CHEMISTRY
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Supporting Information

4-Methyltetrahydropyran (4-MeTHP): Application as an Organic Reaction Solvent

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asia_201901169_sm_miscellaneous_information.pdf

1. A price list of commercially available solvents

Table S1. Price of commercially available solvents[a]

Supplier	Solvent	Grade	Content	Price	
				JPY	USD
Sigma-Aldrich[b]	4-MeTHP	- (unavailable)	-	-	-
	THP	99% (anhydrous)	100 mL	22,400	178.00
	CPME	≧99.90%[e] (ReagentPlus®)	500 mL	11,100	82.40
	2-MeTHF	≧99.5%[e] (ReagentPlus®)	500 mL	20,600	143.00
	THF	≧99.0%[e] (ACS reagent)	500 mL	10,600	84.90
TCI[c]	4-MeTHP	> 99.0% (GC)[e]	500 mL	3,500	-
	THP	> 98.0% (GC)	500 mL	22,300	126.00
	CPME	> 99.5% (GC)[e]	500 mL	3,600	33.00
	2-MeTHF	> 98.0% (GC)[e]	500 mL	10,900	70.00
	THF	> 99.5% (GC)[e]	500 mL	3,100	24.00
Fujifilm Wako[d]	4-MeTHP	> 99.0% (Capillary GC)[e]	500 mL	3,500	39.00
	THP	> 98.0% (Capillary GC)	500 mL	35,000	385.00
	CPME	> 98.0% (Capillary GC)[e]	500 mL	3,600	40.00
	2-MeTHF	> 98.0% (Capillary GC)[e]	500 mL	18,000	198.00
	THF	> 99.5% (Capillary GC)	500 mL	1,950	22.00

[a] The data were collected on September 11, 2019. A safety data sheet (SDS) of solvent is available from the supplier's web page.
[b] https://www.sigmaaldrich.com/united-states.html https://www.sigmaaldrich.com/japan.html
[c] https://www.tcichemicals.com/en/us/index.html https://www.tcichemicals.com/en/jp/index.html
[d] https://labchem-wako.fujifilm.com/us/index.html https://labchem-wako.fujifilm.com/jp/index.html
[e] Stabilized with BHT.

2. Solvent recovery experiments and GC-MS analyses

2.1. Analytical conditions

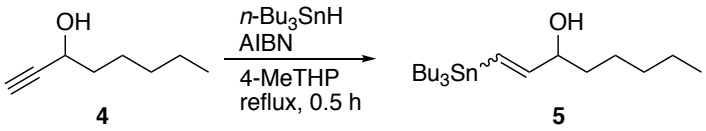
GC conditions

Gas-phase chromatography was performed on a GC-2014 instrument using a DB-WAX column (30 m × 0.25 mm × 0.25 μm film thickness). A temperature of FID detector was adjusted to 250 °C. The oven was heated at 50 °C for 5 min followed by a temperature gradient of 10 °C/min to 200 °C and, finally, at 200 °C for 5 min. Inlet temperature and pressure were 200 °C and 83 kPa, respectively, with a split ratio of 100:1. Helium was used as the carrier gas at a flow rate of 1.0 mL/min.

GC-MS conditions

The gas chromatograph-mass spectrometry model GCMS-QP2010 Ultra (SHIMADZU CORPORATON, Japan), equipped with DB-WAX capillary column with dimensions 30 m × 0.25 mm × 0.25 μm, was used. The oven was maintained at 50 °C for 5 min followed by a temperature gradient of 10 °C/min to 200 °C and, finally, at 200 °C for 5 min. The injection volume of the sample was 0.2 μL with a split ratio of 100:1, using helium as the carrier gas at a flow rate of 1.0 ml/min. Injector temperature was maintained at 200°C. Detector temperature was maintained at 230 °C. The percentage composition was calculated using peak normalization method assuming equal detector response. The samples were analyzed with an electron impact ionization at 70 eV. The compounds separated were characterized from their mass spectral data using the NIST14 mass spectral library.

2.2. Radical addition in 4-MeTHP

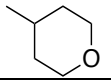


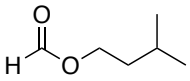
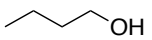
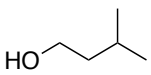
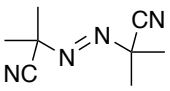
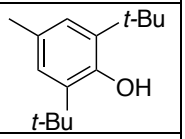
4 **5**

Experimental procedure

Commercially available 4-MeTHP (stabilized with BHT) was stored with molecular sieves 4Å and used for the reaction (sample 1). Oct-1-yn-3-ol (**4**) (126 mg, 0.996 mmol), *n*-Bu_3SnH (378 mg, 1.30 mmol), and AIBN (32.8 mg, 0.200 mmol) were placed in a 100 mL two-necked round bottom flask equipped with a reflux condenser. The flask was flushed with argon and 4-MeTHP (20 mL) was added. After complete dissolution of AIBN at room temperature, the solution was heated at reflux for 30 min. The solution was stood at room temperature and, after attachment of the distillation apparatus, the solvent was distillated under reduced pressure (bp 38-40 °C/8-10 kPa) (sample 2). The residual oil was purified by flash chromatography on silica gel (*n*-hexane/EtOAc/Et_3N = 50/1/0.5) to give stannane **5** (288 mg, 0.691 mmol, 69%, *E*/*Z*=16:1) as a pale yellow oil. The purity of the recovered 4-MeTHP was determined to be 99.94% by the GC analysis. The same experiment was performed with the recovered 4-MeTHP, providing the product **5** (64% yield, *E*/*Z*=8:1) with a recovery of 4-MeTHP (purity: 99.88%) (sample 3).

Compound characterization list analyzed by GC-MS[a]

t (min)	2.2	2.5	2.9	3.6	4.1	4.5
name	acetone[b]	unknown	unknown	4-MeTHP	isobutyronitrile	unknown
structure						
#					**A**	
sample 1	-	0.03%	0.19%	99.21%	-	0.05%
sample 2	0.01%	0.06%	0.15%	98.54%	0.37%	0.05%
sample 3	0.02%	0.14%	0.13%	98.20%	0.62%	0.05%

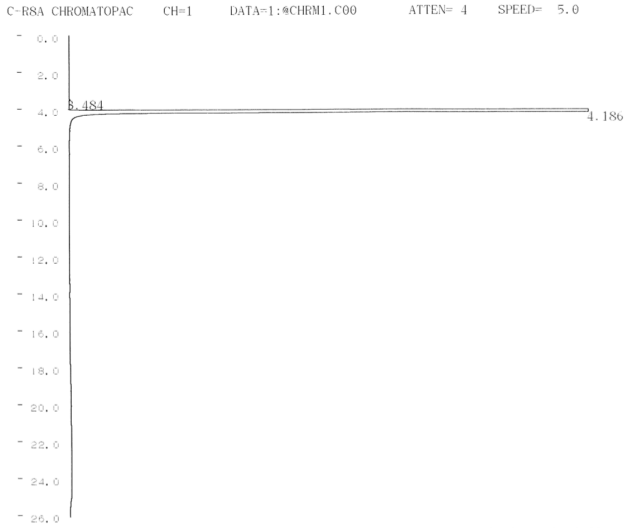
t (min)	5.3	5.8	7.6	9.0	16.0	19.3
name	water	isopentyl formate	1-butanol	isopentanol	AIBN	BHT
structure						
#	**B**	**C**	**D**	**E**		
sample 1	0.27%	0.06%	-	-	-	0.09%
sample 2	0.42%	0.09%	0.09%	0.03%	0.06%	-
sample 3	0.38%	0.13%	0.17%	0.06%	0.04%	-

t (min)						
name						
structure						
#						
sample 1						
sample 2						
sample 3						

[a] Percentage in the table refers to the peak area percentage in GC-MS.
[b] Derived from washing of GC-MS.

