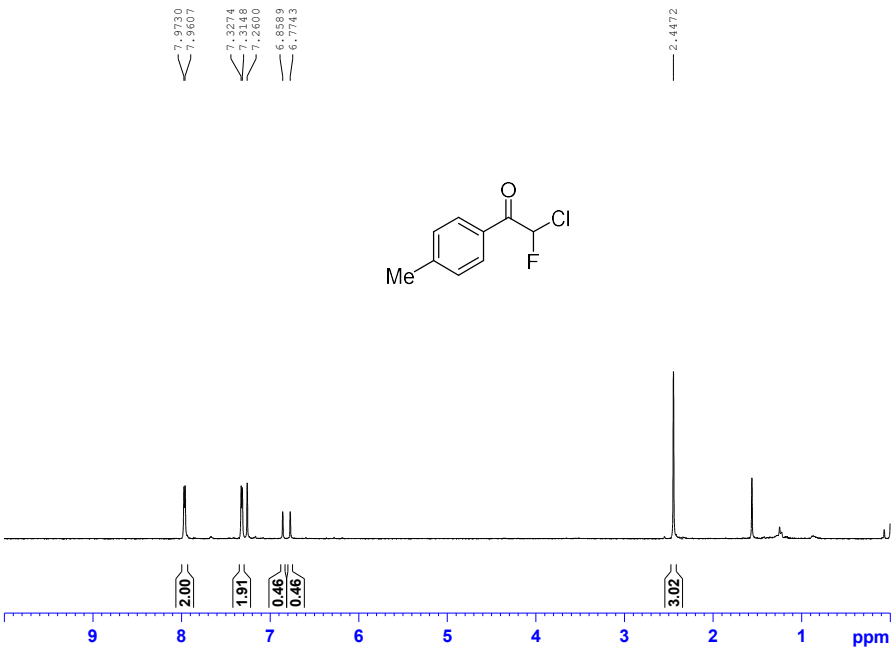



```
Current Data Parameters
NAME         tyf04083-3
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20220228
Time                0.22
INSTRUM            spect
PROBHD   5 mm QNP 1H/15
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                   700
DS                     4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                214.83
DW                20.800 usec
DE                 6.50 usec
TE                299.9 K
D1           3.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6241382 MHz
NUC1                13C
P1                 10.00 usec
PLW1         45.97900009 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          2.08929992 W
PLW12         0.39991000 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40

tyf04083-3
```

^{19}F NMR (376 MHz, $CDCl_3$)

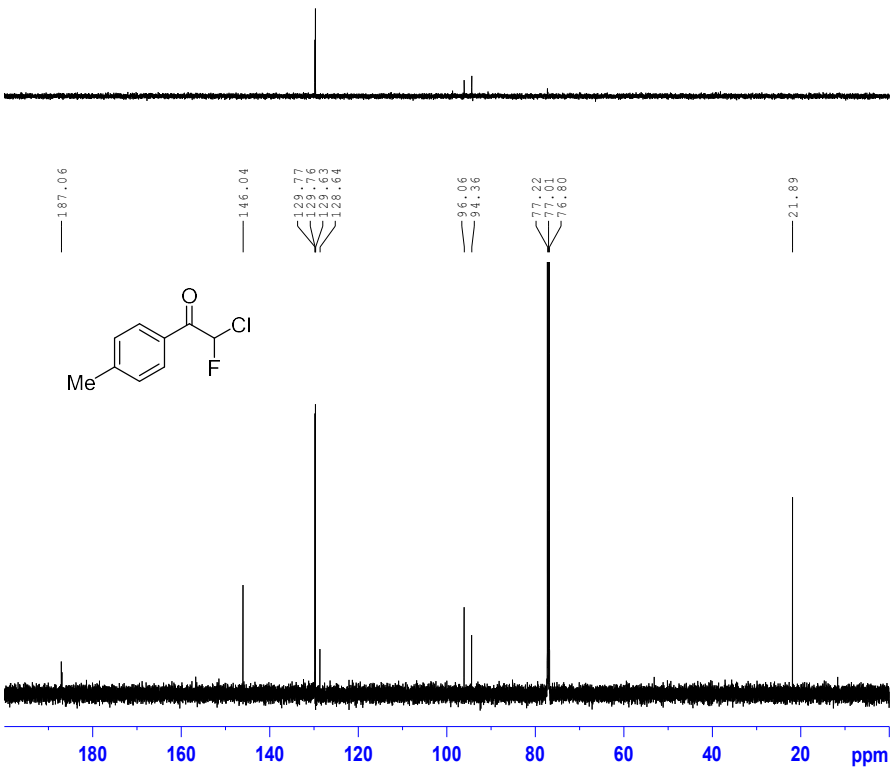


^{1}H-NMR (600 MHz, $CDCl_3$)



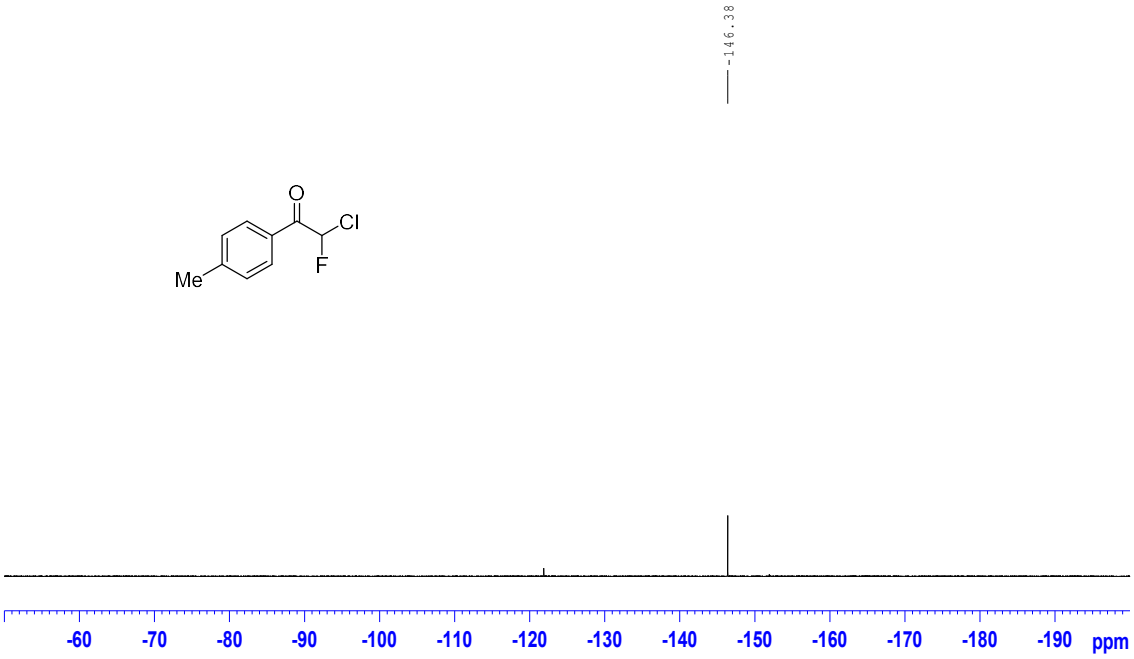

```
Current Data Parameters
NAME      20220228 nmr ynu
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220228
Time_              10.50 h
INSTRUM             spect
PROBHD   Z114607_0222 (
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                     3
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              2.7262976 sec
RG                 188.35
DW                41.600 usec
DE                11.27 usec
TE                290.6 K
D1             1.00000000 sec
TD0                    1
SFO1         600.1737060 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1         26.09399986 W

F2 - Processing parameters
SI                 65536
SF          600.1700169 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
tyf04084-1
```

^{13}C-NMR (150 MHz, $CDCl_3$)

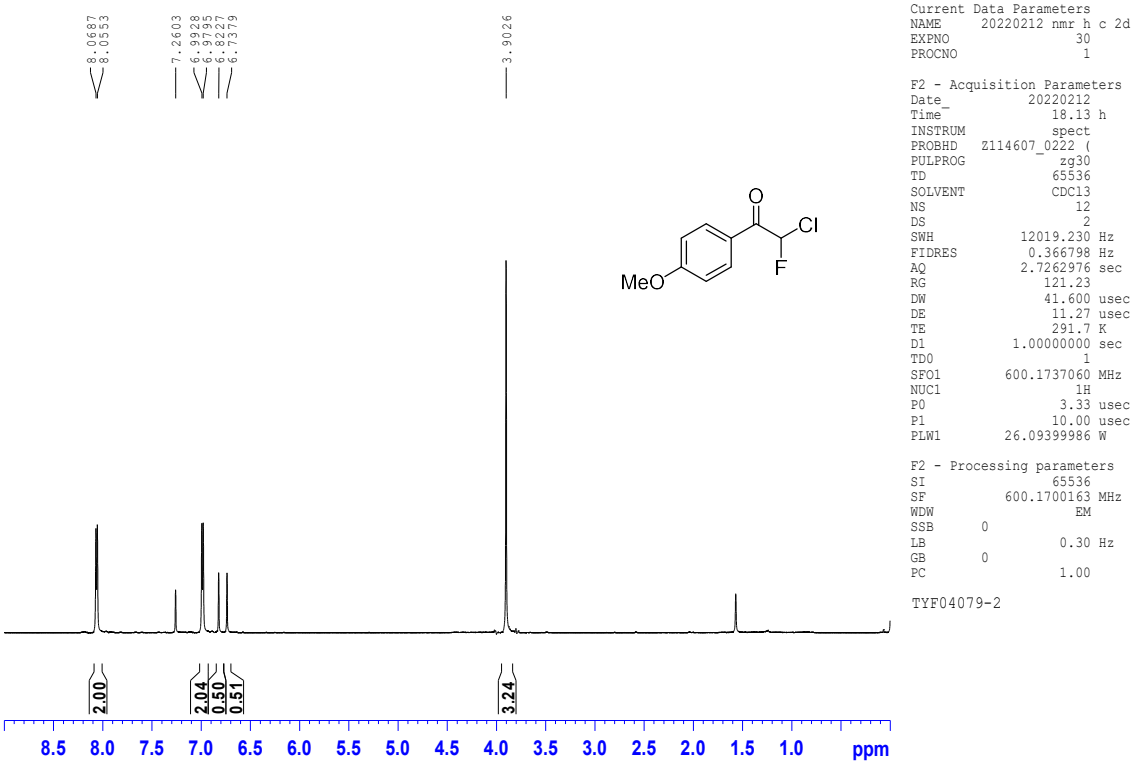



```
Current Data Parameters
NAME      20220228 nmr ynu
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220228
Time_              12.58 h
INSTRUM             spect
PROBHD   Z114607_0222 (
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                  2048
DS                     4
SWH            36231.883 Hz
FIDRES          1.105709 Hz
AQ              0.9043968 sec
RG                 188.35
DW                13.800 usec
DE                 6.50 usec
TE                291.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         150.9279578 MHz
NUC1                 13C
P0                  4.00 usec
P1                 12.00 usec
PLW1         97.67099762 W
SFO2         600.1724007 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2              70.00 usec
PLW2         27.73900032 W
PLW12         0.56610000 W
PLW13         0.28475001 W

F2 - Processing parameters
SI                 32768
SF          150.9128681 MHz
WDW                   GM
SSB       0
LB                -0.30 Hz
GB                 0.3
PC                 1.40
tyf04084-1
```

^{19}F NMR (376 MHz, $CDCl_3$)

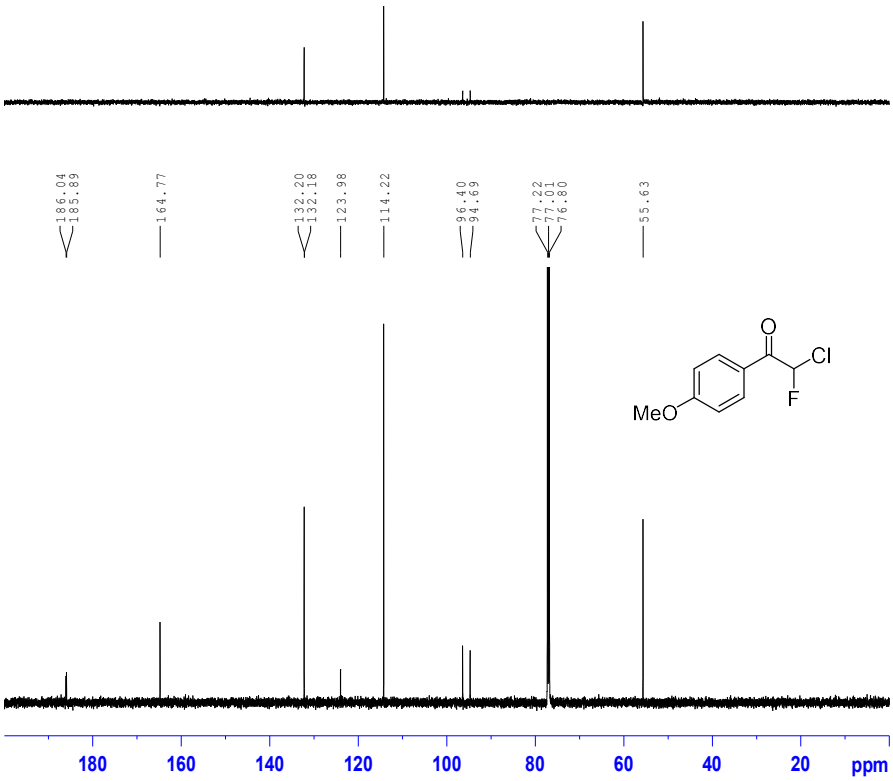


^{1}H-NMR (600 MHz, $CDCl_3$)



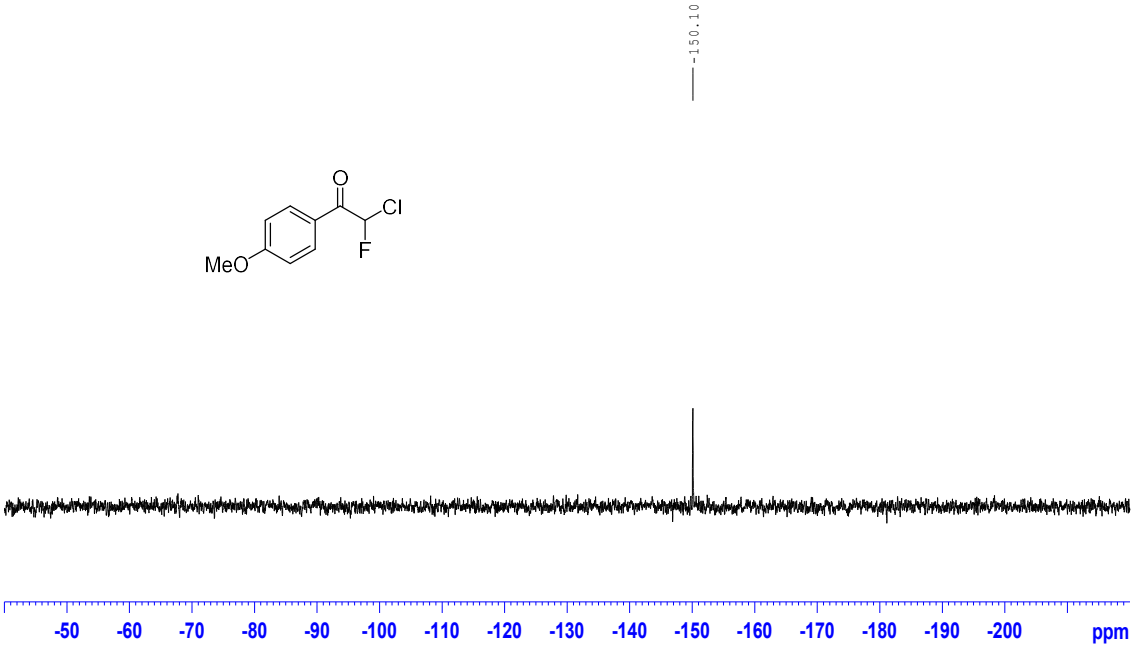

```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                   30
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220212
Time                 18.13 h
INSTRUM              spect
PROBHD    Z114607_0222 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     12
DS                      2
SWH             12019.230 Hz
FIDRES          0.366798 Hz
AQ              2.7262976 sec
RG                 121.23
DW                41.600 usec
DE                11.27 usec
TE                291.7 K
D1             1.00000000 sec
TD0                     1
SFO1         600.1737060 MHz
NUC1                   1H
P0                   3.33 usec
P1                  10.00 usec
PLW1         26.09399986 W

F2 - Processing parameters
SI                  65536
SF           600.1700163 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00

TYF04079-2
```

^{13}C-NMR (150 MHz, $CDCl_3$)

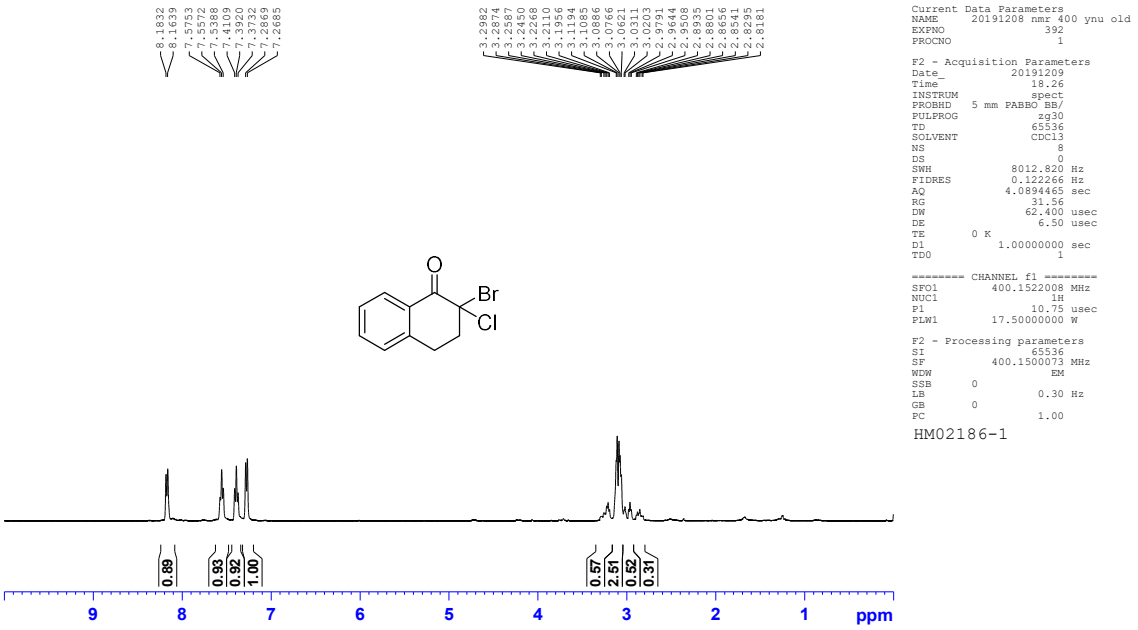



```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                   31
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220212
Time                18.39 h
INSTRUM              spect
PROBHD   Z114607_0222 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            36231.883 Hz
FIDRES          1.105709 Hz
AQ             0.9043968 sec
RG                188.35
DW                13.800 usec
DE                 6.50 usec
TE                293.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         150.9279578 MHz
NUC1                 13C
P0                 4.00 usec
P1                12.00 usec
PLW1          97.67099762 W
SFO2         600.1724007 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2          27.73900032 W
PLW12          0.56610000 W
PLW13          0.28475001 W

F2 - Processing parameters
SI                 32768
SF           150.9128665 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40

TYF04079-2
```

^{19}F NMR (376 MHz, $CDCl_3$)



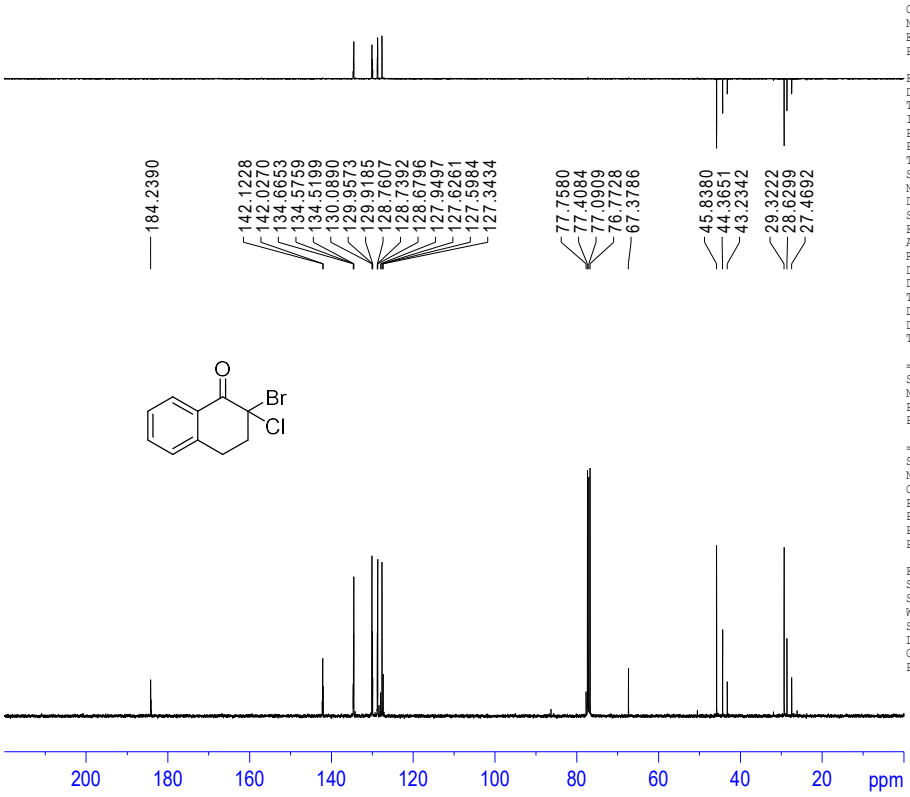
^{1}H-NMR (400 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20191208 nmr 400 ynu old
EXPNO                392
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191209
Time              18.26
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                31.56
DW               62.400 usec
DE                6.50 usec
TE        0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1522008 MHz
NUC1                 1H
P1                10.75 usec
PLW1         17.50000000 W

F2 - Processing parameters
SI                65536
SF           400.1500073 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

HM02186-1

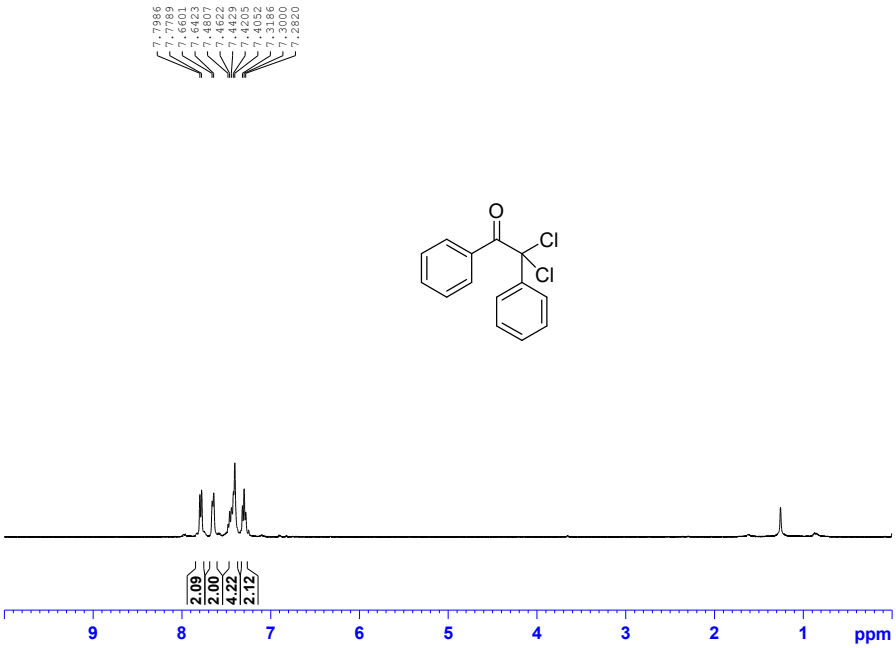
^{13}C-NMR (100 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20191208 nmr 400 ynu old
EXPNO                393
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191209
Time              18.56
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ             1.2976128 sec
RG                195.85
DW               19.800 usec
DE                6.50 usec
TE        0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6283629 MHz
NUC1                 13C
P1                10.50 usec
PLW1         74.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         17.50000000 W
PLW12         0.26142001 W
PLW13         0.13149001 W

F2 - Processing parameters
SI                32768
SF           100.6177980 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

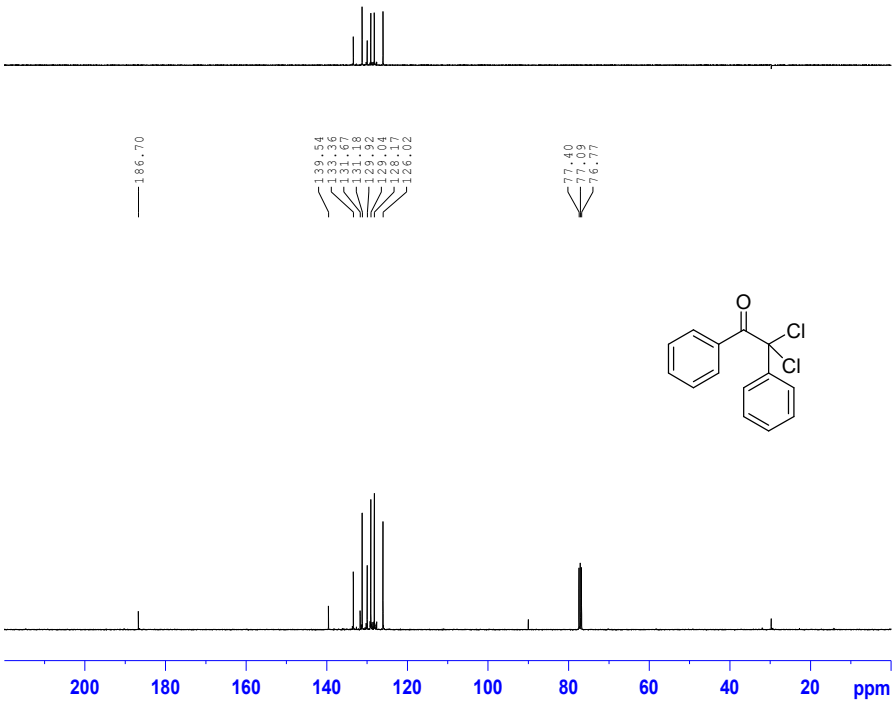
HM02186-1

^{1}H-NMR (400 MHz, $CDCl_3$)



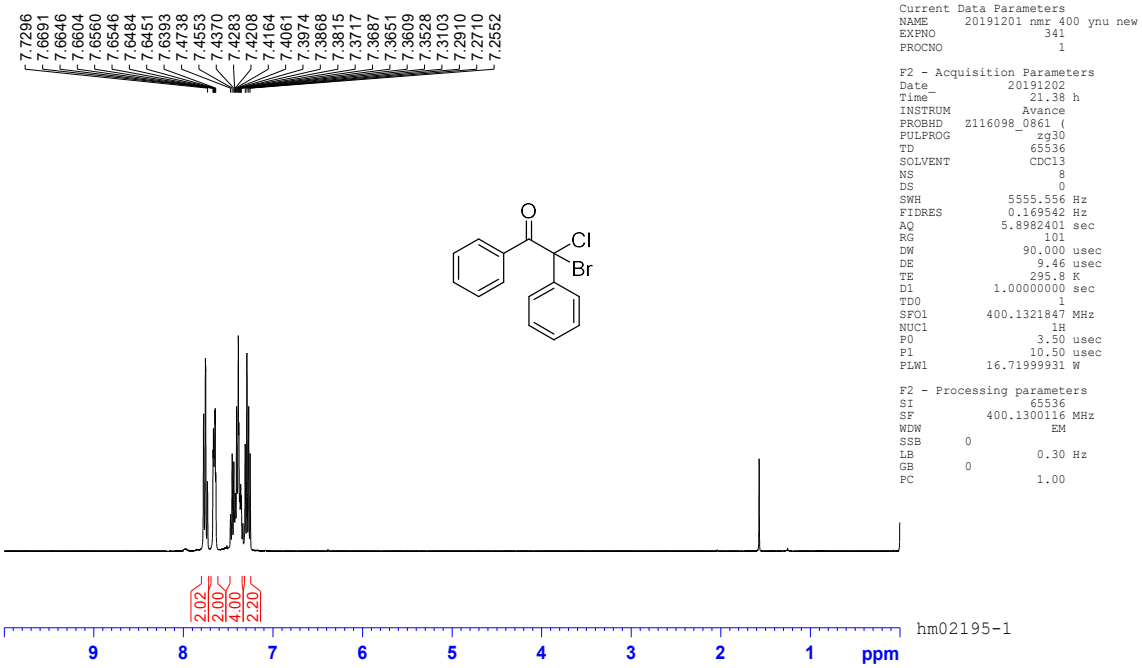

```
Current Data Parameters
NAME      20191208 nmr 400 ynu old
EXPNO              380
PROCNO               1

F2 - Acquisition Parameters
Date_           20191209
Time_              15.32
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                31.56
DW                62.400 usec
DE                 6.50 usec
TE        0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          400.1522008 MHz
NUC1                  1H
P1                10.75 usec
PLW1         17.50000000 W

F2 - Processing parameters
SI                65536
SF          400.1500152 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
HM02174-1
```

^{13}C-NMR (100 MHz, $CDCl_3$)



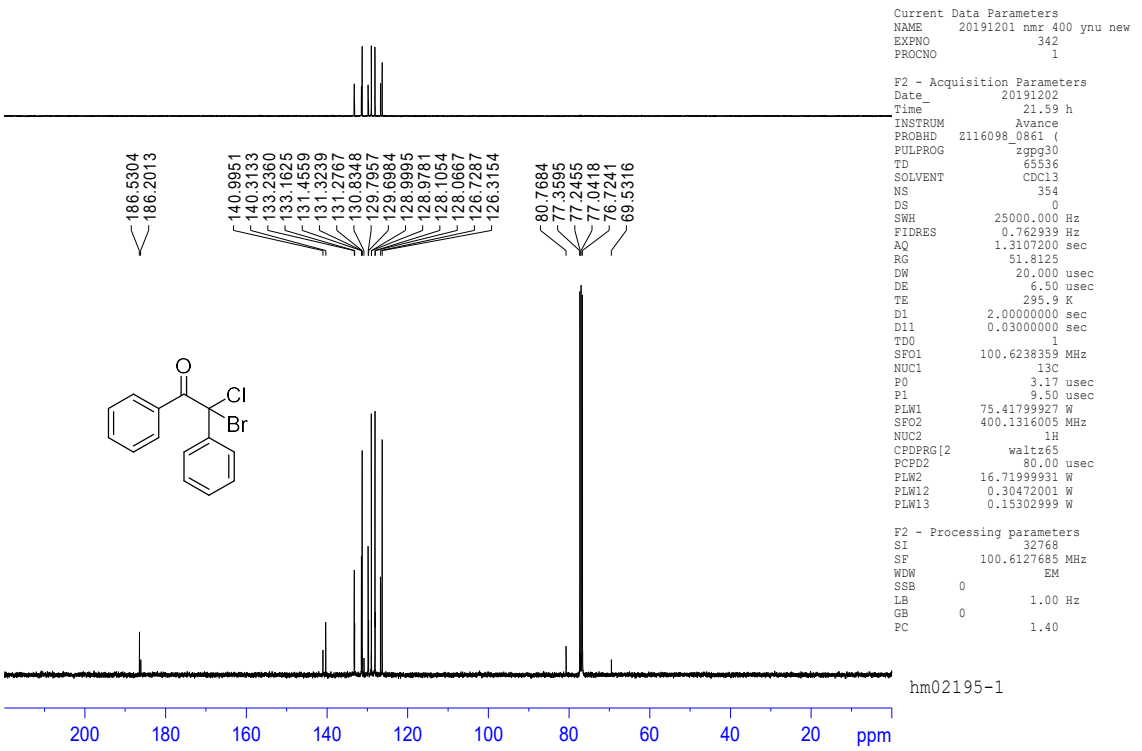

```
Current Data Parameters
NAME      20191208 nmr 400 ynu old
EXPNO              381
PROCNO               1

F2 - Acquisition Parameters
Date_           20191209
Time_              16.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    0
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                195.85
DW                19.800 usec
DE                 6.50 usec
TE        0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          100.6283629 MHz
NUC1                 13C
P1                10.50 usec
PLW1         74.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         17.50000000 W
PLW12         0.26142001 W
PLW13         0.13149001 W

F2 - Processing parameters
SI                32768
SF          100.6177980 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
HM02174-1
```

^{1}H-NMR (400 MHz, $CDCl_3$)