GC spectra

(a) sample 1

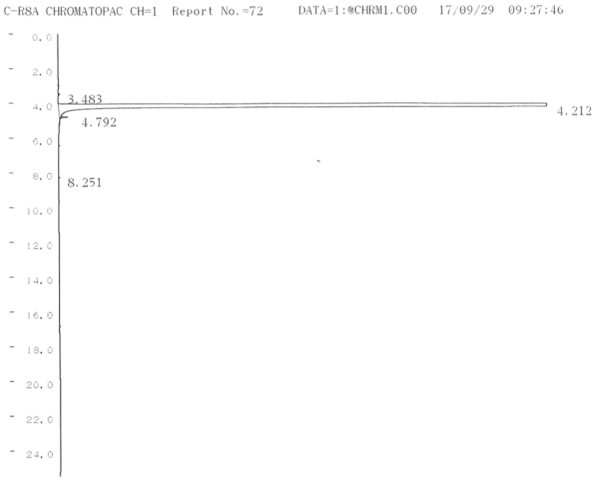


C-R8A CHROMATOPAC CH=1 Report No.=70 DATA=1:@CHRM1.C00 17/09/29 08:50:30

** CALCULATION REPORT **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	3.484	109	41			0.012	
	2	4.186	910963	197676			99.988	
	TOTAL		911072	197717			100	

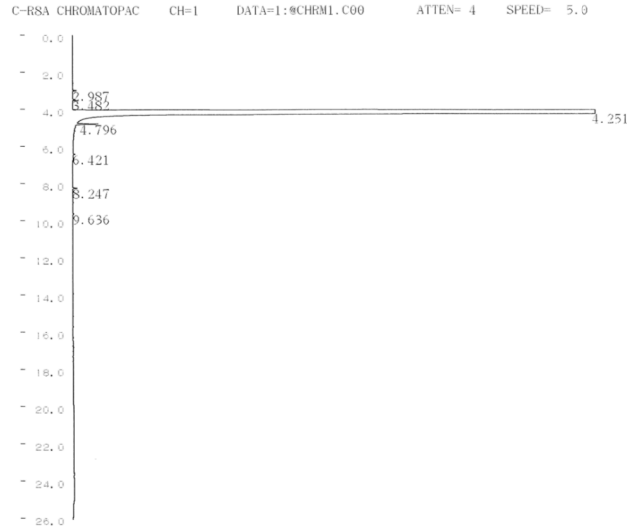
(b) sample 2



** CALCULATION REPORT **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	2	3.483	180	60			0.012	
	3	4.212	1502166	255984	S		99.9425	
	4	4.792	583	225	T		0.0388	
	5	8.251	100	39			0.0067	
	TOTAL		1503030	256308			100	

(c) sample 3



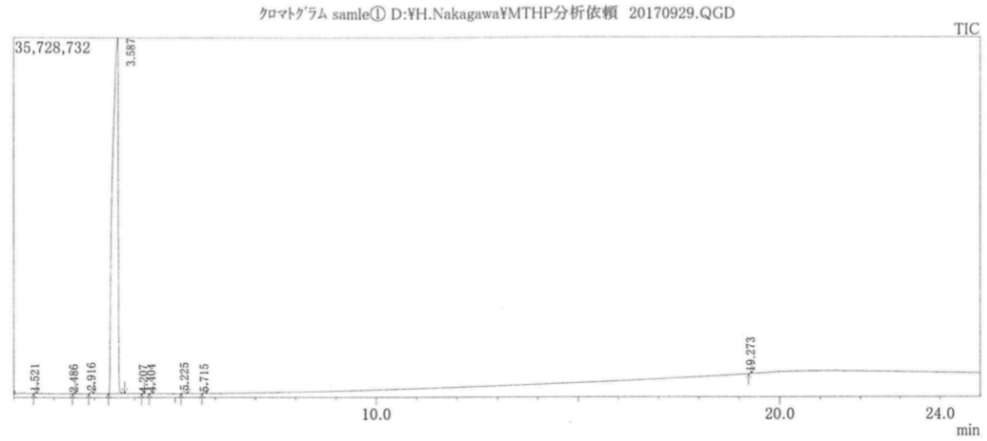
C-R8A CHROMATOPAC CH=1 Report No.=74 DATA=1:@CHRM1.C00 17/09/29 10:36:20

** CALCULATION REPORT **

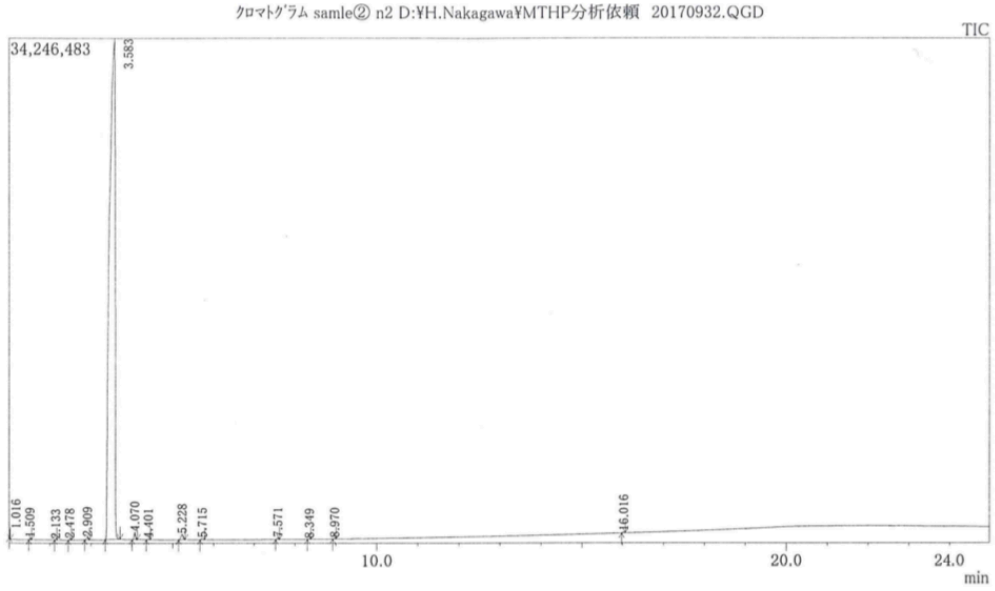
CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.987	304	136			0.0129	
	2	3.482	287	90			0.0122	
	3	4.251	2344774	330156	S		99.8784	
	4	4.796	1619	660	T		0.069	
	5	6.421	211	76			0.009	
	6	8.247	332	134			0.0141	
	7	9.636	103	41			0.0044	
	TOTAL		2347629	331293			100	

GC-MS spectra

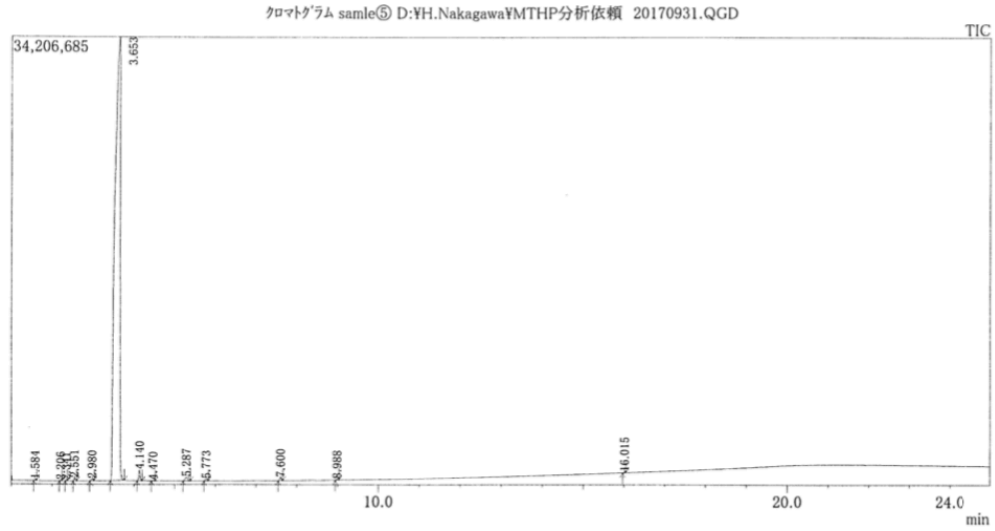
(a) sample 1



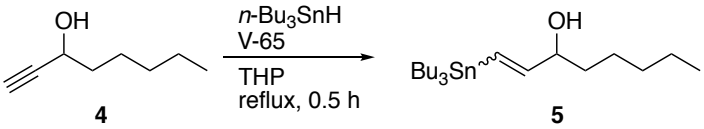
(b) sample 2



(c) sample 3



2.3. Radical addition in THP

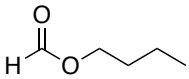


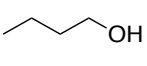
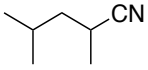
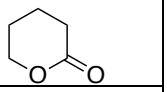
4 **5**

Experimental procedure

Commercially available THP (without stabilizer) was used for the reaction without any pretreatment (sample 4). Oct-1-yn-3-ol (**4**) (126 mg, 0.997 mmol), *n*-Bu_3SnH (380 mg, 1.31 mmol), and V-65 (50.1 mg, 0.202 mmol) were placed in a 100 mL two-necked round bottom flask equipped with a reflux condenser. The flask was flushed with argon and THP (20 mL) was added. After complete dissolution of AIBN at room temperature, the solution was heated at reflux for 30 min. The solution was stood at room temperature and, after attachment of the distillation apparatus, the solvent was distillated under reduced pressure (bp 35-39 °C/17-21 kPa) (sample 5). The residual oil was purified by flash chromatography on silica gel (*n*-hexane/EtOAc/Et_3N = 100/1/1) to give stannane **5** (325 mg, 0.779 mmol, 78%, *E/Z*=10:1) as a pale yellow oil. The purity of the recovered THP was determined to be 99.75% by the GC analysis. The same experiment was performed with the recovered THP, providing the product **5** (79% yield, *E/Z*=10:1) with a recovery of THP (purity: 99.77%) (sample 6).