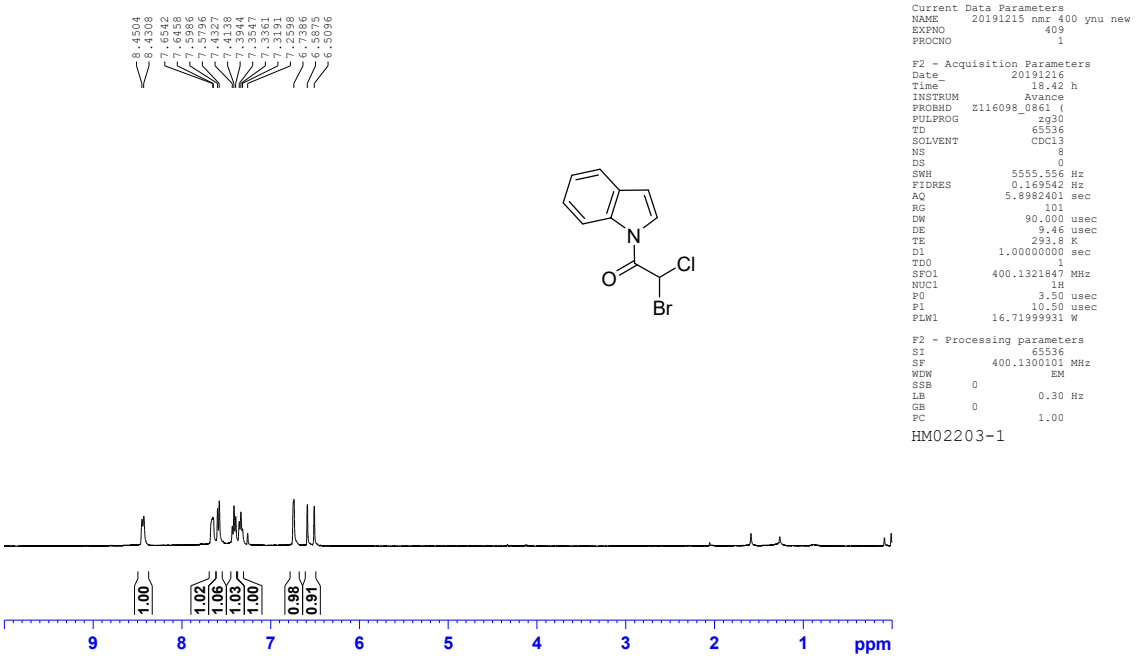

```
Current Data Parameters
NAME      20191201 nmr 400 ynu new
EXPNO              341
PROCNO               1

F2 - Acquisition Parameters
Date_          20191202
Time              21.38 h
INSTRUM          Avance
PROBHD   Z116098_0861 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           5555.556 Hz
FIDRES        0.169542 Hz
AQ            5.8982401 sec
RG                 101
DW              90.000 usec
DE               9.46 usec
TE              295.8 K
D1           1.00000000 sec
TD0                  1
SFO1        400.1321847 MHz
NUC1                1H
P0                3.50 usec
P1               10.50 usec
PLW1        16.71999931 W

F2 - Processing parameters
SI               65536
SF          400.1300116 MHz
WDW                 EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20191201 nmr 400 ynu new
EXPNO              342
PROCNO               1

F2 - Acquisition Parameters
Date_          20191202
Time              21.59 h
INSTRUM          Avance
PROBHD   Z116098_0861 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 354
DS                   0
SWH          25000.000 Hz
FIDRES        0.762939 Hz
AQ            1.3107200 sec
RG              51.8125
DW              20.000 usec
DE               6.50 usec
TE              295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        100.6238359 MHz
NUC1                13C
P0                3.17 usec
P1                9.50 usec
PLW1        75.41799927 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        16.71999931 W
PLW12        0.30472001 W
PLW13        0.15302999 W

F2 - Processing parameters
SI               32768
SF          100.6127685 MHz
WDW                 EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

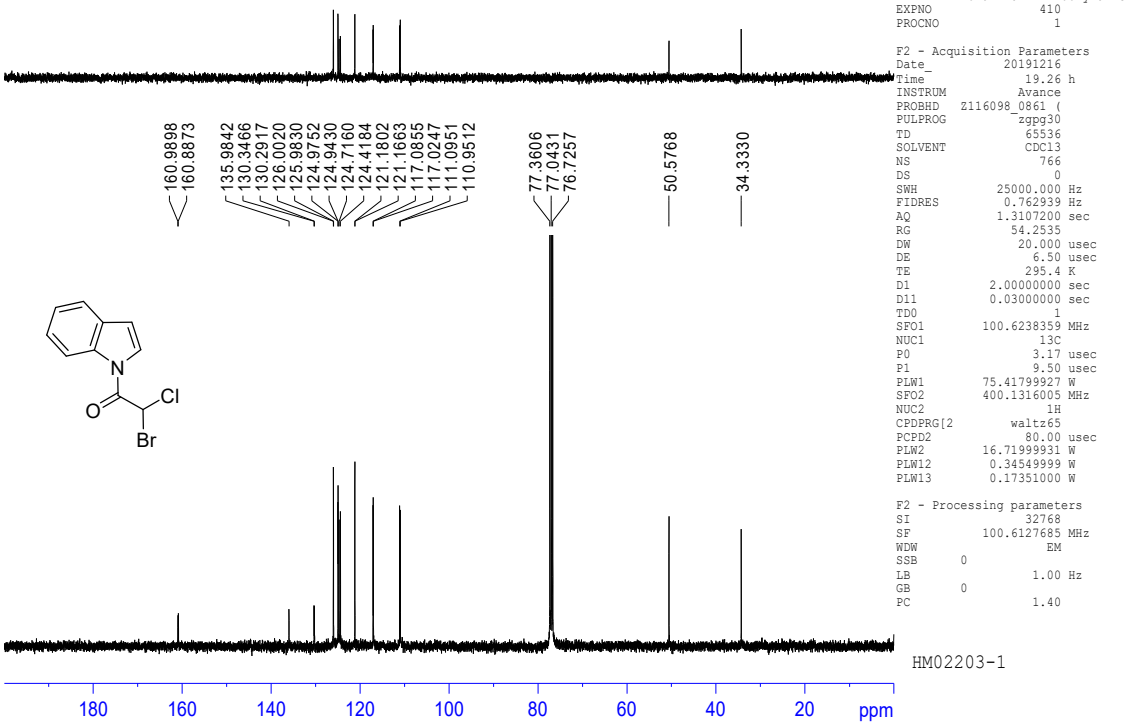
^{1}H-NMR (400 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20191215 nmr 400 ynu new
EXPNO                409
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191216
Time              18.42 h
INSTRUM           Avance
PROBHD   Z116098_0861 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             5555.556 Hz
FIDRES          0.169542 Hz
AQ              5.8982401 sec
RG                   101
DW                90.000 usec
DE                 9.46 usec
TE                293.8 K
D1            1.00000000 sec
TD0                    1
SFO1         400.1321847 MHz
NUC1                  1H
P0                 3.50 usec
P1                10.50 usec
PLW1         16.71999931 W

F2 - Processing parameters
SI                 65536
SF           400.1300101 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

HM02203-1

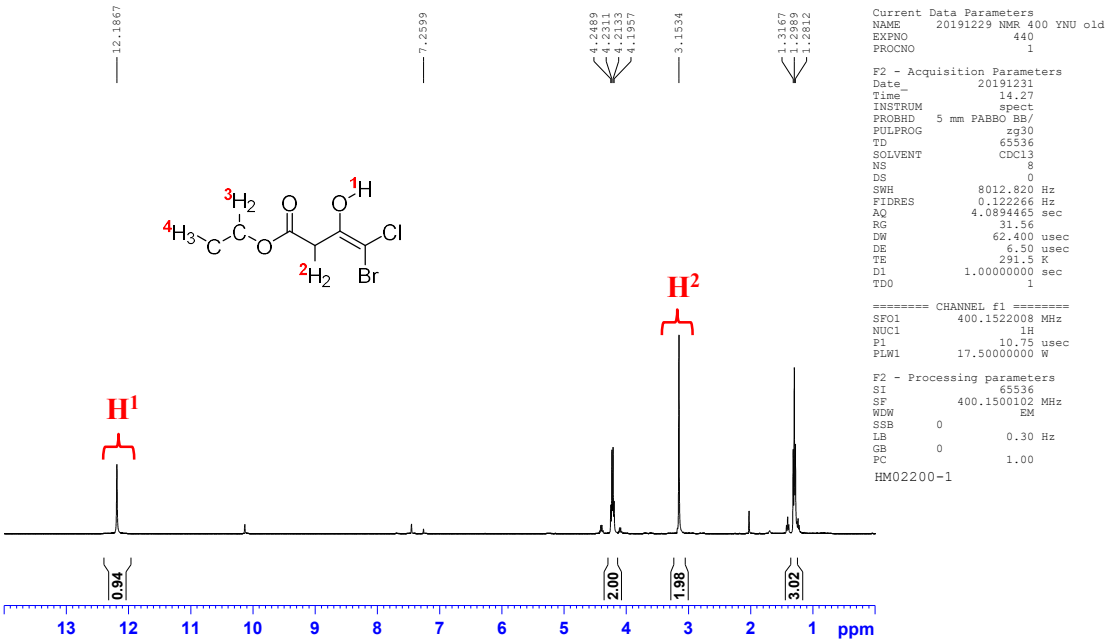
^{13}C-NMR (100 MHz, $CDCl_3$)



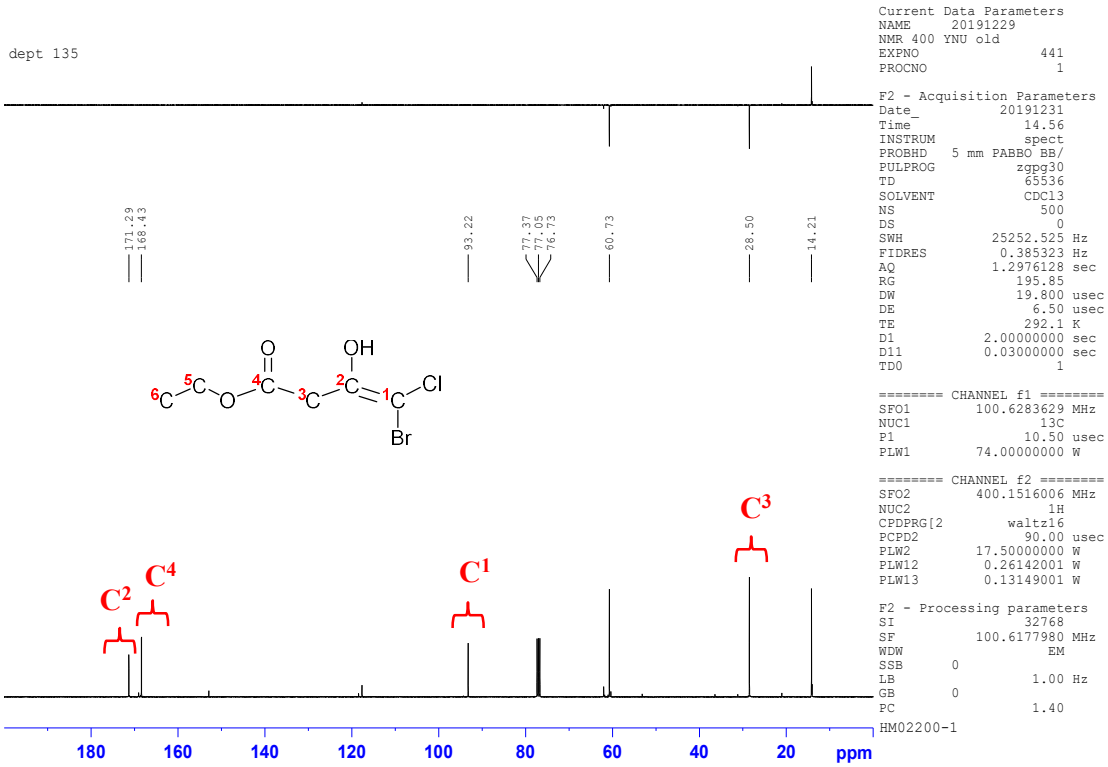

```
Current Data Parameters
NAME      20191215 nmr 400 ynu new
EXPNO                410
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191216
Time              19.26 h
INSTRUM           Avance
PROBHD   Z116098_0861 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   766
DS                     0
SWH            25000.000 Hz
FIDRES          0.762939 Hz
AQ              1.3107200 sec
RG                54.2535
DW                20.000 usec
DE                 6.50 usec
TE                295.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6238359 MHz
NUC1                  13C
P0                 3.17 usec
P1                 9.50 usec
PLW1         75.41799927 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         16.71999931 W
PLW12         0.34549999 W
PLW13         0.17351000 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HM02203-1

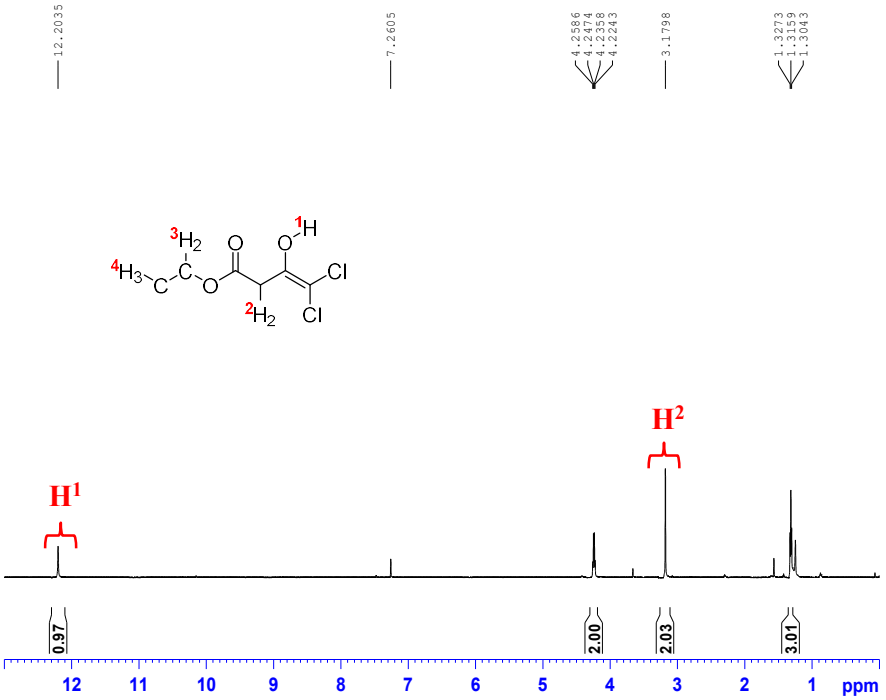
^{1}H-NMR (400 MHz, $CDCl_3$)



^{13}C-NMR (100 MHz, $CDCl_3$)

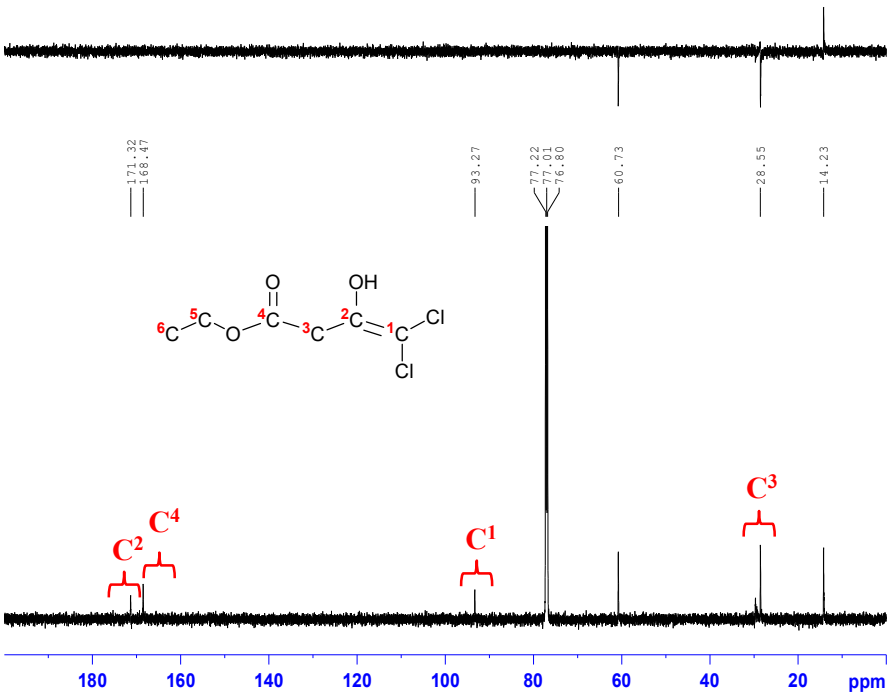


^{1}H-NMR (600 MHz, $CDCl_3$)

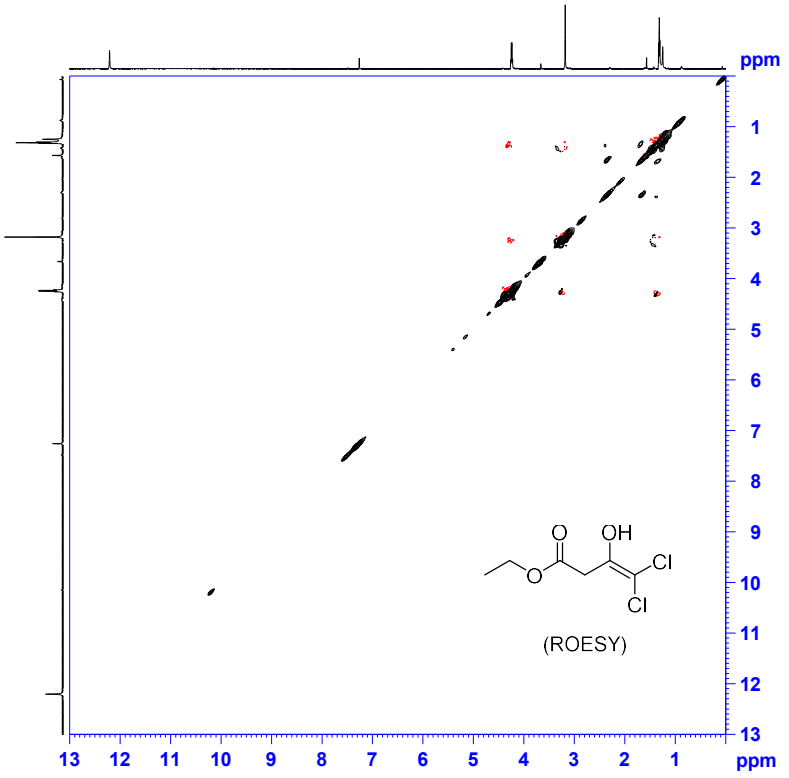



```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                 47
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220212
Time              21.35 h
INSTRUM             spect
PROBHD    Z114607_0222 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            12019.230 Hz
FIDRES             0.366798 Hz
AQ              2.7262976 sec
RG                 121.23
DW                 41.600 usec
DE                 11.27 usec
TE                 291.4 K
D1              1.00000000 sec
TD0                    1
SFO1          600.1737060 MHz
NUC1                  1H
P0                  3.33 usec
P1                 10.00 usec
PLW1          26.09399986 W

F2 - Processing parameters
SI                 65536
SF            600.1700154 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00

TYF04080-1
```

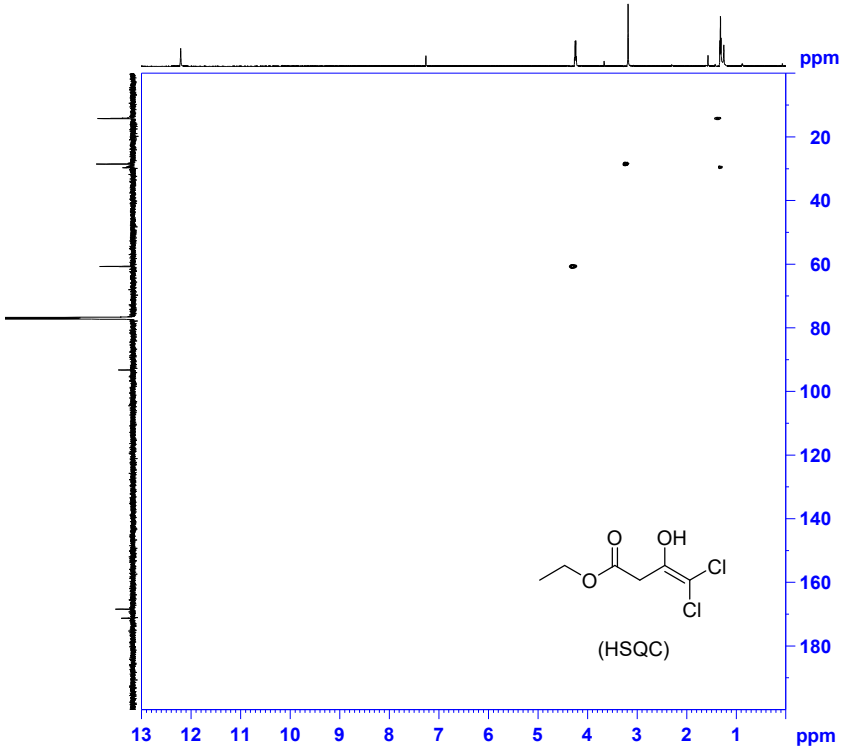
^{13}C-NMR (150 MHz, $CDCl_3$)