Compound characterization list analyzed by GC-MS[a]

t (min)	2.1	2.5	2.96	3.03	3.5	4.4
name	acetone[b]	2-MeTHF	THP	2-MeTHP	3-MeTHP	*n*-butyl formate
structure						
#				**F**	**G**	**H**
sample 4	0.64%	0.34%	93.60%	1.67%	1.51%	0.46%
sample 5	0.07%	0.44%	94.89%	1.56%	1.22%	0.44%
sample 6	0.02%	0.40%	96.07%	1.20%	0.85%	0.28%

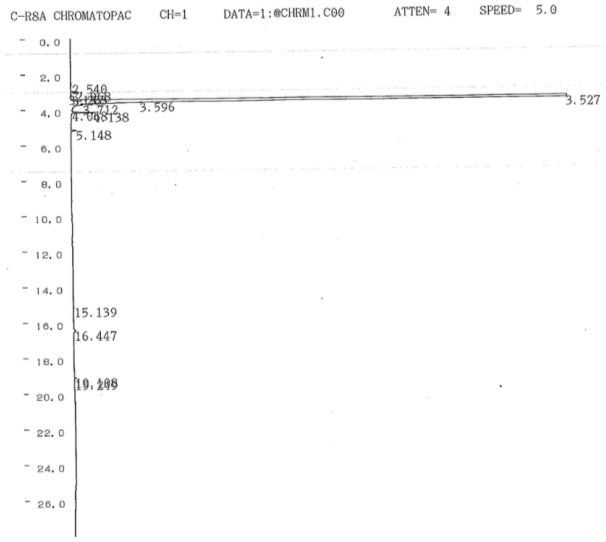
t (min)	5.2	7.6	8.8	14.4	15.6	18.2
name	water	1-butanol	2,4-dimethylpentanenitrile	unknown	unknown	δ-lactone
structure	H_2O					
#	**B**	**D**	**I**			
sample 4	0.54%	0.16%	0.36%	0.16%	0.36%	0.11%
sample 5	0.60%	0.05%	0.10%	-	-	-
sample 6	0.39%	0.05%	0.13%	-	-	-

t (min)						
name						
structure						
#						
sample 4						
sample 5						
sample 6						

[a] Percentage in the table refers to the peak area percentage in GC-MS.
[b] Derived from washing of GC-MS.

GC spectra

(d) sample 4

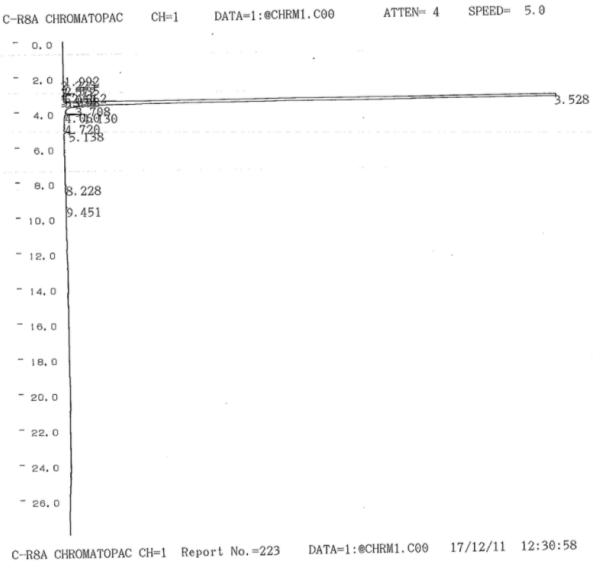


C-R8A CHROMATOPAC CH=1 Report No.=222 DATA=1:@CHRM1.C00 17/12/11 10:59:12

** CALCULATION REPORT **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.54	106	50			0.0081	
	2	2.968	491	227			0.0376	
	3	3.137	33	14			0.0025	
	4	3.203	139	63	V		0.0106	
	5	3.527	1301279	354011	S		99.6302	
	6	3.596	530	393	T		0.0406	
	7	3.712	257	137	T		0.0197	
	8	4.068	86	40	T		0.0065	
	9	4.138	1973	767	TV		0.1511	
	10	5.148	544	184			0.0417	
	11	15.139	72	33			0.0055	
	12	16.447	414	68			0.0317	
	13	19.108	148	64			0.0113	
	14	19.249	39	19			0.003	
		TOTAL	1306109	356069			100	

(e) sample 5



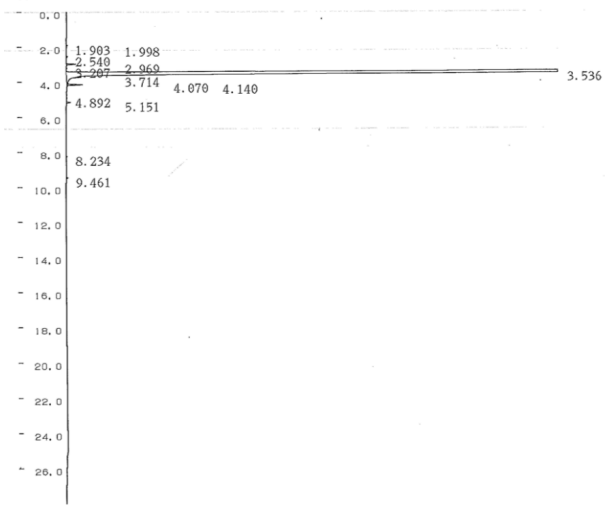
C-R8A CHROMATOPAC CH=1 Report No.=223 DATA=1:@CHRM1.C00 17/12/11 12:30:58

** CALCULATION REPORT **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	1.992	37	29			0.0025	
	3	2.535	98	62			0.0067	
	4	2.572	27	17	V		0.0019	
	5	2.962	700	365			0.0484	
	6	3.052	25	13	V		0.0017	
	7	3.138	28	13			0.0019	
	8	3.198	67	35	V		0.0046	
	9	3.528	1443828	377256	S		99.7453	
	10	3.708	292	166	T		0.0202	
	11	4.06	77	36	T		0.0053	
	12	4.13	1594	658	TV		0.1101	
	13	4.72	36	15			0.0025	
	14	5.138	539	195			0.0372	
	15	8.228	56	24			0.0039	
	16	9.451	114	45			0.0078	
		TOTAL	1447516	378928			100	

(f) sample 6

C-R8A CHROMATOPAC CH=1 Report No.=226 DATA=1:@CHRM1.C00 17/12/11 13:48:40

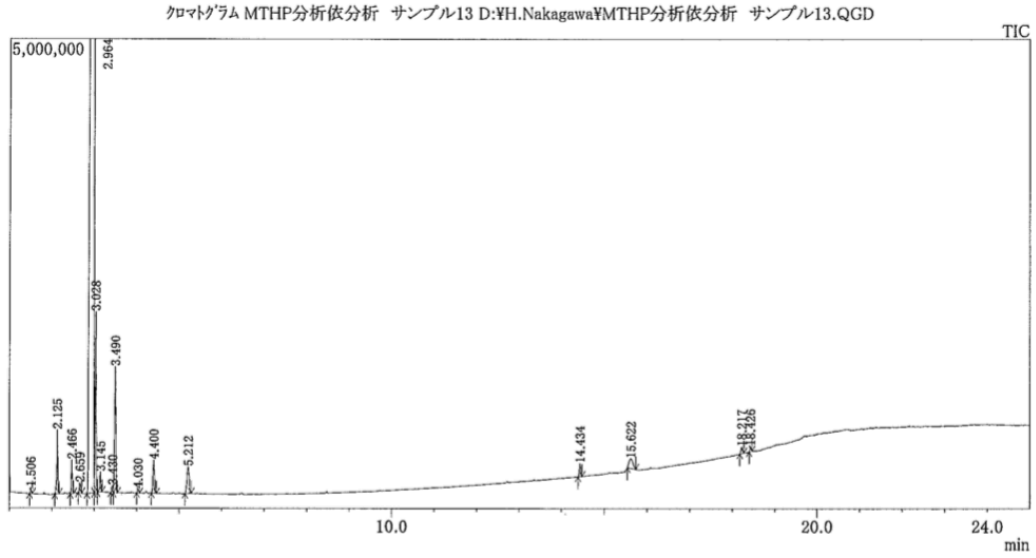


** CALCULATION REPORT **

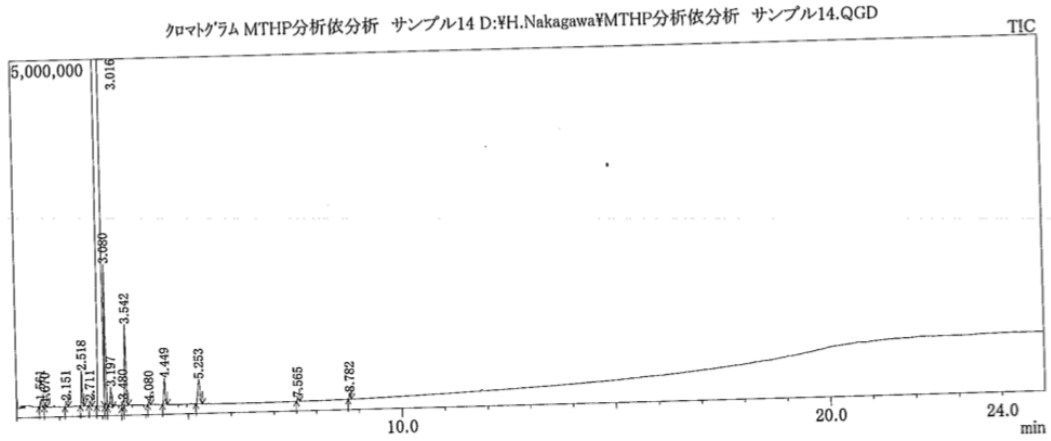
CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	1.903	81	42			0.0052	
	2	1.998	31	18			0.002	
	3	2.54	140	50			0.0091	
	4	2.969	743	304			0.0482	
	5	3.207	48	21			0.0031	
	6	3.536	1537225	389583	S		99.7747	
	7	3.714	310	164	T		0.0201	
	8	4.07	59	27	T		0.0038	
	9	4.14	1297	491	TV		0.0842	
	10	4.892	40	15			0.0026	
	11	5.151	422	142			0.0274	
	12	8.234	100	41			0.0065	
	13	9.461	200	75			0.013	
		TOTAL	1540696	390972			100	

GC-MS spectra

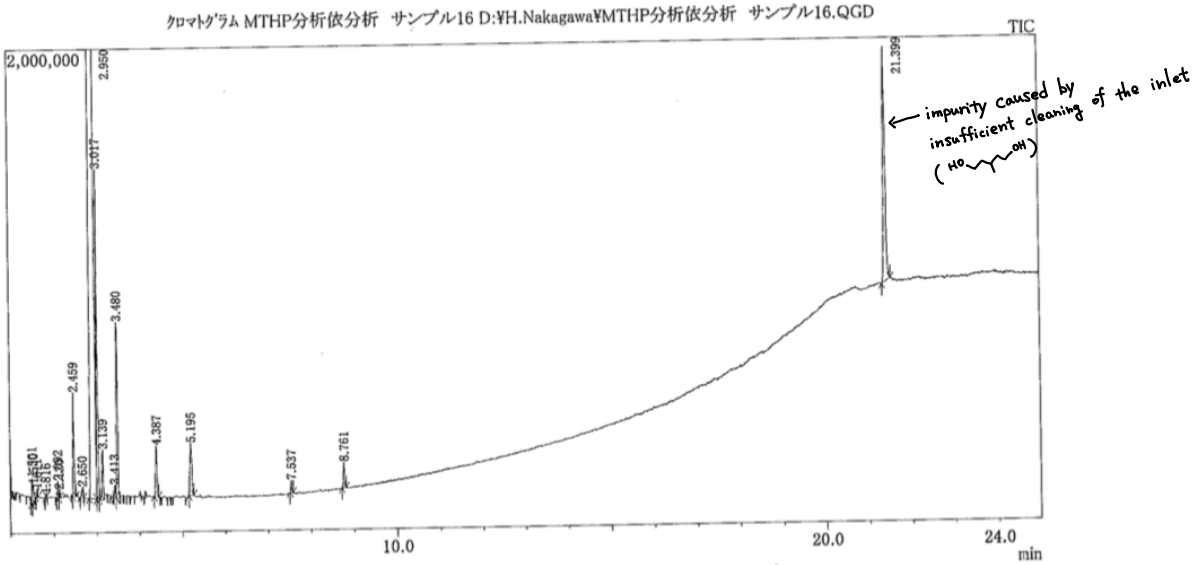
(d) sample 4



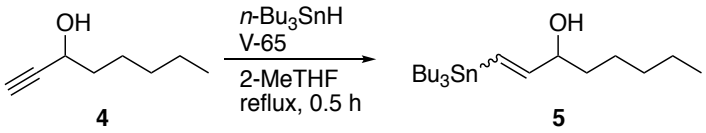
(e) sample 5



(f) sample 6



2.4. Radical addition in 2-MeTHF

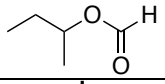
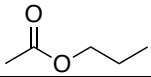
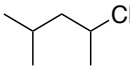
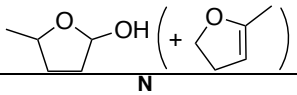
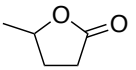
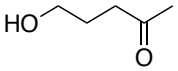
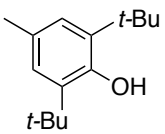
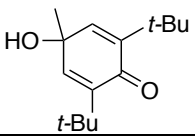


4 **5**

Experimental procedure

Commercially available 2-MeTHF (stabilized with BHT) was stored with molecular sieves 4Å and used for the reaction (sample 7). Oct-1-yn-3-ol (**4**) (126 mg, 0.998 mmol), *n*-Bu_3SnH (379 mg, 1.30 mmol), and V-65 (49.8 mg, 0.201 mmol) were placed in a 100 mL two-necked round bottom flask equipped with a reflux condenser. The flask was flushed with argon and 2-MeTHF (20 mL) was added. After complete dissolution of V-65 at room temperature, the solution was heated at reflux for 30 min. The solution was stood at room temperature and, after attachment of the distillation apparatus, the solvent was distillated under reduced pressure (bp 40-42 °C/25-28 kPa) (sample 8). The residual oil was purified by flash chromatography on silica gel (*n*-hexane/EtOAc/Et_3N = 30/1/0.3) to give stannane **5** (324 mg, 0.821 mmol, 82%, *E*/*Z*=9:1) as a pale yellow oil. The purity of the recovered 2-MeTHF was determined to be 99.96% by the GC analysis. The same experiment was performed with the recovered 2-MeTHF, providing the product **5** (84% yield, *E*/*Z*=10:1) with a recovery of 2-MeTHF (purity: 99.59%) (sample 9).

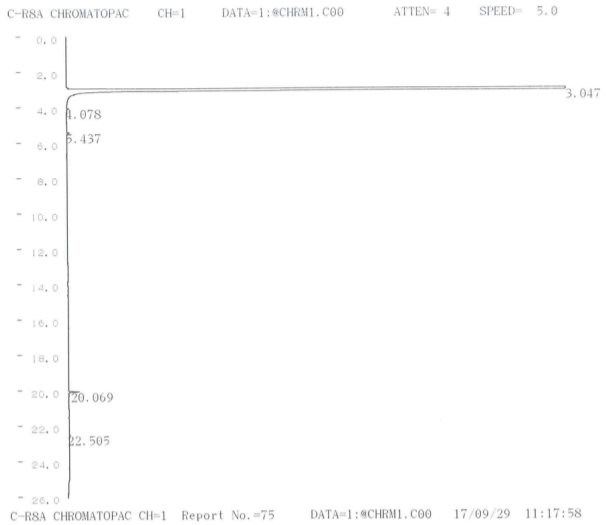
Compound characterization list analyzed by GC-MS[a]

t (min)	2.5	3.2	3.6	4.2	4.6
name	2-MeTHF	*sec*-butyl formate	*n*-propyl acetate	unknown	2-butanol
structure					
#		**J**	**K**	**L**	**M**
sample 7	96.20%	-	-	-	0.24%
sample 8	96.79%	0.11%	0.33%	-	0.20%
sample 9	88.46%	1.55%	3.28%	0.09%	0.09%
t (min)	5.2	8.8	13.5	15.7	16.9
name	water	2,4-dimethylpentanenitrile	5-methyltetrahydrofuran-2-ol (+5-methyl-2,3-dihydrofuran)	γ-valerolactone	5-hydroxypentan-2-one
structure	H_2O				
#	**B**	**I**	**N**	**O**	**P**
sample 7	1.10%	-	-	-	-
sample 8	1.43%	0.42%	0.04%	0.11%	-
sample 9	0.66%	0.19%	1.91%	0.17%	2.84%
t (min)	19.3	21.4			
name	BHT				
structure					
#					
sample 7	1.40%	0.41%			
sample 8	-	-			
sample 9	-	-			

[a] Percentage in the table refers to the peak area percentage in GC-MS.