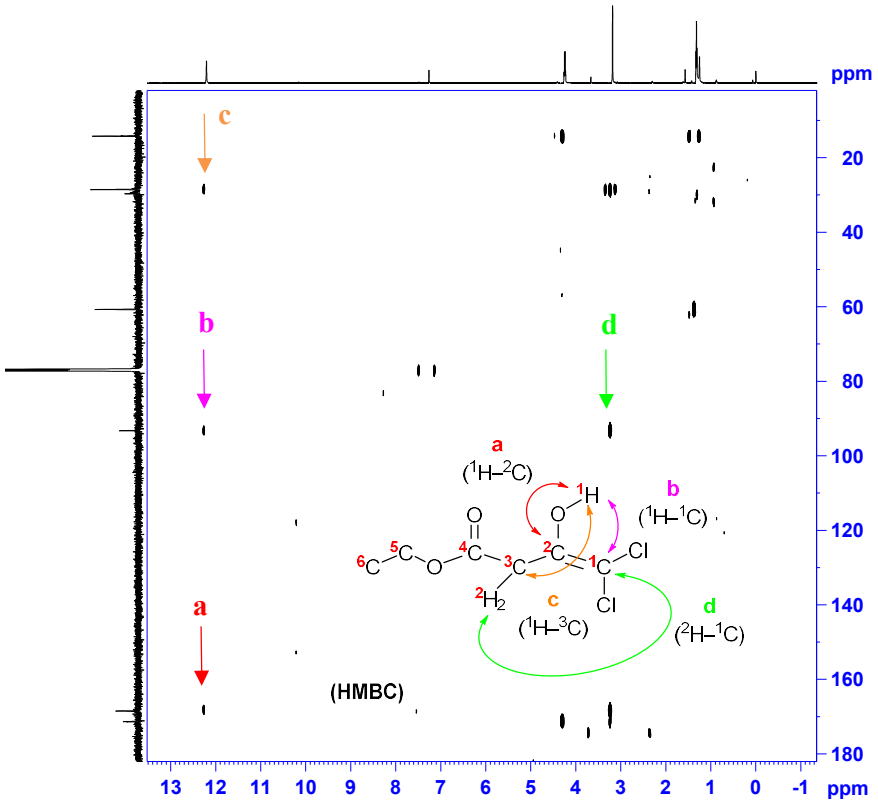

```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                 41
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220212
Time              19.32 h
INSTRUM             spect
PROBHD    Z114607_0222 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   800
DS                     4
SWH            36231.883 Hz
FIDRES             1.105709 Hz
AQ              0.9043968 sec
RG                 188.35
DW                 13.800 usec
DE                 6.50 usec
TE                 293.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1          150.9279578 MHz
NUC1                  13C
P0                  4.00 usec
P1                 12.00 usec
PLW1          97.67099762 W
SFO2          600.1724007 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              70.00 usec
PLW2          27.73900032 W
PLW12          0.56610000 W
PLW13          0.28475001 W

F2 - Processing parameters
SI                 32768
SF            150.9128665 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40

TYF04080-1
```




```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                 44
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220212
Time              20.51
INSTRUM           spect
PROBHD   Z114607_0222 (
PULPROG      roesyphpp.2
TD                2048
SOLVENT           CDCl3
NS                   4
DS                  32
SWH          9259.259 Hz
FIDRES       4.521122 Hz
AQ          0.1105920 sec
RG               61.75
DW             54.000 usec
DE              6.50 usec
TE             291.8 K
d0          -0.00001037 sec
D1           2.05980110 sec
d11          0.03000000 sec
d12          0.00002000 sec
in0       0 sec
14                2556
P15          920000.00 usec
ST1CNT               0
d0orig      -0.00001037 sec
ph1loop              0
t1loop               0
SFO1        600.1736438 MHz
NUC1                 1H
P1                10.00 usec
P17             2500.00 usec
P25              180.00 usec
PLW1        26.09399986 W
PLW10        4.17500019 W
PLW27        0.32214999 W

F1 - Acquisition parameters
TD                 256
SFO1          600.1736 MHz
FIDRES       36.168980 Hz
SW            15.428 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                1024
SF          600.1699832 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
PC                1.00

F1 - Processing parameters
SI                1024
MC2          States-TPPI
SF          600.1699832 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
```

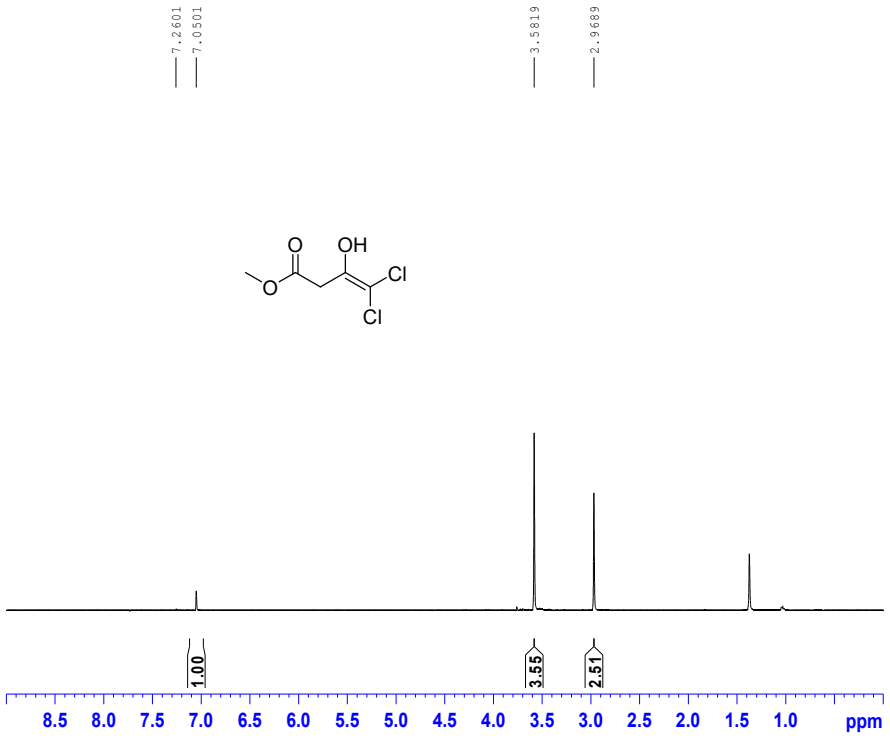



```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO                 45
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220212
Time              21.05
INSTRUM           spect
PROBHD   Z114607_0222 (
PULPROG      hsqcetgpsi2
TD                2048
SOLVENT           CDCl3
NS                   2
DS                  16
SWH          9259.259 Hz
FIDRES       4.521122 Hz
AQ          0.1105920 sec
RG              188.35
DW             54.000 usec
DE              9.85 usec
TE             292.1 K
CNST2       145.0000000
d0          0.00000300 sec
D1          1.50000000 sec
d4          0.00172414 sec
d11         0.03000000 sec
D16         0.00020000 sec
D24         0.00086207 sec
DELTA       0.00127600 sec
DELTA1      0.00121005 sec
DELTA2      0.00006207 sec
DELTA3      0.00052414 sec
in0       0 sec
ST1CNT               0
ZGOPTNS
d0orig      0.00000300 sec
ph1loop              0
t1loop               0
SFO1        600.1736438 MHz
NUC1                 1H
P1                10.00 usec
p2                20.00 usec
P28             1000.00 usec
PLW1        26.09399986 W
SFO2        150.9267505 MHz
NUC2                13C
CPDPRG[2            garp
P3                12.00 usec
p4                24.00 usec
PCPD2             60.00 usec
PLW2        97.67099762 W
PLW12        3.90680003 W
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                 256
SFO1          150.9268 MHz
FIDRES       106.148094 Hz
SW            180.047 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                2048
SF          600.1699832 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          150.9128665 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
```



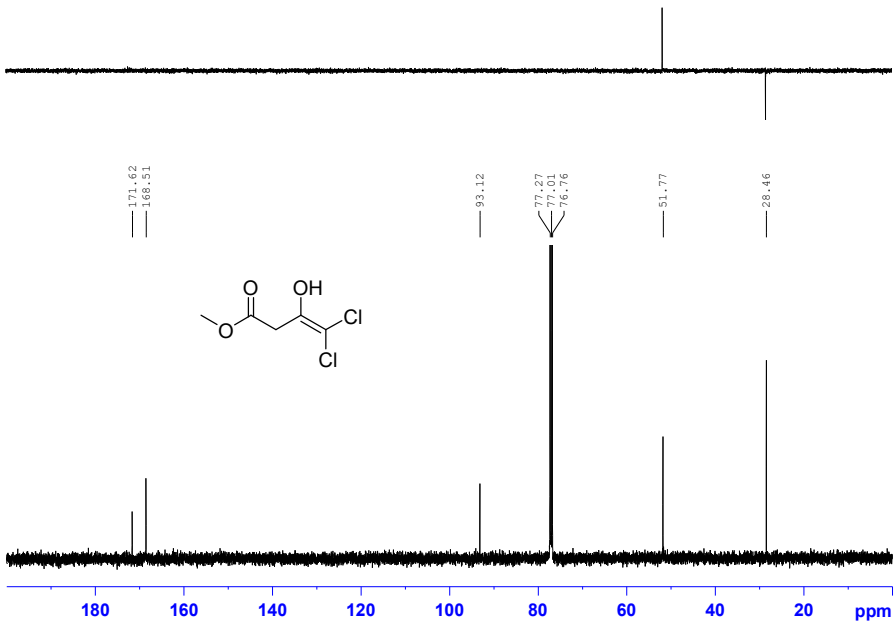

```
Current Data Parameters
NAME      20220212 nmr h c 2d
EXPNO               48
PROCNO               1

F2 - Acquisition Parameters
Date_          20220212
Time_             22.29
INSTRUM           spect
PROBHD   Z114607_0222 (
PULPROG    hmbcgplpndqf
TD                8192
SOLVENT           CDCl3
NS                  12
DS                  16
SWH            8928.571 Hz
FIDRES         1.089913 Hz
AQ             0.4587520 sec
RG               188.35
DW                56.000 usec
DE                 6.50 usec
TE               291.3 K
CNST2        145.0000000
CNST13        10.0000000
d0             0.00000300 sec
D1             1.50000000 sec
d2             0.00344828 sec
d6             0.05000000 sec
D16            0.00020000 sec
in0       0 sec
ST1CNT              0
d0orig         0.00000300 sec
phlloop             0
tlloop              0
SFO1         600.1736359 MHz
NUC1                1H
P1                10.00 usec
p2                20.00 usec
PLW1         26.09399986 W
SFO2         150.9296179 MHz
NUC2                13C
P3                12.00 usec
PLW2         97.67099762 W
GPNAM[1]     SMSQ10.100
GPNAM[2]     SMSQ10.100
GPNAM[3]     SMSQ10.100
GPZ1               50.00 %
GPZ2               30.00 %
GPZ3               40.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1          150.9296 MHz
FIDRES        258.692047 Hz
SW              219.391 ppm
FnMODE              QF

F2 - Processing parameters
SI                 8192
SF           600.1699832 MHz
WDW                QSINE
SSB        0
LB         0 Hz
GB         0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2                QF
SF           150.9128665 MHz
WDW                QSINE
SSB        0
LB         0 Hz
GB         0
```

^{1}H-NMR (500 MHz, $CDCl_3$)



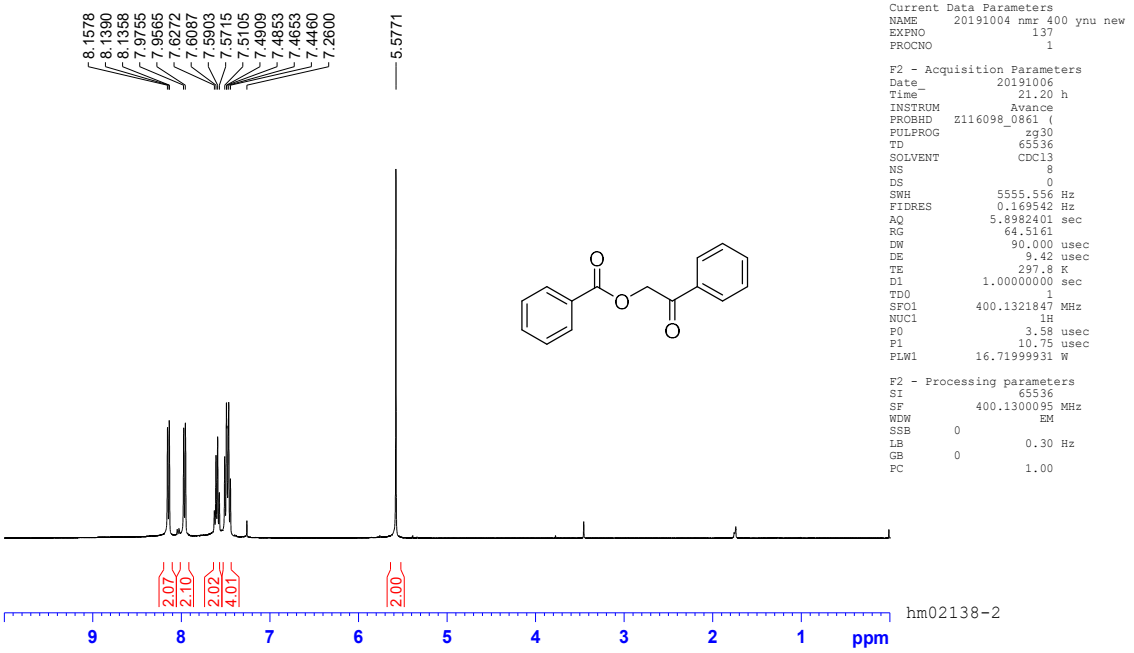

```
Current Data Parameters
NAME      20211125 nmr h
EXPNO                70
PROCNO                1

F2 - Acquisition Parameters
Date_          20211125
Time              12.17 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   3
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               169.48
DW               50.000 usec
DE               13.89 usec
TE               296.3 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1301173 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
TYF04052-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



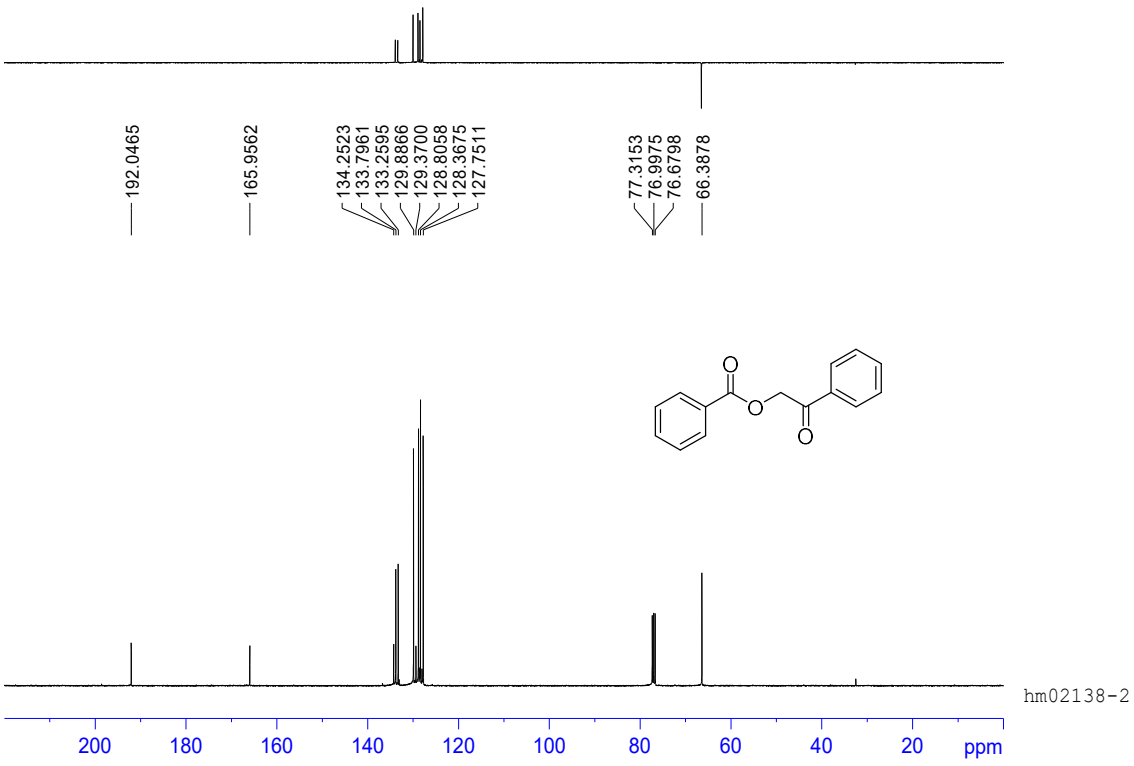

```
Current Data Parameters
NAME      20211125 nmr c
EXPNO                72
PROCNO                1

F2 - Acquisition Parameters
Date_          20211125
Time              19.23 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 221
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40

TYF04052-1
```

^{1}H-NMR (400 MHz, $CDCl_3$)

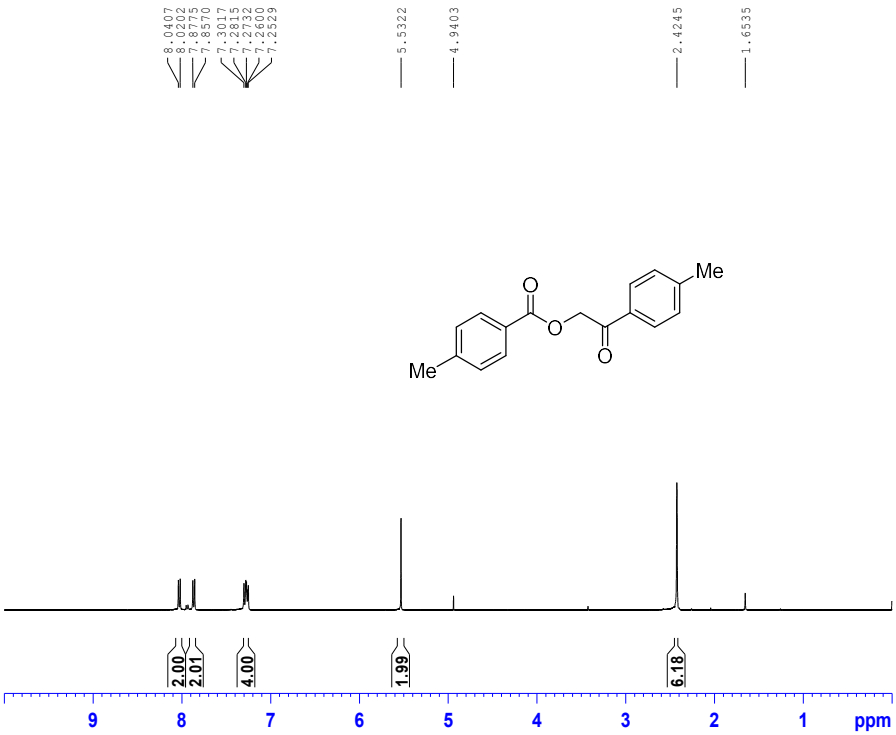



```
Current Data Parameters
NAME      20191004 nmr 400 ynu new
EXPNO              137
PROCNO               1

F2 - Acquisition Parameters
Date_          20191006
Time             21.20 h
INSTRUM          Avance
PROBHD    Z116098_0861 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            5555.556 Hz
FIDRES         0.169542 Hz
AQ             5.8982401 sec
RG               64.5161
DW               90.000 usec
DE                9.42 usec
TE               297.8 K
D1            1.00000000 sec
TD0                   1
SFO1         400.1321847 MHz
NUC1                 1H
P0                3.58 usec
P1               10.75 usec
PLW1         16.71999931 W

F2 - Processing parameters
SI                65536
SF           400.1300095 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)

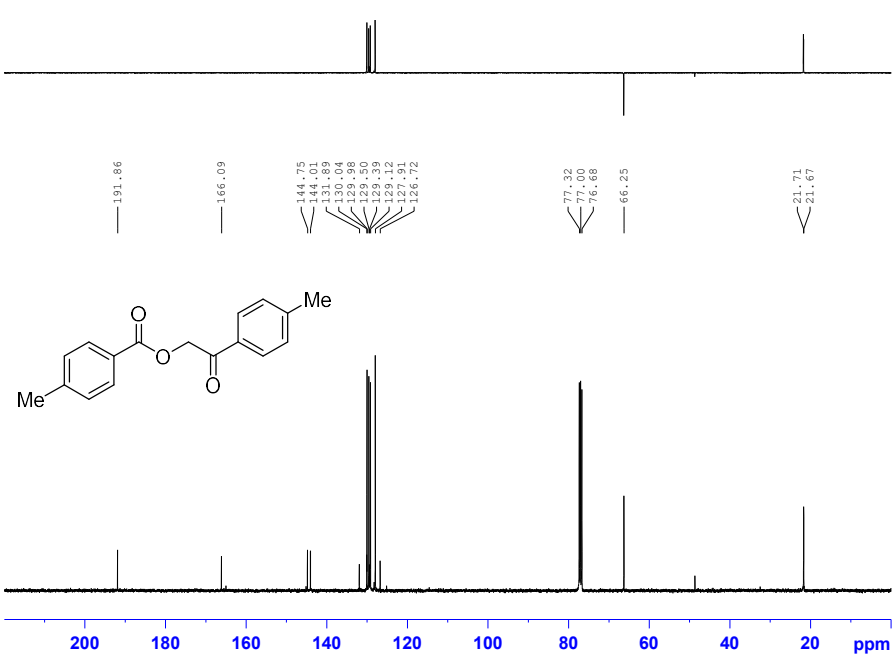


^{1}H-NMR (400 MHz, $CDCl_3$)