GC spectra

(g) sample 7

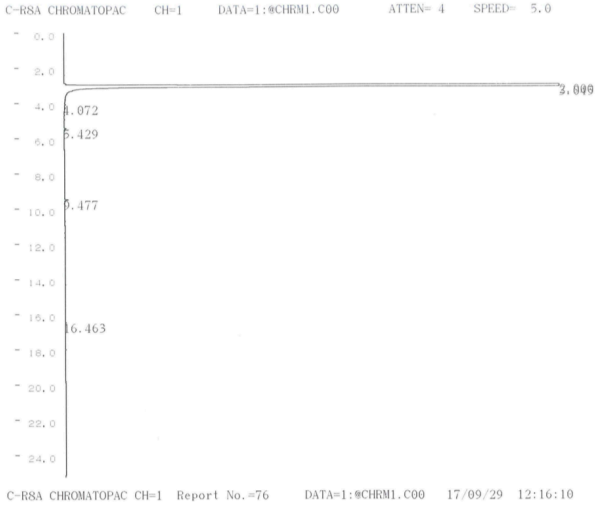


C-R8A CHROMATOPAC CH=1 Report No.=75 DATA=1:@CHRM1.C00 17/09/29 11:17:58

** CALCULATION REPORT **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	3.047	2147333	629114			99.9321	
	2	4.078	215	81			0.01	
	3	5.437	277	100			0.0129	
	4	20.069	867	351			0.0404	
	5	22.505	100	35			0.0047	
	TOTAL		2148793	629681			100	

(h) sample 8

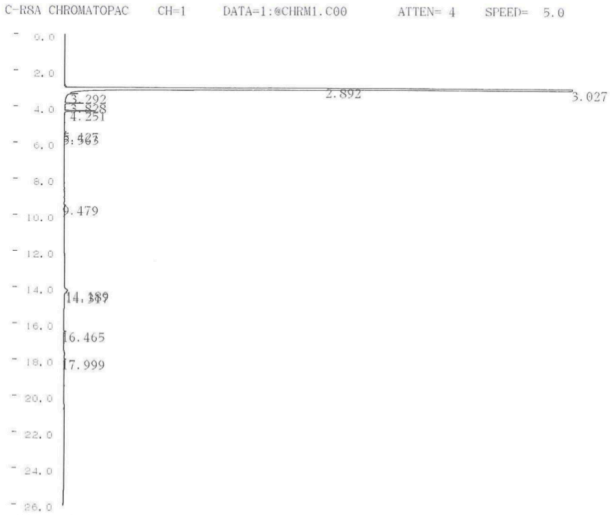


C-R8A CHROMATOPAC CH=1 Report No.=76 DATA=1:@CHRM1.C00 17/09/29 12:16:10

** CALCULATION REPORT **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.9	299	77			0.0132	
	2	3.045	2259035	661781	V		99.9576	
	3	4.072	120	45			0.0053	
	4	5.429	203	74			0.009	
	5	9.477	337	123			0.0149	
	TOTAL		2259994	662099			100	

(i) sample 9



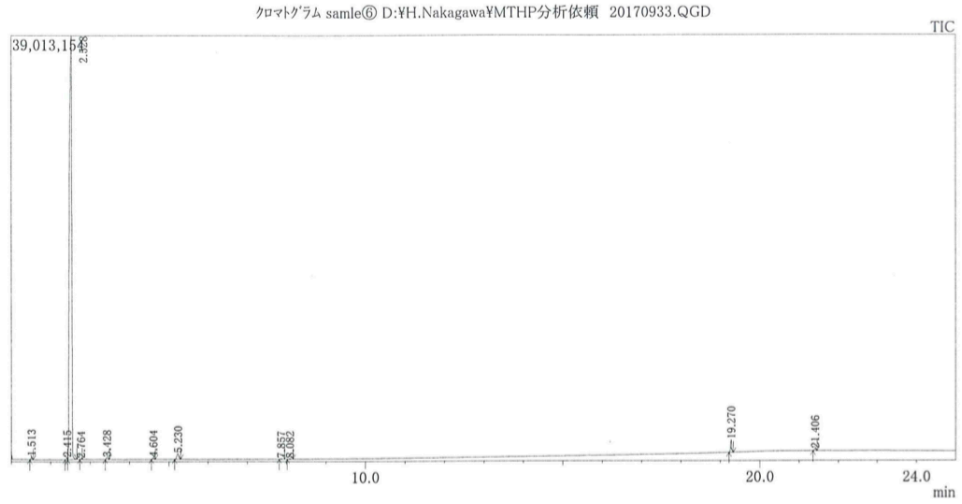
C-R8A CHROMATOPAC CH=1 Report No.=77 DATA=1:@CHRM1.C00 17/09/29 12:50:40

** CALCULATION REPORT **

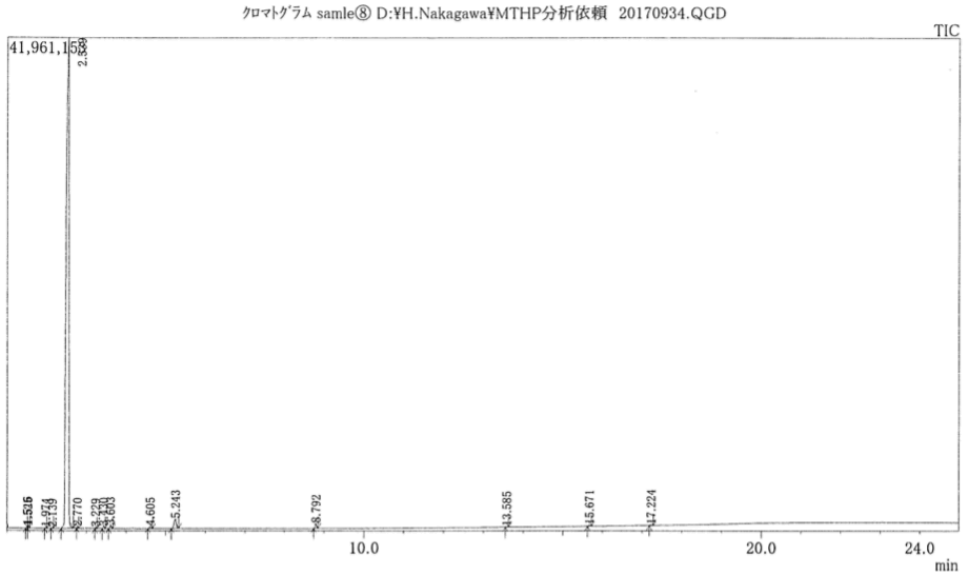
CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.892	176	65			0.0114	
	2	3.027	1539656	528535	SV		99.5878	
	3	3.292	493	263	T		0.0319	
	4	3.828	1338	579			0.0866	
	5	4.251	2471	976			0.1598	
	6	5.427	172	63			0.0111	
	8	9.479	148	55			0.0096	
	9	14.189	964	103			0.0624	
	10	14.317	256	79	V		0.0166	
	11	16.465	190	80			0.0123	
	12	17.999	165	70			0.0106	
	TOTAL		1546028	530866			100	

GC-MS spectra

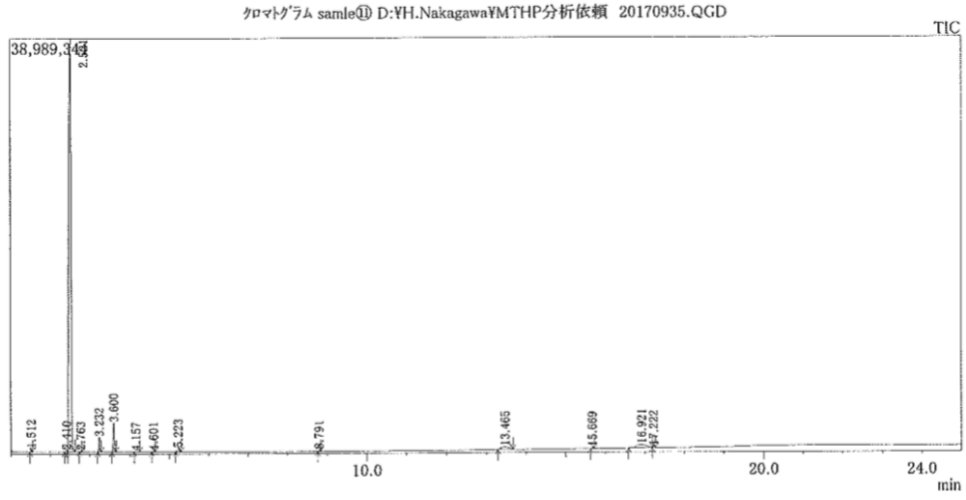
(g) sample 7



(h) sample 8



(i) sample 9



3. ^{1}H and ^{13}C NMR spectra of synthetic compounds

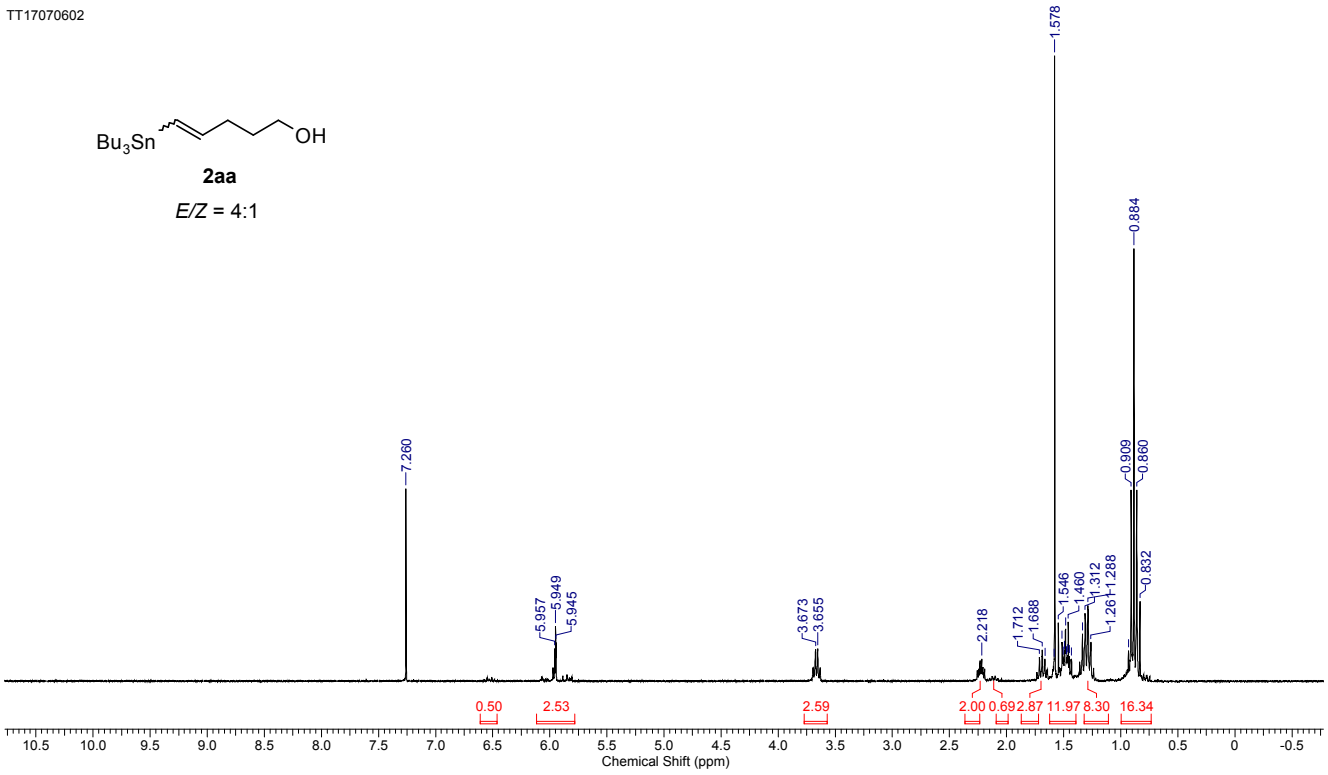
2019/02/28 17:29:39

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jul 6 2017
Date Stamp	Jul 6 2017	*File Name*	¥¥Mac¥iCloud¥[redacted]NMR¥[redacted]¥2017NMR K¥2017NMR(agilent)¥tamura¥TT17070602.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	28.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1698.4518	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

TT17070602

2aa

E/*Z* = 4:1



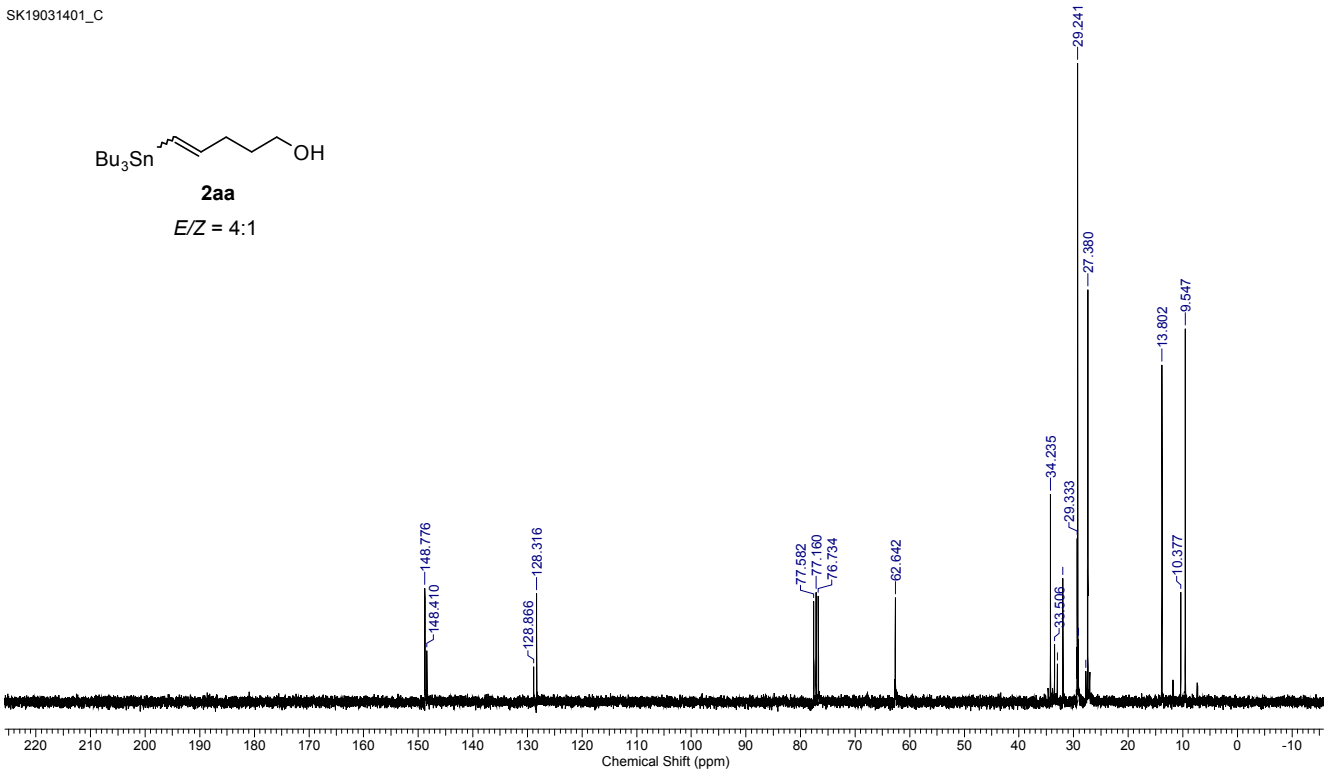
2019/03/14 16:36:06

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Mar 14 2019	*Date Stamp*	Mar 14 2019
File Name	¥¥Mac¥iCloud¥[redacted]NMR¥[redacted]¥2019NMR K¥koba¥SK19031401_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	128	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8956.2578
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