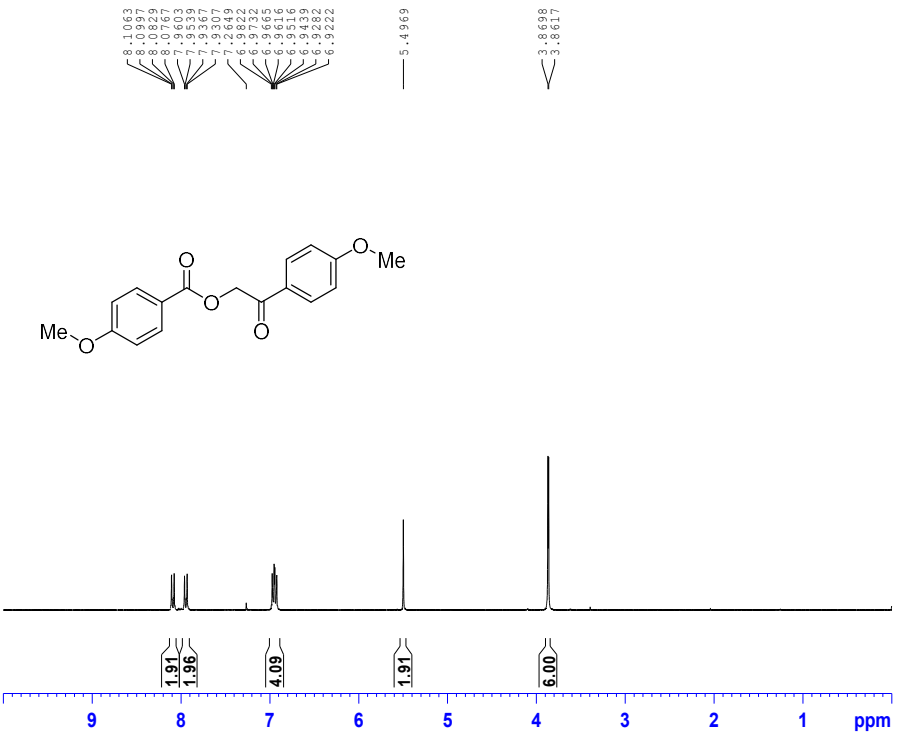

```
Current Data Parameters
NAME      20191013 nmr 400 ynu new
EXPNO                189
PROCNO                 1

F2 - Acquisition Parameters
Date_              20191014
Time                  9.45 h
INSTRUM              Avance
PROBHD    Z116098_0861 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                5555.556 Hz
FIDRES            0.169542 Hz
AQ                5.8982401 sec
RG                      101
DW                   90.000 usec
DE                    9.42 usec
TE                   297.2 K
D1                1.00000000 sec
TD0                       1
SFO1           400.1321847 MHz
NUC1                     1H
P0                    3.58 usec
P1                   10.75 usec
PLW1           16.71999931 W

F2 - Processing parameters
SI                    65536
SF             400.1300095 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
hm02145-2
```

^{13}C-NMR (100 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20191013 nmr 400 ynu new
EXPNO                190
PROCNO                 1

F2 - Acquisition Parameters
Date_              20191014
Time                 10.15 h
INSTRUM              Avance
PROBHD    Z116098_0861 (
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      512
DS                        0
SWH               25000.000 Hz
FIDRES            0.762939 Hz
AQ                1.3107200 sec
RG                      101
DW                   20.000 usec
DE                    6.50 usec
TE                   298.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1           100.6238359 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           75.41799927 W
SFO2           400.1316005 MHz
NUC2                     1H
CPDPRG[2            waltz65
PCPD2                80.00 usec
PLW2           16.71999931 W
PLW12           0.34549999 W
PLW13           0.17351000 W

F2 - Processing parameters
SI                    32768
SF             100.6127726 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
hm02145-2
```

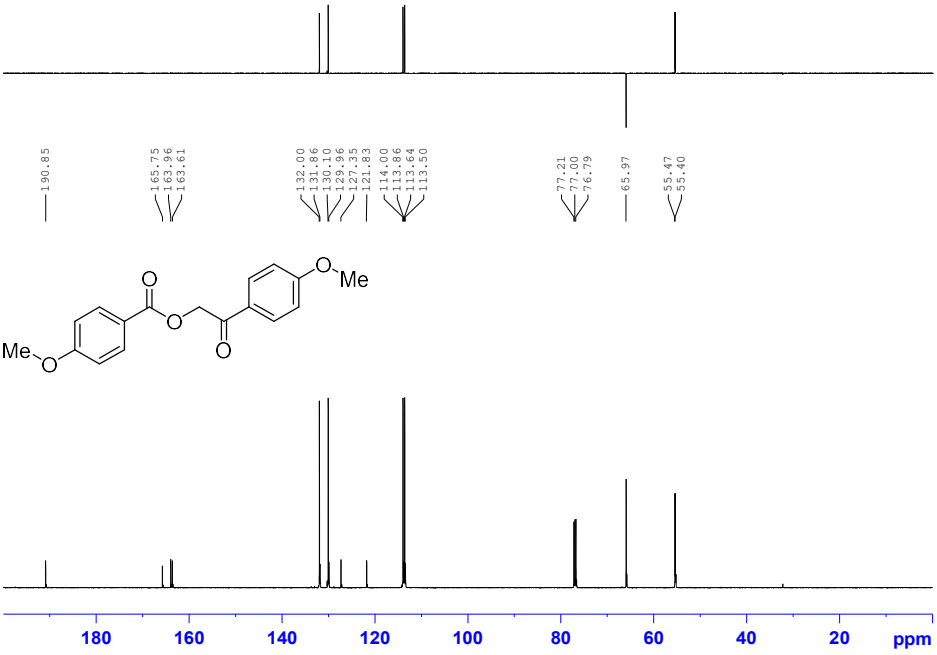
^{1}H-NMR (300 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20181221-20190530 NMR 300 YNU
EXPNO                541
PROCNO                 1

F2 - Acquisition Parameters
Date_              20190401
Time                   2.22
INSTRUM               av300
PROBHD    5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6172.839 Hz
FIDRES           0.094190 Hz
AQ               5.3084159 sec
RG                    181
DW                 81.000 usec
DE                  6.50 usec
TE                 294.7 K
D1            1.00000000 sec
TD0                     1
SFO1          300.1318534 MHz
NUC1                   1H
P1                  8.25 usec
PLW1         -1.00000000 W

F2 - Processing parameters
SI                  32768
SF            300.1300106 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

bzhm02011

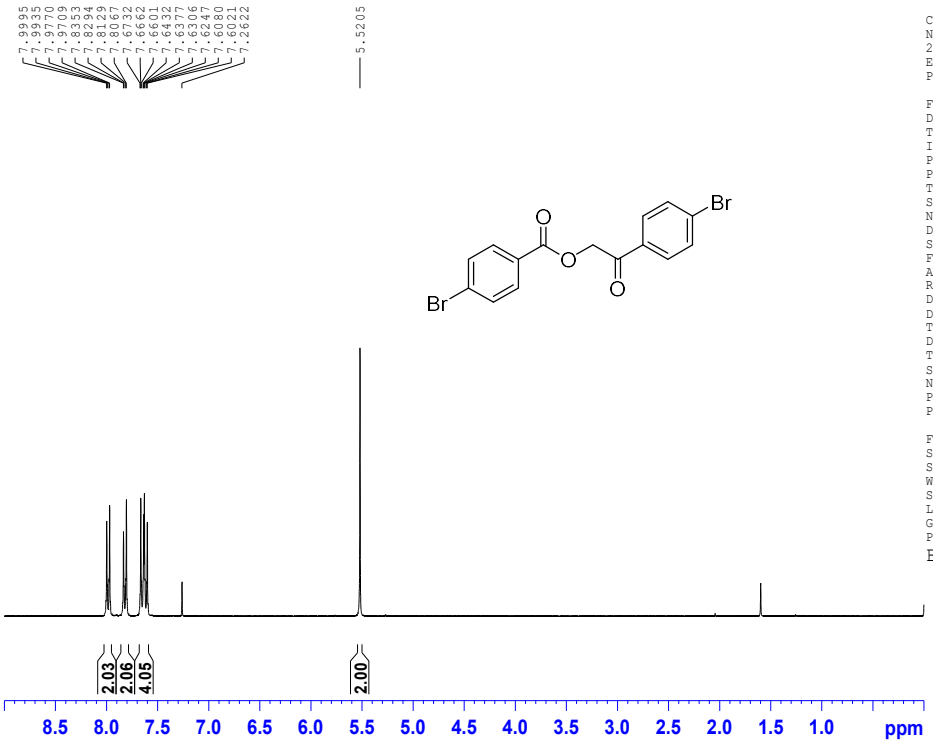
^{13}C-NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      bzhm02011
20190410-2 600 KIB chen
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_              20190412
Time                   2.30
INSTRUM               spect
PROBHD    5 mm CPQCI 1H-
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                    800
DS                      4
SWH              36231.883 Hz
FIDRES           0.552855 Hz
AQ               0.9043968 sec
RG                  199.06
DW                 13.800 usec
DE                  18.00 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          150.9438010 MHz
NUC1                   13C
P1                  11.20 usec
PLW1          94.00000000 W

======== CHANNEL f2 ========
SFO2          600.2294009 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2           2.89730000 W
PLW12          0.06519000 W

F2 - Processing parameters
SI                 131072
SF            150.9272810 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

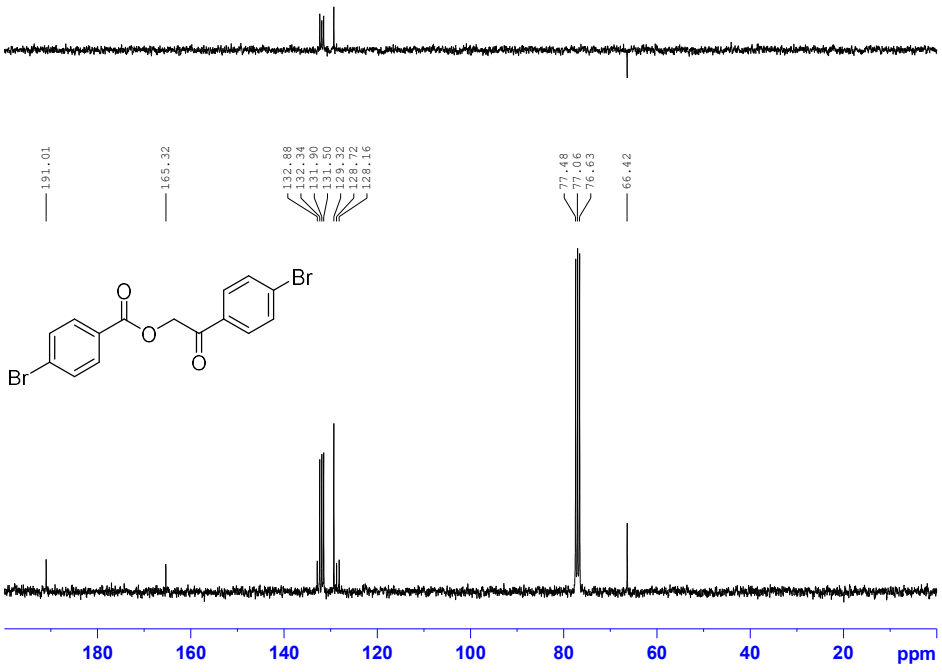
hm02011

^{1}H-NMR (300 MHz, $CDCl_3$)



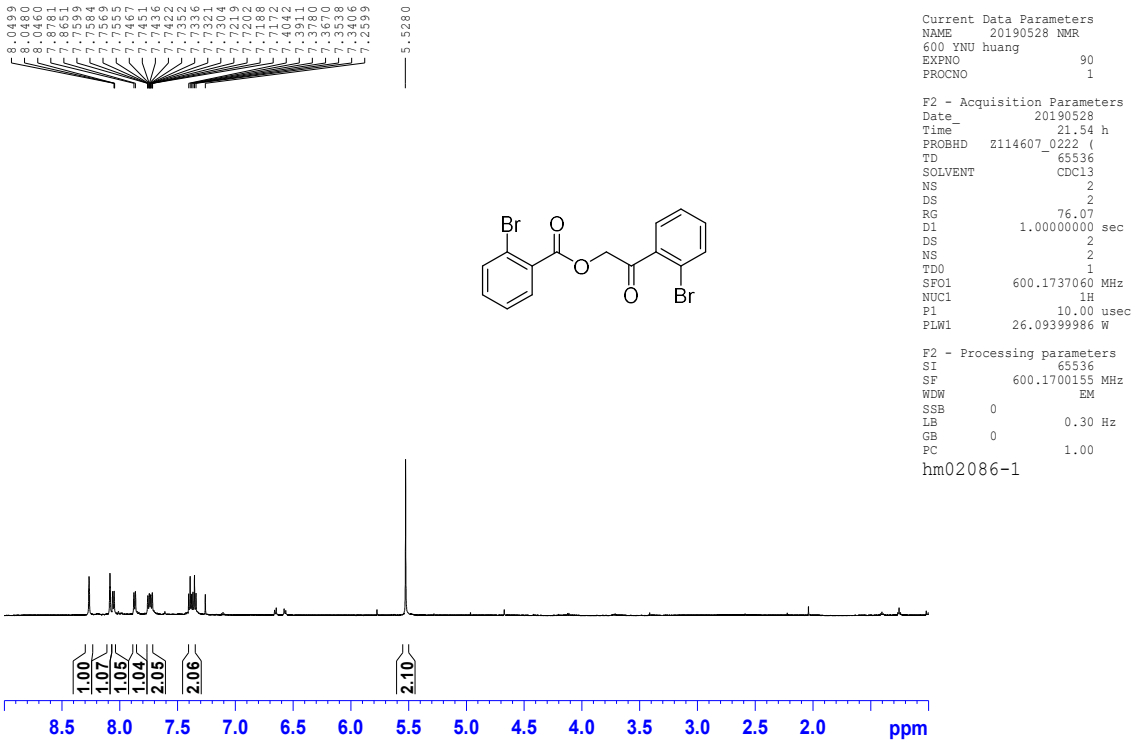

```
Current Data Parameters
NAME      20181221-
20190530 NMR 300 YNU
EXPNO                767
PROCNO                 1

F2 - Acquisition Parameters
Date_              20190509
Time                   1.15
INSTRUM              av300
PROBHD    5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH             6172.839 Hz
FIDRES             0.094190 Hz
AQ              5.3084159 sec
RG                  456.1
DW                 81.000 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1
SFO1          300.1318534 MHz
NUC1                   1H
P1                  8.25 usec
PLW1          -1.00000000 W

F2 - Processing parameters
SI                  32768
SF            300.1300114 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
BZHM02083
```

^{13}C-NMR (75 MHz, $CDCl_3$)



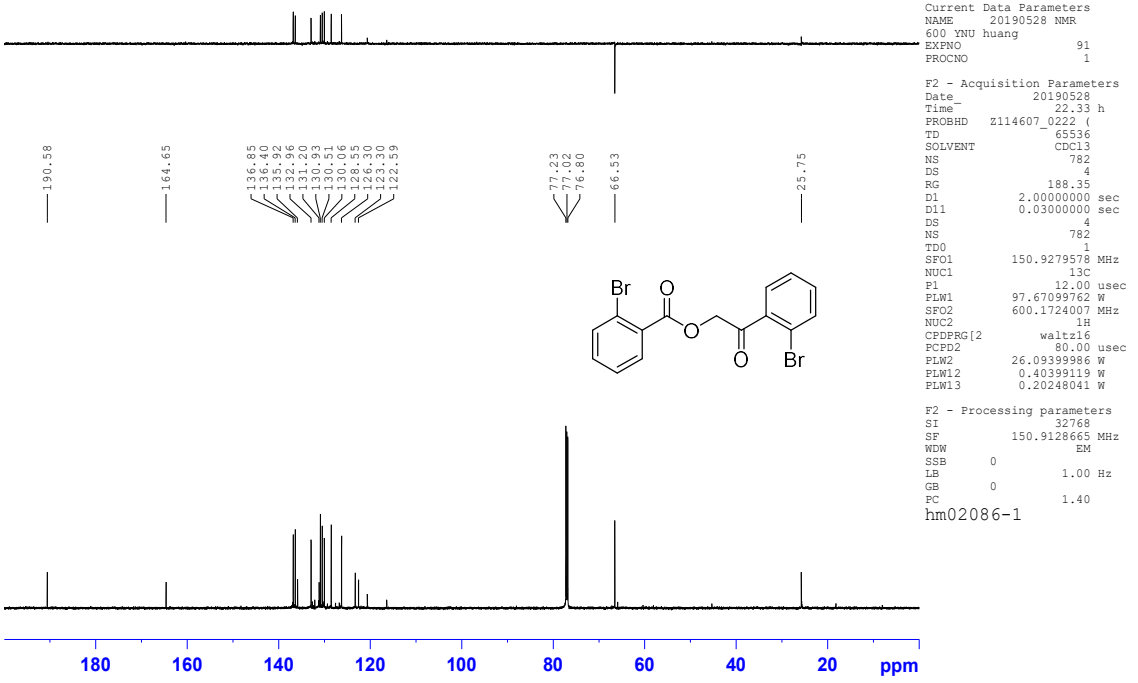

```
Current Data Parameters
NAME      20181221-
20190530 NMR 300 YNU
EXPNO                768
PROCNO                 1

F2 - Acquisition Parameters
Date_              20190509
Time                   1.22
INSTRUM              av300
PROBHD    5 mm QNP 1H/13
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    377
DS                      0
SWH            20325.203 Hz
FIDRES             0.310138 Hz
AQ              1.6121856 sec
RG                  16384
DW                 24.600 usec
DE                  6.50 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1
SFO1          75.4752953 MHz
NUC1                   13C
P1                 28.00 usec
PLW1          -1.00000000 W
SFO2         300.1312005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          -1.00000000 W
PLW12         -1.00000000 W
PLW13         -1.00000000 W

F2 - Processing parameters
SI                  32768
SF            75.4677490 MHz
WDW                    EM
SSB       0
LB                  3.00 Hz
GB        0
PC                  1.40

BZHM02083
```

^{1}H-NMR (600 MHz, $CDCl_3$)



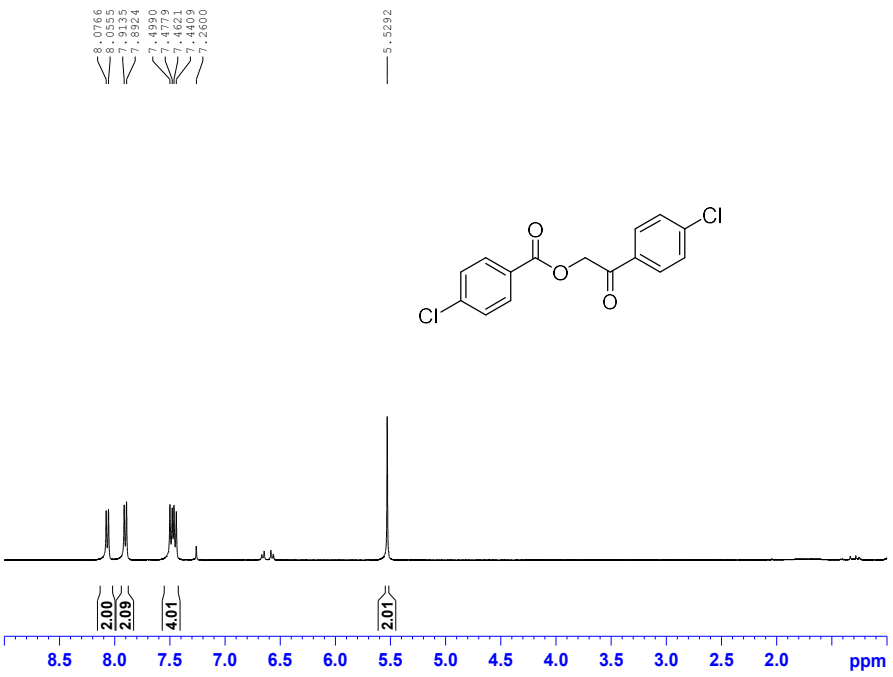

```
Current Data Parameters
NAME      20190528 NMR
600 YNU huang
EXPNO                90
PROCNO                1

F2 - Acquisition Parameters
Date_            20190528
Time               21.54 h
PROBHD   Z114607_0222 (
TD                 65536
SOLVENT            CDCl3
NS                     2
DS                     2
RG                 76.07
D1          1.00000000 sec
DS                     2
NS                     2
TD0                    1
SFO1         600.1737060 MHz
NUC1                  1H
P1                10.00 usec
PLW1         26.09399986 W

F2 - Processing parameters
SI                 65536
SF           600.1700155 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
hm02086-1
```

^{13}C-NMR (150 MHz, $CDCl_3$)



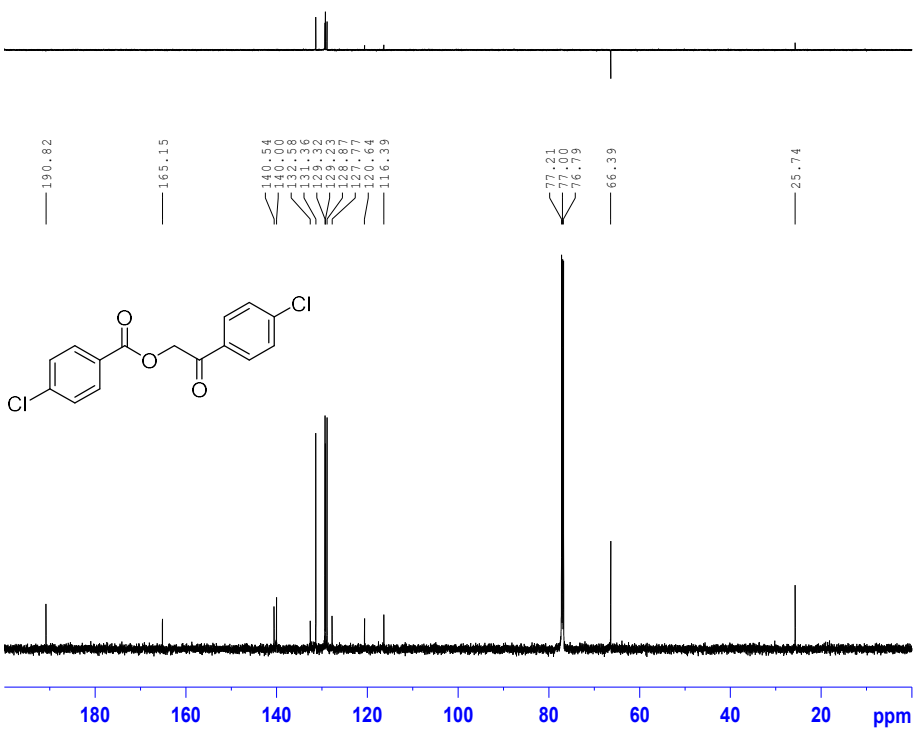

```
Current Data Parameters
NAME      20190528 NMR
600 YNU huang
EXPNO                91
PROCNO                1

F2 - Acquisition Parameters
Date_            20190528
Time               22.33 h
PROBHD   Z114607_0222 (
TD                 65536
SOLVENT            CDCl3
NS                   782
DS                     4
RG                 188.35
D1          2.00000000 sec
D11         0.03000000 sec
DS                     4
NS                   782
TD0                    1
SFO1         150.9279578 MHz
NUC1                  13C
P1                12.00 usec
PLW1         97.67099762 W
SFO2         600.1724007 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         26.09399986 W
PLW12         0.40399119 W
PLW13         0.20248041 W

F2 - Processing parameters
SI                 32768
SF           150.9128665 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
hm02086-1
```

^{1}H-NMR (400 MHz, $CDCl_3$)



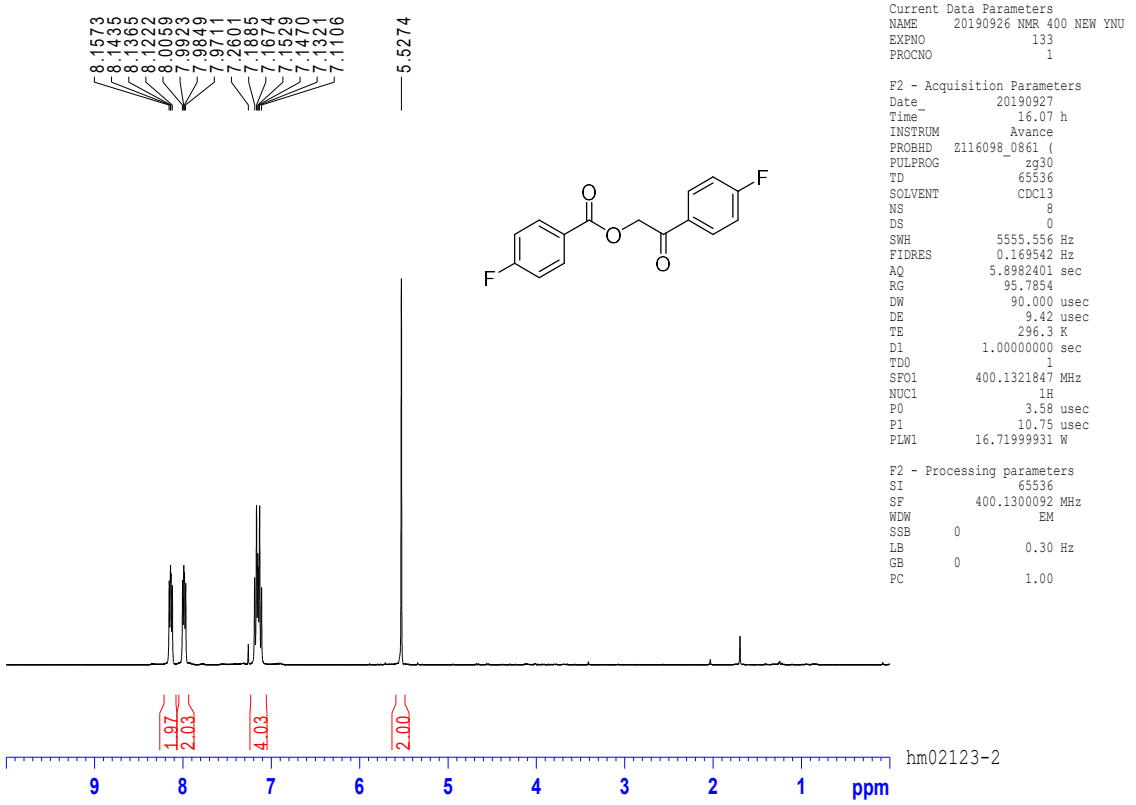

```
Current Data Parameters
NAME          bzhm02085
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190526
Time               4.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ             4.0894465 sec
RG                50.87
DW               62.400 usec
DE                6.50 usec
TE                295.8 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1318812 MHz
NUC1                 1H
P1                12.00 usec
PLW1         11.69999981 W

F2 - Processing parameters
SI                65536
SF           400.1300098 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
bzhm02085
```

^{13}C-NMR (150 MHz, $CDCl_3$)



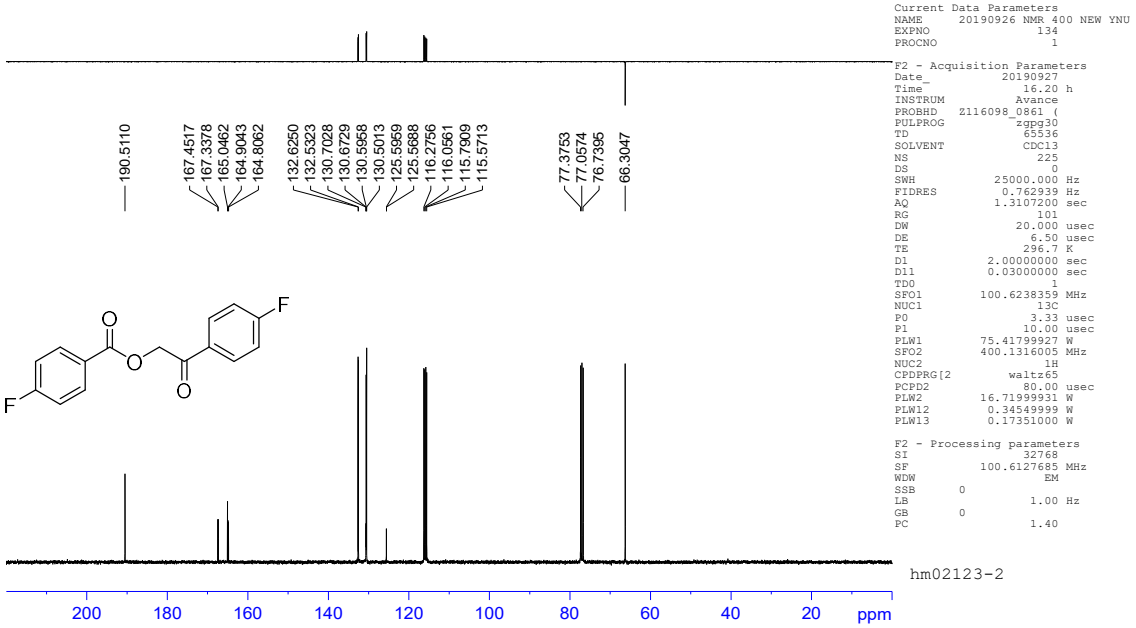

```
Current Data Parameters
NAME      20190528 NMR
600 YNU huang
EXPNO               121
PROCNO                1

F2 - Acquisition Parameters
Date_          20190529
Time               8.55 h
PROBHD   Z114607_0222 (
TD                65536
SOLVENT           CDCl3
NS                  240
DS                    4
RG               188.35
D1            2.00000000 sec
D11           0.03000000 sec
DS                    4
NS                  240
TD0                   1
SFO1         150.9279578 MHz
NUC1                 13C
P1                12.00 usec
PLW1         97.67099762 W
SFO2         600.1724007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         26.09399986 W
PLW12         0.40399119 W
PLW13         0.20248041 W

F2 - Processing parameters
SI                32768
SF           150.9128665 MHz
WDW                  EM
SSB       0
LB                1.40 Hz
GB        0
PC                1.40
hm02085
```

^{1}H-NMR (400 MHz, $CDCl_3$)



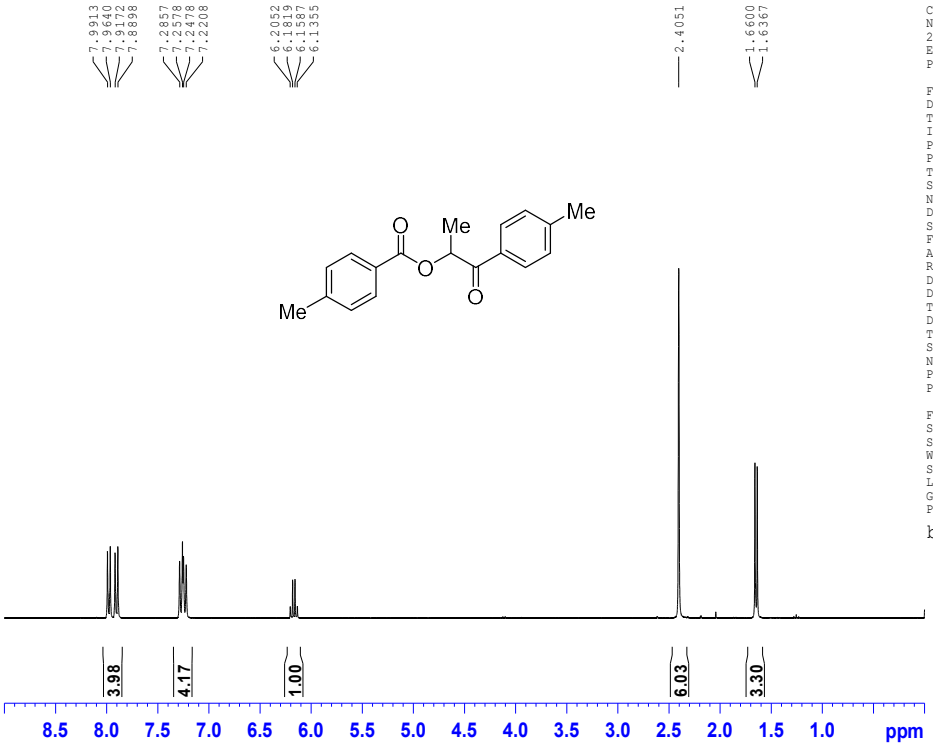

```
Current Data Parameters
NAME      20190926 NMR 400 NEW YNU
EXPNO              133
PROCNO               1

F2 - Acquisition Parameters
Date_          20190927
Time             16.07 h
INSTRUM          Avance
PROBHD   Z116098_0861 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           5555.556 Hz
FIDRES        0.169542 Hz
AQ            5.8982401 sec
RG              95.7854
DW               90.000 usec
DE                9.42 usec
TE               296.3 K
D1           1.00000000 sec
TD0                  1
SFO1        400.1321847 MHz
NUC1                1H
P0                3.58 usec
P1               10.75 usec
PLW1        16.71999931 W