SK19031401_C

2aa

E/*Z* = 4:1



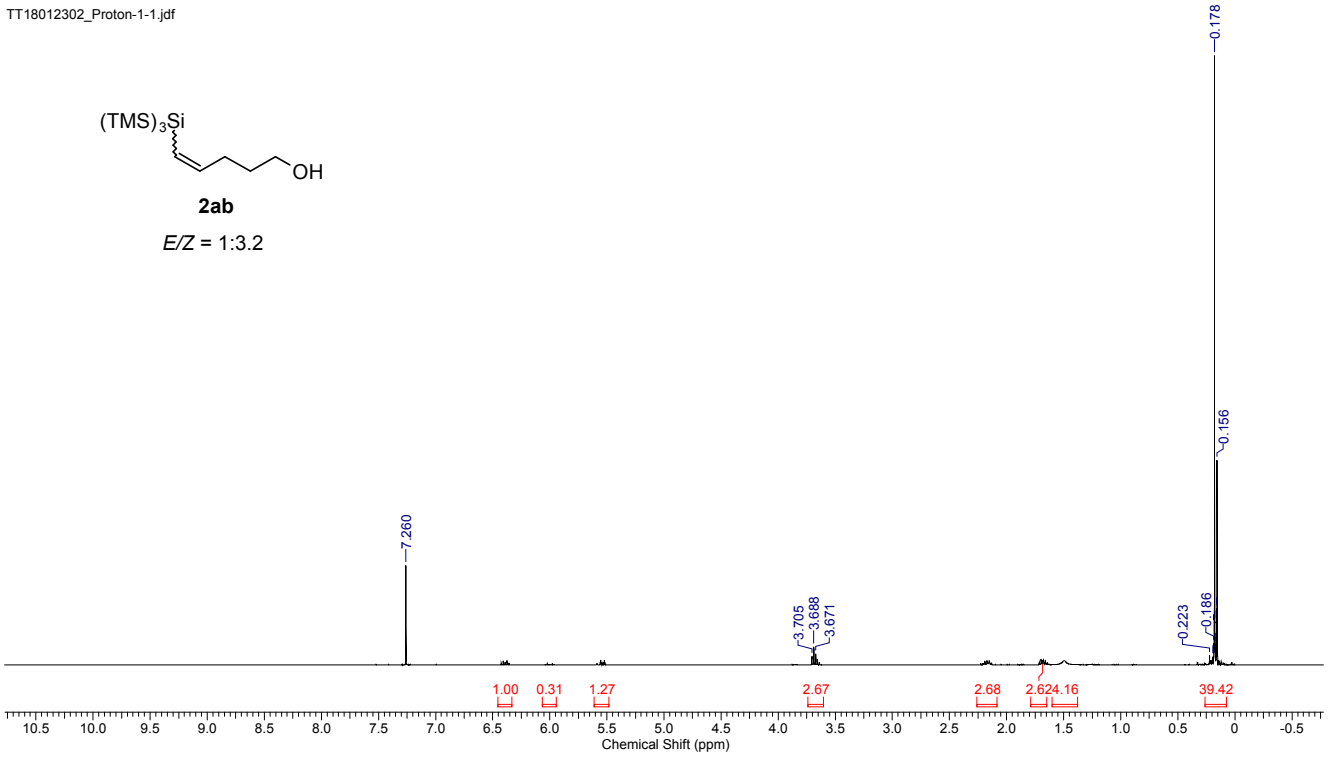
2019/03/01 10:58:30

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	23 Jan 2018 12:28:31		
Date Stamp	23 Jan 2018 12:27:40						
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2017NMR K¥2017NMR(JEOL)¥[redacted]TT18012302 Proton-1-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4902	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	18.400		

TT18012302_Proton-1-1.jdf

2ab

E/*Z* = 1:3.2



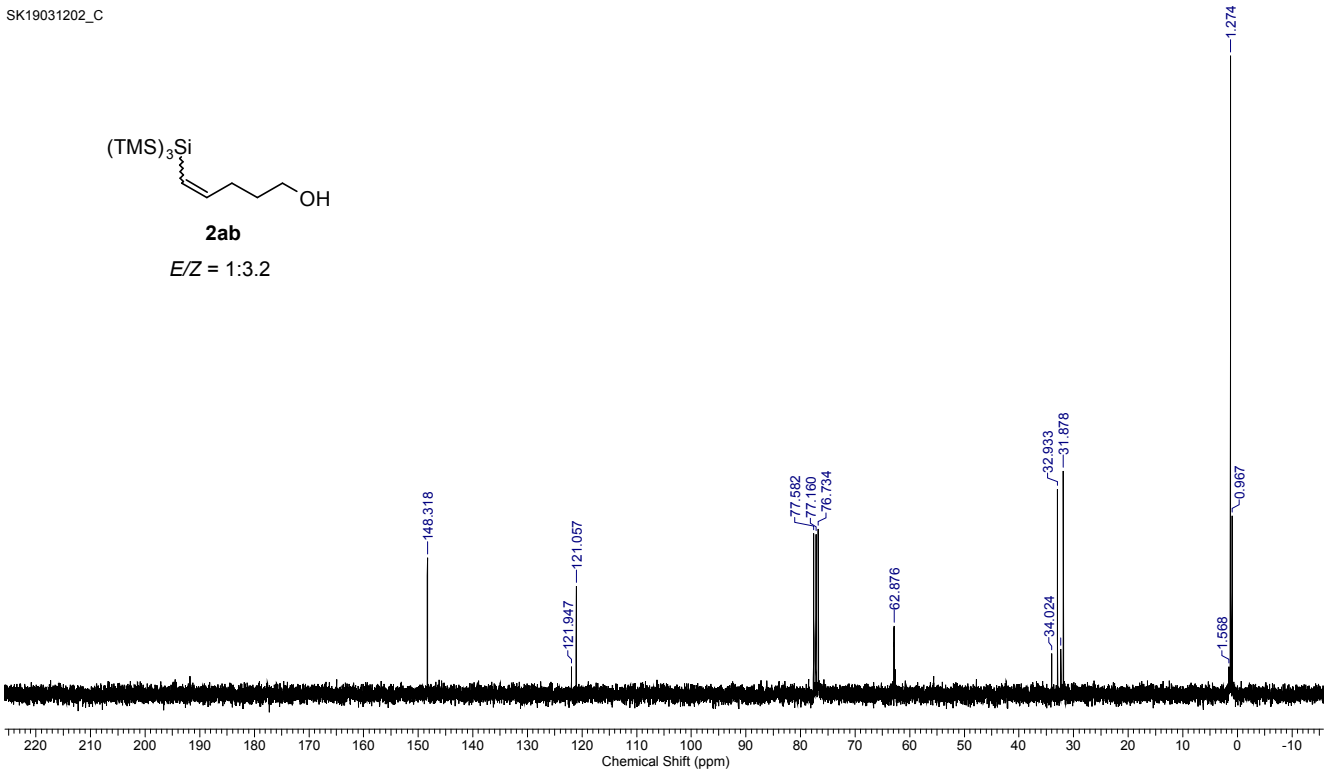
2019/03/13 11:21:27

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Mar 12 2019	*Date Stamp*	Mar 12 2019		
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2019NMR K¥koba¥SK19031202 C.fid¥fid					*Frequency (MHz)*	75.46	*Nucleus*	13C
Number of Transients	128	*Original Points Count*	19335	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	30.00
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	8956.9492	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74
Temperature (degree C)	AMBIENT TEMPERATURE								

SK19031202_C

2ab

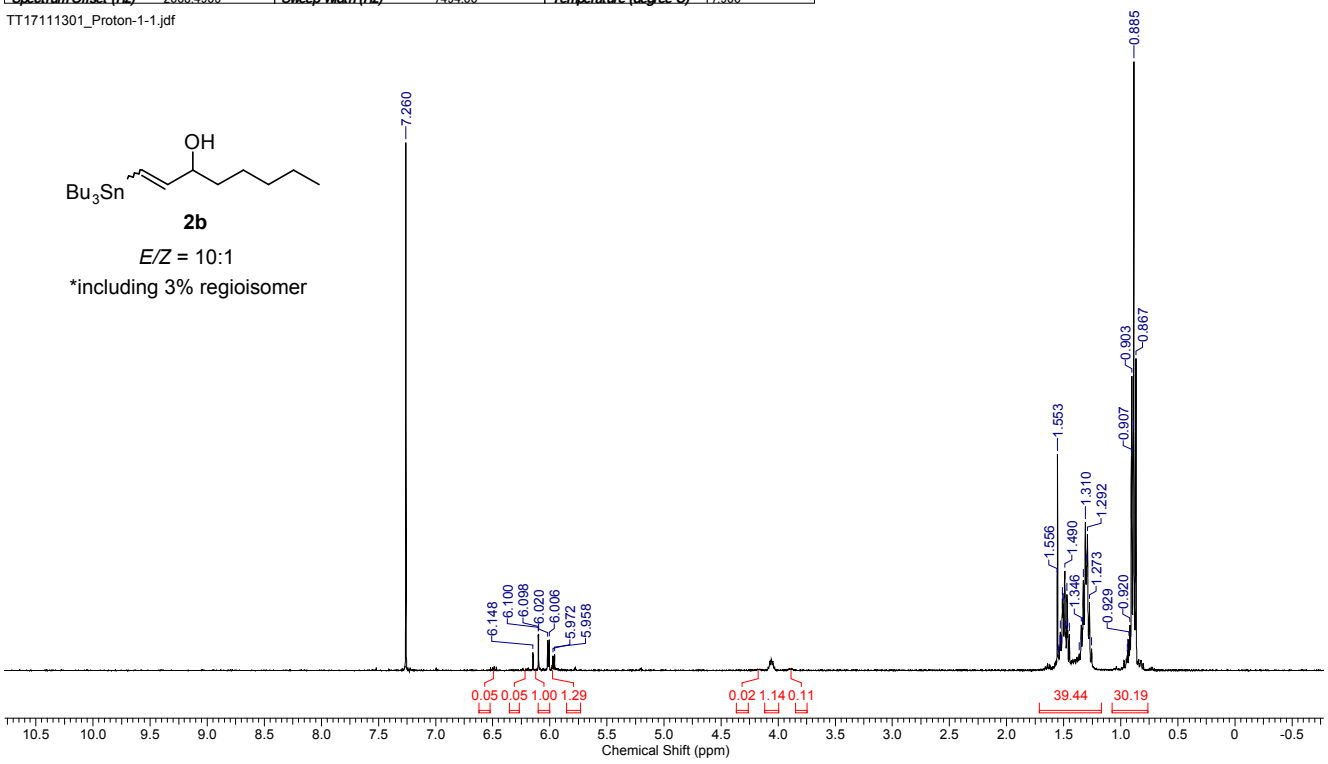
E/*Z* = 1:3.2



2019/03/01 11:58:58

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	13 Nov 2017 13:07:39		
Date Stamp	13 Nov 2017 13:06:48						
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2017NMR K¥2017NMR(JEOL)¥[redacted]TT17111301 Proton-1-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	17.900		