F2 - Processing parameters
SI               65536
SF          400.1300092 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
```

^{13}C-NMR (100 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20190926 NMR 400 NEW YNU
EXPNO              134
PROCNO               1

F2 - Acquisition Parameters
Date_          20190927
Time             16.20 h
INSTRUM          Avance
PROBHD   Z116098_0861 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 225
DS                   0
SWH          25000.000 Hz
FIDRES        0.762939 Hz
AQ            1.3107200 sec
RG                 101
DW               20.000 usec
DE                6.50 usec
TE               296.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        100.6238359 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        75.41799927 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2        16.71999931 W
PLW12        0.34549999 W
PLW13        0.17351000 W

F2 - Processing parameters
SI               32768
SF          100.6127685 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```

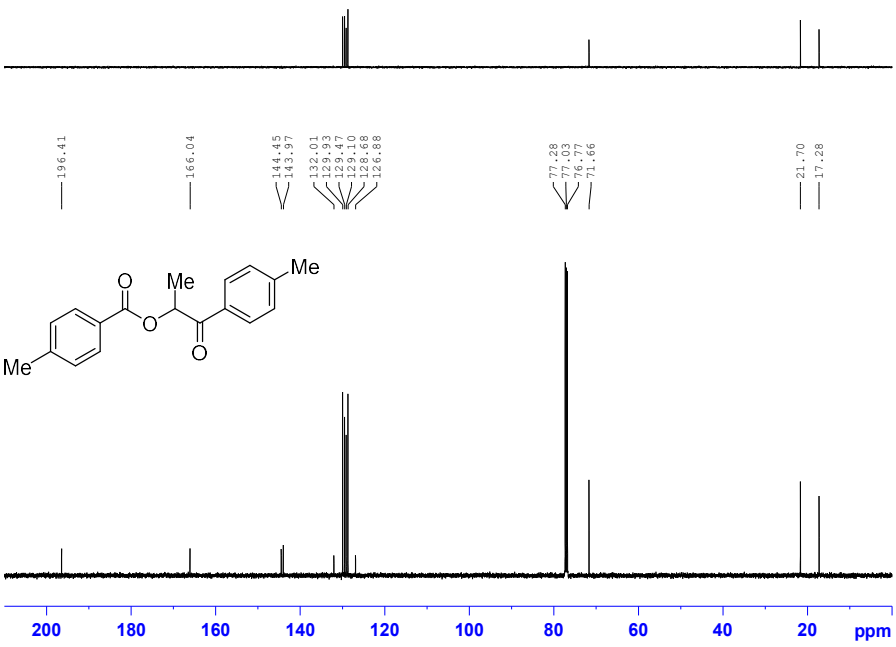
^{1}H-NMR (300 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20181221-
20190530 NMR 300 YNU
EXPNO                488
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190315
Time                2.32
INSTRUM           av300
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             6172.839 Hz
FIDRES             0.094190 Hz
AQ              5.3084159 sec
RG                   181
DW                81.000 usec
DE                 6.50 usec
TE                294.3 K
D1             1.00000000 sec
TD0                    1
SFO1          300.1318534 MHz
NUC1                  1H
P1                 8.25 usec
PLW1          -1.00000000 W

F2 - Processing parameters
SI                 32768
SF            300.1300129 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

bzhm02023-1

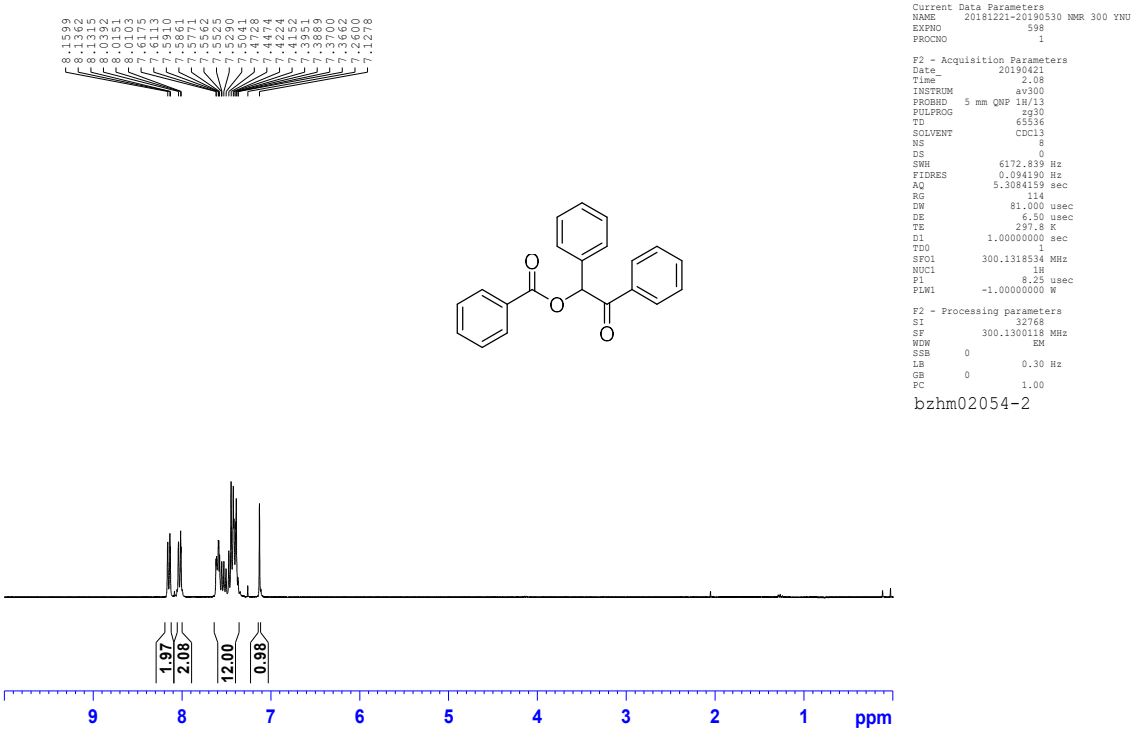
^{13}C-NMR (125 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20210914-2 c nmr
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210914
Time               19.35 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   159
DS                     4
SWH            29761.904 Hz
FIDRES             0.908261 Hz
AQ              1.1010048 sec
RG                 190.79
DW                16.800 usec
DE                 6.50 usec
TE                298.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          125.7703643 MHz
NUC1                  13C
P1                10.00 usec
PLW1          96.79299927 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          24.22500038 W
PLW12          0.37852001 W
PLW13          0.19039001 W

F2 - Processing parameters
SI                 32768
SF            125.7577885 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

HM02023-1

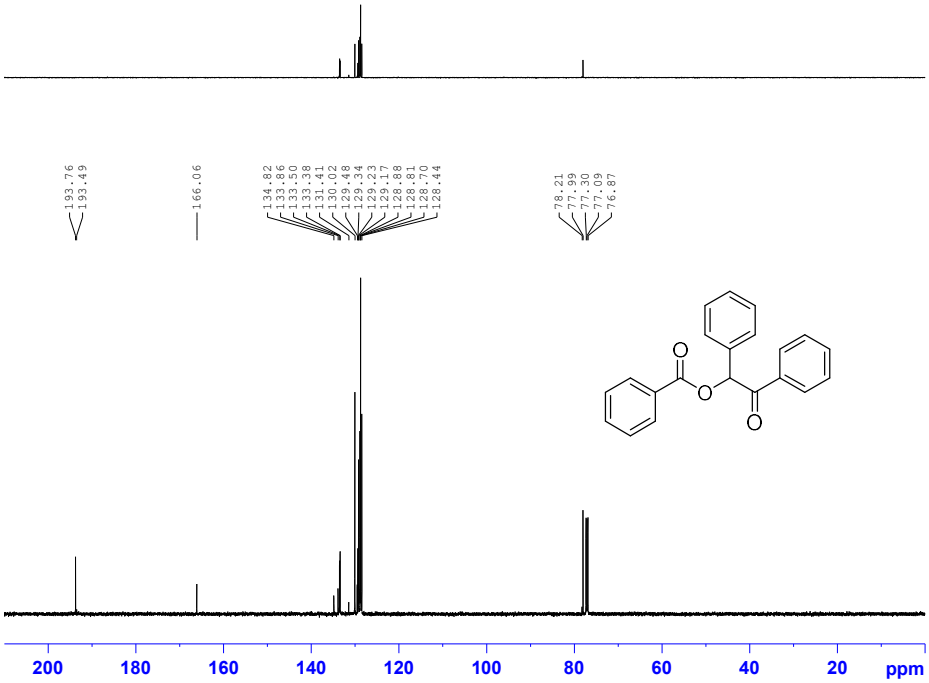
^{1}H-NMR (300 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20181221-20190530 NMR 300 YNU
EXPNO                598
PROCNO                 1

F2 - Acquisition Parameters
Date_              20190421
Time                  2.08
INSTRUM             av300
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             6172.839 Hz
FIDRES             0.094190 Hz
AQ                5.3084159 sec
RG                   114
DW                  81.000 usec
DE                   6.50 usec
TE                  297.8 K
D1             1.00000000 sec
TD0                    1
SFO1           300.1318534 MHz
NUC1                  1H
P1                   8.25 usec
PLW1          -1.00000000 W

F2 - Processing parameters
SI                 32768
SF             300.1300118 MHz
WDW                   EM
SSB        0
LB                  0.30 Hz
GB         0
PC                  1.00
```

bzhm02054-2

^{13}C-NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20190429 500
NMR YNU huang rong
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_              20190423
Time                 17.22 h
PROBHD    Z114607_0222 (
TD                 65536
SOLVENT            CDCl3
NS                    71
DS                     4
RG                188.35
D1             2.00000000 sec
D11            0.03000000 sec
DS                     4
NS                    71
TD0                    1
SFO1          150.9279578 MHz
NUC1                  13C
P1                  12.00 usec
PLW1           97.67099762 W
SFO2          600.1724007 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2           26.09399986 W
PLW12           0.40399119 W
PLW13           0.20248041 W

F2 - Processing parameters
SI                 32768
SF            150.9128665 MHz
WDW                   EM
SSB        0
LB                  1.00 Hz
GB         0
PC                  1.40
```

hm02054-2

5. DFT calculations

DFT calculations of geometries and energies for all optimized starting materials, transition states, intermediates, and target materials

Single Point Energy■,Δ (*E*M06, in Hartree)

Zero-point correction (*E*0, in Hartree)

Thermal correction to Enthalpy (*H*, in Hartree)

Thermal correction to Gibbs Free Energy (*G*, in Hartree)

Sum of electronic and zero-point Energies (*E*M06+*E*0, in Hartree)

Sum of electronic and thermal Enthalpies (*E*M06+*H*, in Hartree)

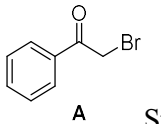
Sum of electronic and thermal Free Energies (*E*M06+*G*, in Hartree)

■ The single-point energies and solvent effects were computed at the M06-2X/def2-TZVP level

Δ The single-point energies and solvent effects were computed at the M06-2X/def2-TZVP level

Methods: Gaussian program[1] was employed for DFT calculations, and /M06-2X/def2-SVP level was used for geometry optimization and frequency calculations. Frequency calculations were performed to ensure minimums were found. The single point calculations were at M06-2X/def2-TZVP level. The SMD implicit solvent model was used to take account of the solvation effect of water.

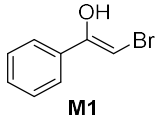
Standard orientation, imaginary frequencies, thermodynamic energies and single-point energies of all stationary points.



A Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.477831	0.473945	-0.603946
2	6	0	2.216356	1.059673	-0.596556
3	6	0	1.161980	0.462069	0.107441
4	6	0	1.386682	-0.731240	0.807521
5	6	0	2.652080	-1.313692	0.801778
6	6	0	3.696379	-0.714386	0.096494
7	1	0	4.293591	0.943344	-1.155489
8	1	0	2.029960	1.988462	-1.137252
9	1	0	0.582517	-1.220107	1.358698
10	1	0	2.822820	-2.241578	1.349077
11	1	0	4.685361	-1.175566	0.093374
12	6	0	-0.164554	1.150706	0.085211
13	8	0	-0.304659	2.230759	-0.448910
14	6	0	-1.365758	0.482951	0.747584
15	1	0	-1.072326	-0.004179	1.683600
16	1	0	-2.837531	1.874794	-0.005544
17	35	0	-1.876653	-0.997663	-0.456167

Zero-point correction= 0.158338 (Hartree/Particle)
Thermal correction to Energy= 0.168492
Thermal correction to Enthalpy= 0.169436
Thermal correction to Gibbs Free Energy= 0.121014
Sum of electronic and zero-point Energies= -2996.844625
Sum of electronic and thermal Energies= -2996.834471
Sum of electronic and thermal Enthalpies= -2996.833526
Sum of electronic and thermal Free Energies= -2996.881948

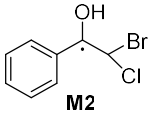


M1 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.314048	0.402462	0.770108
2	6	0	-2.076094	1.036908	0.682278
3	6	0	-1.051173	0.516807	-0.120272
4	6	0	-1.315172	-0.635516	-0.871832
5	6	0	-2.560177	-1.262260	-0.803063
6	6	0	-3.560971	-0.752347	0.025408

7	1	0	-4.092316	0.814535	1.415403
8	1	0	-1.890818	1.957329	1.239385
9	1	0	-0.540712	-1.039218	-1.525413
10	1	0	-2.752339	-2.152587	-1.405106
11	1	0	-4.531839	-1.247712	0.083523
12	6	0	0.234775	1.305531	-0.214340
13	8	0	0.081705	2.579779	-0.355365
14	6	0	1.470024	0.703673	-0.138001
15	1	0	3.327102	1.420310	0.730437
16	35	0	1.724777	-1.161371	0.258375

Zero-point correction= 0.144446 (Hartree/Particle)
Thermal correction to Energy= 0.154671
Thermal correction to Enthalpy= 0.155615
Thermal correction to Gibbs Free Energy= 0.107180
Sum of electronic and zero-point Energies= -2996.354856
Sum of electronic and thermal Energies= -2996.344632
Sum of electronic and thermal Enthalpies= -2996.343687
Sum of electronic and thermal Free Energies= -2996.392122



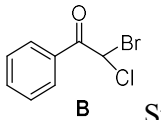
M2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.770588	0.507551	0.394721
2	6	0	-2.524209	1.118025	0.449323
3	6	0	-1.356451	0.421308	0.059615
4	6	0	-1.494624	-0.918263	-0.372121
5	6	0	-2.748090	-1.517742	-0.421302
6	6	0	-3.893524	-0.813850	-0.042647
7	1	0	-4.656736	1.069669	0.694514
8	1	0	-2.442383	2.149598	0.789414
9	1	0	-0.620346	-1.499231	-0.659527
10	1	0	-2.829821	-2.552792	-0.757192
11	1	0	-4.873214	-1.291519	-0.088032
12	6	0	-0.083291	1.099442	0.140344
13	8	0	-0.093839	2.262659	0.819996
14	6	0	1.213461	0.580414	-0.327558
15	1	0	2.531673	1.880732	0.786639
16	35	0	1.781935	-1.017847	0.853783
17	17	0	1.113806	-0.047508	-2.010481
18	1	0	0.727293	2.764506	0.705623

Zero-point correction= 0.159406 (Hartree/Particle)
Thermal correction to Energy= 0.171064
Thermal correction to Enthalpy= 0.172008
Thermal correction to Gibbs Free Energy= 0.119970
Sum of electronic and zero-point Energies= -3456.848267

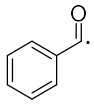
Sum of electronic and thermal Energies= -3456.836610
Sum of electronic and thermal Enthalpies= -3456.835665
Sum of electronic and thermal Free Energies= -3456.887703



B Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.734925	0.541684	-0.446020
2	6	0	2.471421	1.110777	-0.561949
3	6	0	1.334047	0.423522	-0.111416
4	6	0	1.484321	-0.850873	0.457653
5	6	0	2.750966	-1.418871	0.567902
6	6	0	3.876073	-0.726707	0.118929
7	1	0	4.611602	1.088277	-0.795938
8	1	0	2.350296	2.099982	-1.004014
9	1	0	0.625273	-1.413457	0.817489
10	1	0	2.858072	-2.410755	1.008729
11	1	0	4.865834	-1.176853	0.212251
12	6	0	0.027958	1.131216	-0.295224
13	8	0	-0.032914	2.190976	-0.873373
14	6	0	-1.307517	0.558299	0.240822
15	1	0	-2.578922	1.752603	-1.016692
16	35	0	-1.684477	-1.085288	-0.775285
17	17	0	-1.140351	0.191141	1.985596

Zero-point correction= 0.148703 (Hartree/Particle)
Thermal correction to Energy= 0.159929
Thermal correction to Enthalpy= 0.160873
Thermal correction to Gibbs Free Energy= 0.109728
Sum of electronic and zero-point Energies= -3456.292158
Sum of electronic and thermal Energies= -3456.280932
Sum of electronic and thermal Enthalpies= -3456.279988
Sum of electronic and thermal Free Energies= -3456.331133

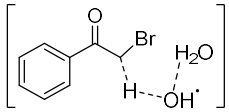


M3 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.268769	1.335045	0.000000
2	6	0	-0.099907	1.090144	0.000000
3	6	0	-0.559554	-0.236145	0.000000

4	6	0	0.339201	-1.307527	0.000000
5	6	0	1.708961	-1.053284	0.000000
6	6	0	2.169174	0.264600	0.000000
7	1	0	1.639817	2.360909	0.000000
8	1	0	-0.820719	1.909923	0.000000
9	1	0	-0.045636	-2.329075	0.000000
10	1	0	2.418163	-1.881793	0.000000
11	1	0	3.242583	0.461764	0.000000
12	6	0	-2.009494	-0.512125	0.000000
13	8	0	-2.917138	0.249253	0.000000

Zero-point correction= 0.098664 (Hartree/Particle)
Thermal correction to Energy= 0.104923
Thermal correction to Enthalpy= 0.105867
Thermal correction to Gibbs Free Energy= 0.067472
Sum of electronic and zero-point Energies= -344.419147
Sum of electronic and thermal Energies= -344.412888
Sum of electronic and thermal Enthalpies= -344.411944
Sum of electronic and thermal Free Energies= -344.450339

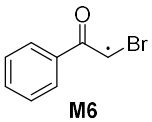


M5 (HAT)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.022685	0.239000	-0.081796
2	6	0	2.868538	0.987589	0.122419
3	6	0	1.630803	0.347160	0.275742
4	6	0	1.561660	-1.052141	0.229858
5	6	0	2.721113	-1.798319	0.032063
6	6	0	3.949031	-1.155053	-0.127056
7	1	0	4.982990	0.741014	-0.206911
8	1	0	2.910017	2.076866	0.162353
9	1	0	0.612827	-1.572582	0.361765
10	1	0	2.664479	-2.886973	0.001896
11	1	0	4.854576	-1.742526	-0.287431
12	6	0	0.434118	1.204535	0.510924
13	8	0	0.532490	2.390475	0.738407
14	6	0	-0.966038	0.594347	0.464091
15	1	0	-0.968770	-0.407169	1.058319
17	1	0	-2.119161	2.415108	0.407857
18	35	0	-1.325426	0.019271	-1.366053
19	1	0	-3.120705	-1.447253	1.065315
20	8	0	-3.953998	-1.280848	0.590234
21	1	0	-3.665425	-1.164141	-0.324179
22	8	0	-1.384511	-1.539974	1.842401
23	1	0	-1.479612	-1.072615	2.698958

Zero-point correction= 0.189710 (Hartree/Particle)
Thermal correction to Energy= 0.205051
Thermal correction to Enthalpy= 0.205996
Thermal correction to Gibbs Free Energy= 0.145352
Sum of electronic and zero-point Energies= -3148.800360
Sum of electronic and thermal Energies= -3148.785019
Sum of electronic and thermal Enthalpies= -3148.784075
Sum of electronic and thermal Free Energies= -3148.844718

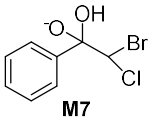


M6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.747070	0.328701	-0.458234
2	6	0	2.497608	0.923816	-0.602798
3	6	0	1.332552	0.322735	-0.100439
4	6	0	1.463420	-0.907264	0.551520
5	6	0	2.716133	-1.516189	0.689937
6	6	0	3.862309	-0.903578	0.191035
7	1	0	4.635696	0.824639	-0.853891
8	1	0	2.405393	1.880098	-1.121578
9	1	0	0.593298	-1.413662	0.963582
10	1	0	2.789095	-2.480186	1.197572
11	1	0	4.838031	-1.379370	0.305589
12	6	0	0.029506	1.120545	-0.387957
13	8	0	-0.116414	1.420920	-1.652831
14	6	0	-1.300674	0.455608	0.188597
15	1	0	-2.576315	1.495622	-1.169925
16	35	0	-1.642292	-1.290724	-0.675001
17	1	0	-0.237109	3.003167	-0.119938

Zero-point correction= 0.162515 (Hartree/Particle)
Thermal correction to Energy= 0.174932
Thermal correction to Enthalpy= 0.175876
Thermal correction to Gibbs Free Energy= 0.123156
Sum of electronic and zero-point Energies= -3532.140751
Sum of electronic and thermal Energies= -3532.128334
Sum of electronic and thermal Enthalpies= -3532.127390
Sum of electronic and thermal Free Energies= -3532.180110



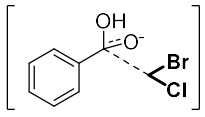
M7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.817764	0.161236	-0.506764
2	6	0	2.620738	0.809102	-0.807358
3	6	0	1.406613	0.327389	-0.303283
4	6	0	1.397532	-0.833932	0.481414
5	6	0	2.594823	-1.488948	0.766154
6	6	0	3.805959	-0.990326	0.281414
7	1	0	4.760869	0.551978	-0.892727
8	1	0	2.619333	1.701898	-1.435454
9	1	0	0.440641	-1.231384	0.825504
10	1	0	2.583479	-2.399638	1.367818
11	1	0	4.740407	-1.504407	0.513466
12	6	0	0.150926	1.047223	-0.702989
13	8	0	0.065962	1.513644	-1.851842
14	8	0	-0.935540	1.234271	0.219487
15	6	0	-2.160656	1.978250	-0.169521
16	1	0	-3.024937	1.595600	0.387067
17	35	0	-2.085973	-1.354491	-0.372140
18	17	0	-0.672811	1.071525	1.924610

Zero-point correction= 0.146112 (Hartree/Particle)
Thermal correction to Energy= 0.158464
Thermal correction to Enthalpy= 0.159409
Thermal correction to Gibbs Free Energy= 0.104463
Sum of electronic and zero-point Energies= -3456.412566
Sum of electronic and thermal Energies= -3456.400214
Sum of electronic and thermal Enthalpies= -3456.399270
Sum of electronic and thermal Free Energies= -3456.454215



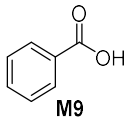
M8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.722365	-0.484265	1.438456
2	6	0	1.979743	0.618060	1.014177
3	6	0	1.507173	0.678216	-0.300966
4	6	0	1.796338	-0.363640	-1.188749
5	6	0	2.533710	-1.462564	-0.762599
6	6	0	2.998493	-1.525948	0.553396
7	1	0	3.094466	-0.523231	2.463646
8	1	0	1.790634	1.436705	1.710272
9	1	0	1.421576	-0.306791	-2.211593
10	1	0	2.746885	-2.276849	-1.457264
11	1	0	3.580690	-2.387043	0.886677
12	6	0	0.760494	1.863931	-0.817802
13	8	0	0.731963	2.156957	-1.996969
14	8	0	-1.448309	0.407560	-0.131736

15	1	0	-3.670082	0.326740	0.067041
16	1	0	-2.949629	1.907285	-0.359084
17	35	0	-1.382322	-1.602437	-0.299041
18	17	0	-1.343102	0.734201	1.736445
19	6	0	0.301989	2.750860	0.087865

Zero-point correction= 0.159869 (Hartree/Particle)
Thermal correction to Energy= 0.172875
Thermal correction to Enthalpy= 0.173819
Thermal correction to Gibbs Free Energy= 0.117823
Sum of electronic and zero-point Energies= -3532.108983
Sum of electronic and thermal Energies= -3532.095977
Sum of electronic and thermal Enthalpies= -3532.095032
Sum of electronic and thermal Free Energies= -3532.151028



M9 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836728	1.235735	-0.000052
2	6	0	-0.444006	1.202843	-0.000095
3	6	0	0.219012	-0.029527	-0.000028
4	6	0	-0.510420	-1.223463	0.000080
5	6	0	-1.901906	-1.185179	0.000053
6	6	0	-2.564079	0.044276	0.000023
7	1	0	-2.357900	2.193929	-0.000099
8	1	0	0.129471	2.129877	-0.000189
9	1	0	0.024348	-2.174279	0.000082
10	1	0	-2.473239	-2.114387	0.000078
11	1	0	-3.654928	0.073785	0.000035
12	6	0	1.706541	-0.114259	-0.000007
13	8	0	2.325716	-1.154471	-0.000152
14	8	0	2.305835	1.075773	0.000179
15	1	0	3.269360	0.938091	0.000038

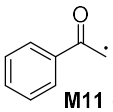
Zero-point correction= 0.116781 (Hartree/Particle)
Thermal correction to Energy= 0.123817
Thermal correction to Enthalpy= 0.124761
Thermal correction to Gibbs Free Energy= 0.084814
Sum of electronic and zero-point Energies= -420.236407
Sum of electronic and thermal Energies= -420.229371
Sum of electronic and thermal Enthalpies= -420.228427
Sum of electronic and thermal Free Energies= -420.268375

$^{\bullet}$CHBrCl

M10 Standard orientation:

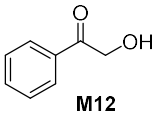
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.586512	0.416229	0.443946
2	1	0	-0.166776	2.502954	0.211111
3	35	0	1.219050	-0.174563	-0.031444
4	17	0	-1.781906	-0.805118	-0.074563

Zero-point correction= 0.057215 (Hartree/Particle)
Thermal correction to Energy= 0.062156
Thermal correction to Enthalpy= 0.063100
Thermal correction to Gibbs Free Energy= 0.027507
Sum of electronic and zero-point Energies= -3112.390793
Sum of electronic and thermal Energies= -3112.385852
Sum of electronic and thermal Enthalpies= -3112.384908
Sum of electronic and thermal Free Energies= -3112.420501


M11 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.482951	1.010446	0.080407
2	6	0	1.103742	1.195457	0.062222
3	6	0	0.237213	0.096121	-0.010039
4	6	0	0.778390	-1.195310	-0.073254
5	6	0	2.160527	-1.379069	-0.059825
6	6	0	3.014823	-0.279235	0.019661
7	1	0	3.147192	1.874020	0.139999
8	1	0	0.679347	2.199030	0.106722
9	1	0	0.131879	-2.070312	-0.143690
10	1	0	2.570371	-2.388746	-0.113939
11	1	0	4.095922	-0.427208	0.032258
12	6	0	-1.239451	0.371430	-0.032934
13	8	0	-1.641993	1.537839	-0.149381
14	6	0	-2.173775	-0.716608	0.094845
15	1	0	-4.088685	-1.114305	-0.742138
16	1	0	-4.099094	-0.831619	0.993861

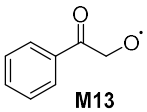
Zero-point correction= 0.154471 (Hartree/Particle)
Thermal correction to Energy= 0.163555
Thermal correction to Enthalpy= 0.164499
Thermal correction to Gibbs Free Energy= 0.118696
Sum of electronic and zero-point Energies= -422.906952
Sum of electronic and thermal Energies= -422.897868
Sum of electronic and thermal Enthalpies= -422.896924
Sum of electronic and thermal Free Energies= -422.942727



M12 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.768014	-0.935258	0.301830
2	6	0	1.407795	-1.221217	0.253424
3	6	0	0.488006	-0.221999	-0.094073
4	6	0	0.946084	1.066721	-0.400256
5	6	0	2.310238	1.348553	-0.355633
6	6	0	3.219891	0.350680	-0.004618
7	1	0	3.479525	-1.715069	0.576709
8	1	0	1.039210	-2.221004	0.487083
9	1	0	0.248408	1.856233	-0.682401
10	1	0	2.663962	2.351171	-0.599100
11	1	0	4.287367	0.574846	0.029572
12	6	0	-0.956574	-0.584801	-0.144550
13	8	0	-1.321710	-1.743130	-0.061382
14	6	0	-2.020346	0.503887	-0.241876
15	1	0	-1.180758	1.756890	1.348601
17	1	0	-1.741921	1.211279	-1.037504
18	8	0	-3.252258	-0.081400	-0.590790
19	1	0	-3.208898	-1.003515	-0.287366

Zero-point correction= 0.172953 (Hartree/Particle)
Thermal correction to Energy= 0.183003
Thermal correction to Enthalpy= 0.183948
Thermal correction to Gibbs Free Energy= 0.137052
Sum of electronic and zero-point Energies= -498.678195
Sum of electronic and thermal Energies= -498.668145
Sum of electronic and thermal Enthalpies= -498.667201
Sum of electronic and thermal Free Energies= -498.714097

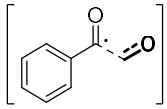


M13 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.727771	-0.915925	0.295505
2	6	0	1.371466	-1.216720	0.235887
3	6	0	0.441799	-0.224236	-0.106365
4	6	0	0.886520	1.073394	-0.392975
5	6	0	2.247115	1.369591	-0.335272
6	6	0	3.166707	0.378580	0.008283
7	1	0	3.445747	-1.691525	0.565329

8	1	0	1.013149	-2.222856	0.456946
9	1	0	0.185990	1.862686	-0.667392
10	1	0	2.589586	2.379761	-0.562785
11	1	0	4.231169	0.614838	0.052099
12	6	0	-0.996347	-0.627213	-0.152141
13	8	0	-1.339301	-1.783370	-0.062348
14	6	0	-2.056126	0.497056	-0.249917
15	1	0	-1.262850	1.647288	1.425094
16	1	0	-1.713144	1.210912	-1.019111
17	8	0	-3.231446	-0.103869	-0.654252

Zero-point correction= 0.156890 (Hartree/Particle)
Thermal correction to Energy= 0.166511
Thermal correction to Enthalpy= 0.167455
Thermal correction to Gibbs Free Energy= 0.120704
Sum of electronic and zero-point Energies= -498.009657
Sum of electronic and thermal Energies= -498.000036
Sum of electronic and thermal Enthalpies= -497.999092
Sum of electronic and thermal Free Energies= -498.045843

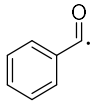


M14 (Bz-release) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.860358	0.823331	0.229428
2	6	0	-1.531293	1.227069	0.191495
3	6	0	-0.528181	0.284247	-0.089122
4	6	0	-0.856454	-1.054266	-0.334627
5	6	0	-2.191523	-1.446918	-0.296085
6	6	0	-3.189088	-0.512718	-0.013418
7	1	0	-3.643444	1.550557	0.447014
8	1	0	-1.254137	2.265419	0.379495
9	1	0	-0.084310	-1.791259	-0.553960
10	1	0	-2.452573	-2.488110	-0.487496
11	1	0	-4.233170	-0.828400	0.016557
12	6	0	0.860896	0.788410	-0.102602
13	8	0	1.257838	1.887884	0.025122
14	6	0	2.347758	-0.578878	-0.307445
15	8	0	3.322641	0.096718	-0.698529

Zero-point correction= 0.156743 (Hartree/Particle)
Thermal correction to Energy= 0.166729
Thermal correction to Enthalpy= 0.167673
Thermal correction to Gibbs Free Energy= 0.119904
Sum of electronic and zero-point Energies= -498.000007
Sum of electronic and thermal Energies= -497.990021
Sum of electronic and thermal Enthalpies= -497.989077

Sum of electronic and thermal Free Energies= -498.036846



M15 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.828668	1.208071	0.000045
2	6	0	0.433854	1.205681	0.000043
3	6	0	-0.275007	0.000017	-0.000001
4	6	0	0.434033	-1.205725	-0.000047
5	6	0	1.828676	-1.208057	-0.000051
6	6	0	2.528595	0.000084	-0.000002
7	1	0	2.373521	2.153947	0.000082
8	1	0	-0.122960	2.143679	0.000072
9	1	0	-0.122914	-2.143659	-0.000083
10	1	0	2.373675	-2.153850	-0.000091
11	1	0	3.620084	0.000172	-0.000002
12	6	0	-1.805690	-0.000122	0.000001
13	8	0	-2.372419	-1.116446	-0.000010

Zero-point correction= 0.104108 (Hartree/Particle)
Thermal correction to Energy= 0.110869
Thermal correction to Enthalpy= 0.111813
Thermal correction to Gibbs Free Energy= 0.072283
Sum of electronic and zero-point Energies= -419.781501
Sum of electronic and thermal Energies= -419.774739
Sum of electronic and thermal Enthalpies= -419.773795
Sum of electronic and thermal Free Energies= -419.813326

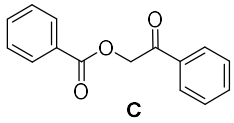
C1 (HCHO)

M16 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160175	-0.151889	-0.000023
2	1	0	1.695389	0.227765	0.883543
3	1	0	1.144703	-1.248338	-0.000142
4	8	0	-1.230589	-0.274916	-0.000004

Zero-point correction= 0.055942 (Hartree/Particle)
Thermal correction to Energy= 0.059782
Thermal correction to Enthalpy= 0.060726
Thermal correction to Gibbs Free Energy= 0.031099
Sum of electronic and zero-point Energies= -153.586213
Sum of electronic and thermal Energies= -153.582372

Sum of electronic and thermal Enthalpies= -153.581428
Sum of electronic and thermal Free Energies= -153.611055



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.795722	2.482452	0.871441
2	6	0	-2.758426	1.092882	0.925799
3	6	0	-2.138604	0.364396	-0.097781
4	6	0	-1.566926	1.038470	-1.185154
5	6	0	-1.618619	2.430396	-1.242180
6	6	0	-2.225690	3.152065	-0.213951
7	1	0	-3.271368	3.046158	1.675301
8	1	0	-3.203222	0.555531	1.764968
9	1	0	-1.090401	0.484495	-1.995138
10	1	0	-1.179976	2.953236	-2.093156
11	1	0	-2.255609	4.241983	-0.258255
12	6	0	-2.134125	-1.126235	0.014462
13	8	0	-2.944068	-1.709001	0.702632
14	6	0	-1.118057	-1.927138	-0.806506
15	1	0	-1.994880	-3.859602	-0.494536
16	8	0	0.167696	-1.290977	-0.826536
17	6	0	0.704246	-0.924656	0.339271
18	8	0	0.144638	-1.098368	1.399325
19	6	0	2.032899	-0.272742	0.191049
20	6	0	2.694366	0.136945	1.354233
21	6	0	2.615035	-0.062212	-1.064732
22	6	0	3.937884	0.755070	1.262434
23	1	0	2.225139	-0.033967	2.324163
24	6	0	3.859243	0.557888	-1.150292
25	1	0	2.094782	-0.382216	-1.967497
26	6	0	4.519288	0.965585	0.010257
27	1	0	4.456362	1.073669	2.167662
28	1	0	4.316346	0.723210	-2.126880
29	1	0	5.494395	1.450202	-0.062535
30	1	0	-1.452407	-1.870301	-1.853529

Zero-point correction= 0.265010 (Hartree/Particle)
Thermal correction to Energy= 0.281091
Thermal correction to Enthalpy= 0.282035
Thermal correction to Gibbs Free Energy= 0.218970
Sum of electronic and zero-point Energies= -842.601794
Sum of electronic and thermal Energies= -842.585713
Sum of electronic and thermal Enthalpies= -842.584769
Sum of electronic and thermal Free Energies= -842.647834

OH_radical_H_2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.456857	-0.170539	0.007052
2	8	0	-1.424601	-0.095257	-0.018258
3	1	0	-1.567166	0.847908	0.132849
4	8	0	1.486171	-0.098205	0.016871
5	1	0	1.531460	0.870324	-0.128803

Zero-point correction= 0.032580 (Hartree/Particle)
Thermal correction to Energy= 0.037921
Thermal correction to Enthalpy= 0.038865
Thermal correction to Gibbs Free Energy= 0.006091
Sum of electronic and zero-point Energies= -151.951522
Sum of electronic and thermal Energies= -151.946181
Sum of electronic and thermal Enthalpies= -151.945237
Sum of electronic and thermal Free Energies= -151.978012

OH_anion_H_2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.115645	-0.118459	0.012077
2	8	0	-1.214742	-0.078865	0.068666
3	1	0	-1.402224	0.684168	-0.490767
4	8	0	1.232769	-0.079565	-0.068811
5	1	0	1.373658	0.701728	0.479846

Zero-point correction= 0.031760 (Hartree/Particle)
Thermal correction to Energy= 0.035780
Thermal correction to Enthalpy= 0.036724
Thermal correction to Gibbs Free Energy= 0.008021
Sum of electronic and zero-point Energies= -152.136076
Sum of electronic and thermal Energies= -152.132056
Sum of electronic and thermal Enthalpies= -152.131112
Sum of electronic and thermal Free Energies= -152.159815

H_2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.753364	-0.483677	0.000000
2	8	0	0.000000	0.120916	0.000000
3	1	0	-0.753364	-0.483653	0.000000

Zero-point correction= 0.021290 (Hartree/Particle)
Thermal correction to Energy= 0.024126
Thermal correction to Enthalpy= 0.025070
Thermal correction to Gibbs Free Energy= 0.002972
Sum of electronic and zero-point Energies= -76.314093
Sum of electronic and thermal Energies= -76.311257
Sum of electronic and thermal Enthalpies= -76.310313
Sum of electronic and thermal Free Energies= -76.332411

H, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.000000

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -0.496666
Sum of electronic and thermal Energies= -0.495249
Sum of electronic and thermal Enthalpies= -0.494305
Sum of electronic and thermal Free Energies= -0.507320

H_2, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.376835
2	1	0	0.000000	0.000000	-0.376835

Zero-point correction= 0.010244 (Hartree/Particle)
Thermal correction to Energy= 0.012604
Thermal correction to Enthalpy= 0.013548
Thermal correction to Gibbs Free Energy= -0.001271
Sum of electronic and zero-point Energies= -1.153268
Sum of electronic and thermal Energies= -1.150907
Sum of electronic and thermal Enthalpies= -1.149963
Sum of electronic and thermal Free Energies= -1.164782

Cl radical H2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.275059	0.004703	-0.000004
2	1	0	1.296455	-0.214622	0.000224

3	8	0	2.254618	-0.091964	-0.000025
4	1	0	2.342604	0.870378	0.000034

Zero-point correction= 0.023422 (Hartree/Particle)
Thermal correction to Energy= 0.027696
Thermal correction to Enthalpy= 0.028640
Thermal correction to Gibbs Free Energy= -0.003139
Sum of electronic and zero-point Energies= -536.290007
Sum of electronic and thermal Energies= -536.285733
Sum of electronic and thermal Enthalpies= -536.284789
Sum of electronic and thermal Free Energies= -536.316568

Cl H_2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.085588	0.005320	0.000000
2	1	0	0.935006	-0.136464	0.000000
3	8	0	1.928785	-0.100678	0.000000
4	1	0	2.089715	0.851440	0.000000

Zero-point correction= 0.022866 (Hartree/Particle)
Thermal correction to Energy= 0.026690
Thermal correction to Enthalpy= 0.027634
Thermal correction to Gibbs Free Energy= -0.001793
Sum of electronic and zero-point Energies= -536.510141
Sum of electronic and thermal Energies= -536.506317
Sum of electronic and thermal Enthalpies= -536.505373
Sum of electronic and thermal Free Energies= -536.534800

Br radical H2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.457141	2.099482	0.000000
2	8	0	0.026562	2.934687	0.000000
3	1	0	-0.685037	3.588904	0.000000
4	35	0	0.026562	-0.833311	0.000000

Zero-point correction= 0.022545 (Hartree/Particle)
Thermal correction to Energy= 0.027287
Thermal correction to Enthalpy= 0.028231
Thermal correction to Gibbs Free Energy= -0.006056
Sum of electronic and zero-point Energies= -2650.156221
Sum of electronic and thermal Energies= -2650.151478
Sum of electronic and thermal Enthalpies= -2650.150534
Sum of electronic and thermal Free Energies= -2650.184822

Br H_2O, Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.523403	-0.178407	0.000036
2	8	0	2.509309	-0.096174	-0.000004
3	1	0	2.618981	0.863277	0.000004
4	35	0	-0.691910	0.002415	0.000000

Zero-point correction= 0.023125 (Hartree/Particle)
Thermal correction to Energy= 0.026993
Thermal correction to Enthalpy= 0.027937
Thermal correction to Gibbs Free Energy= -0.002794
Sum of electronic and zero-point Energies= -2650.361806
Sum of electronic and thermal Energies= -2650.357938
Sum of electronic and thermal Enthalpies= -2650.356994
Sum of electronic and thermal Free Energies= -2650.387725