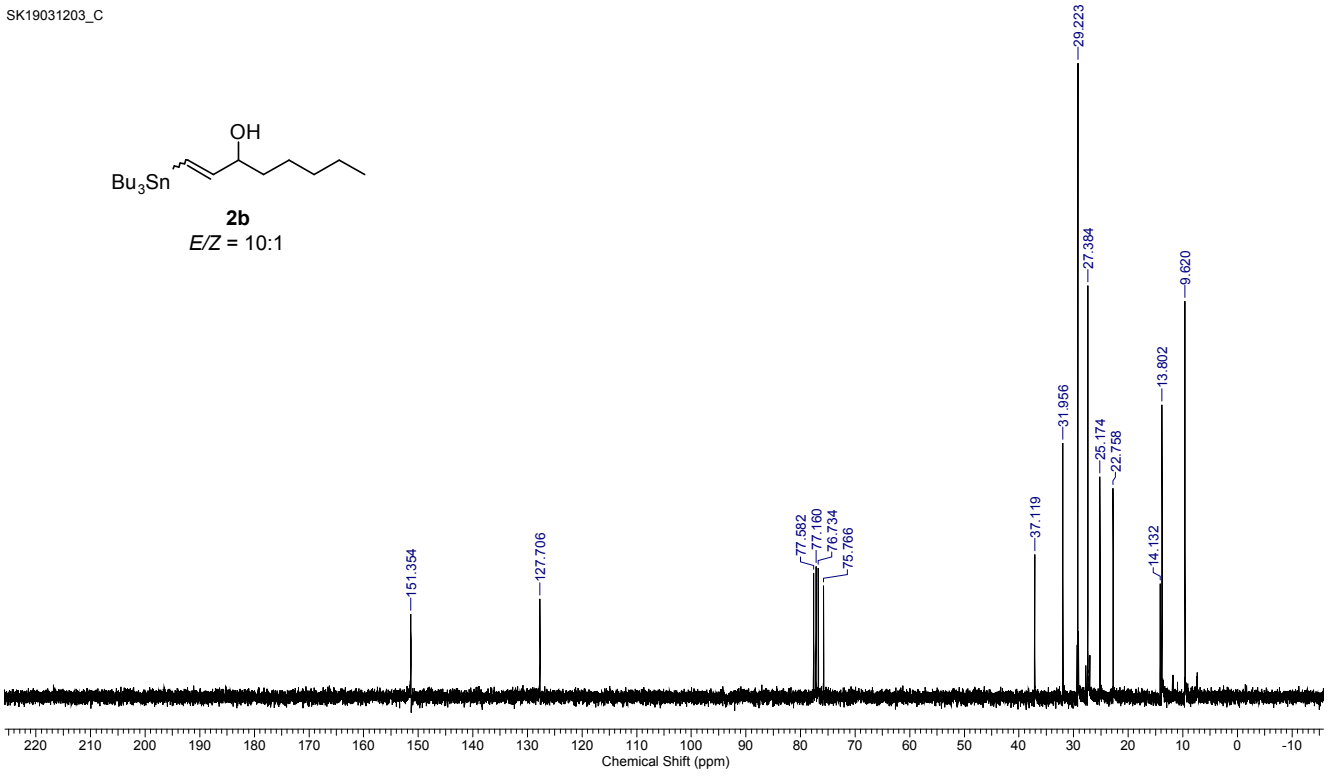
TT17111301_Proton-1-1.jdf



2019/03/13 11:39:36

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Mar 12 2019	*Date Stamp*	Mar 12 2019		
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2019NMR K¥koba¥SK19031203 C.fid¥fid					*Frequency (MHz)*	75.46	*Nucleus*	13C
Number of Transients	128	*Original Points Count*	19335	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	30.00
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	8956.9492	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74
Temperature (degree C)	AMBIENT TEMPERATURE								

SK19031203_C

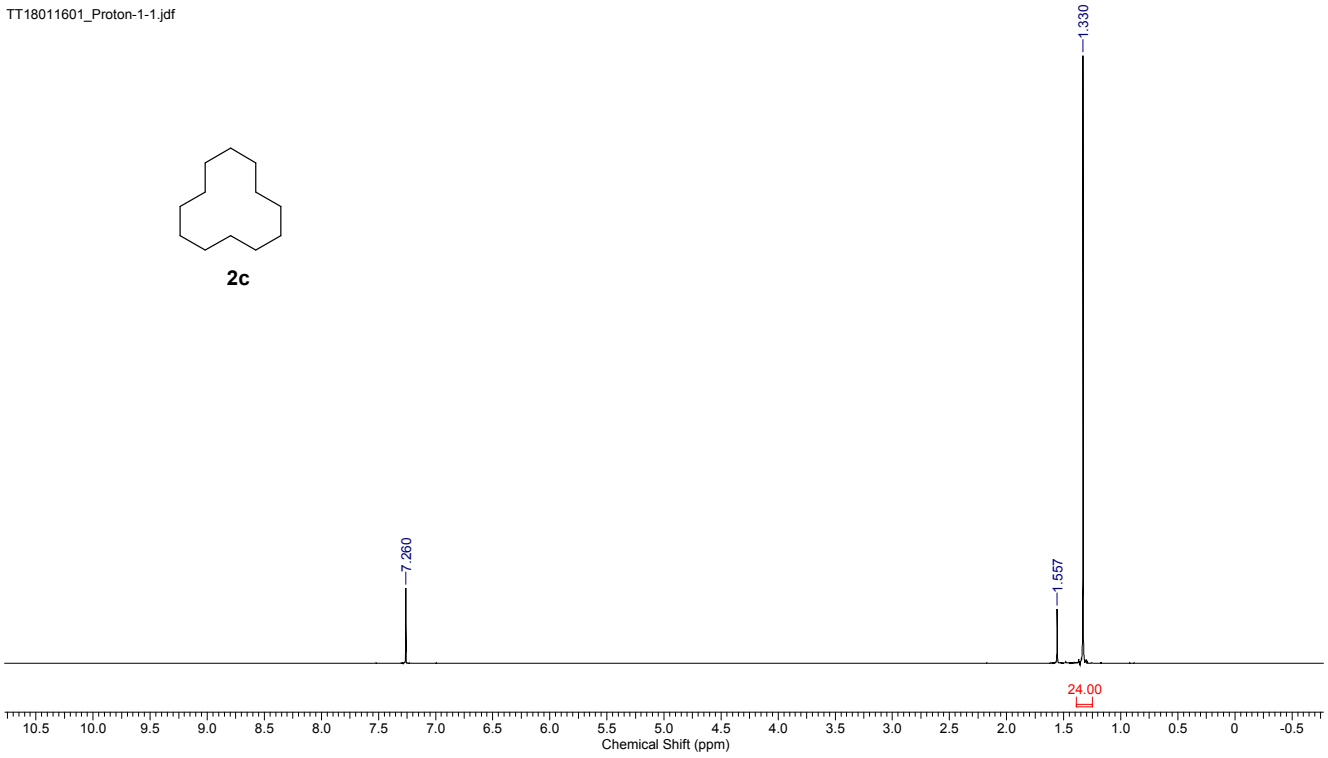


2019/03/01 14:14:08

Acquisition Time (sec)	2.1863	***Comment***	single_pulse	***Date***	16 Jan 2018 07:48:07		
Date Stamp	16 Jan 2018 07:47:16						
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2017NMR K¥2017NMR(JEOL)¥[redacted]TT18011601 Proton-1-1.jdf					***Frequency (MHz)***	399.78
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA	***Original Points Count***	16384
Owner	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4905	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	16.500		

TT18011601_Proton-1-1.jdf

2c

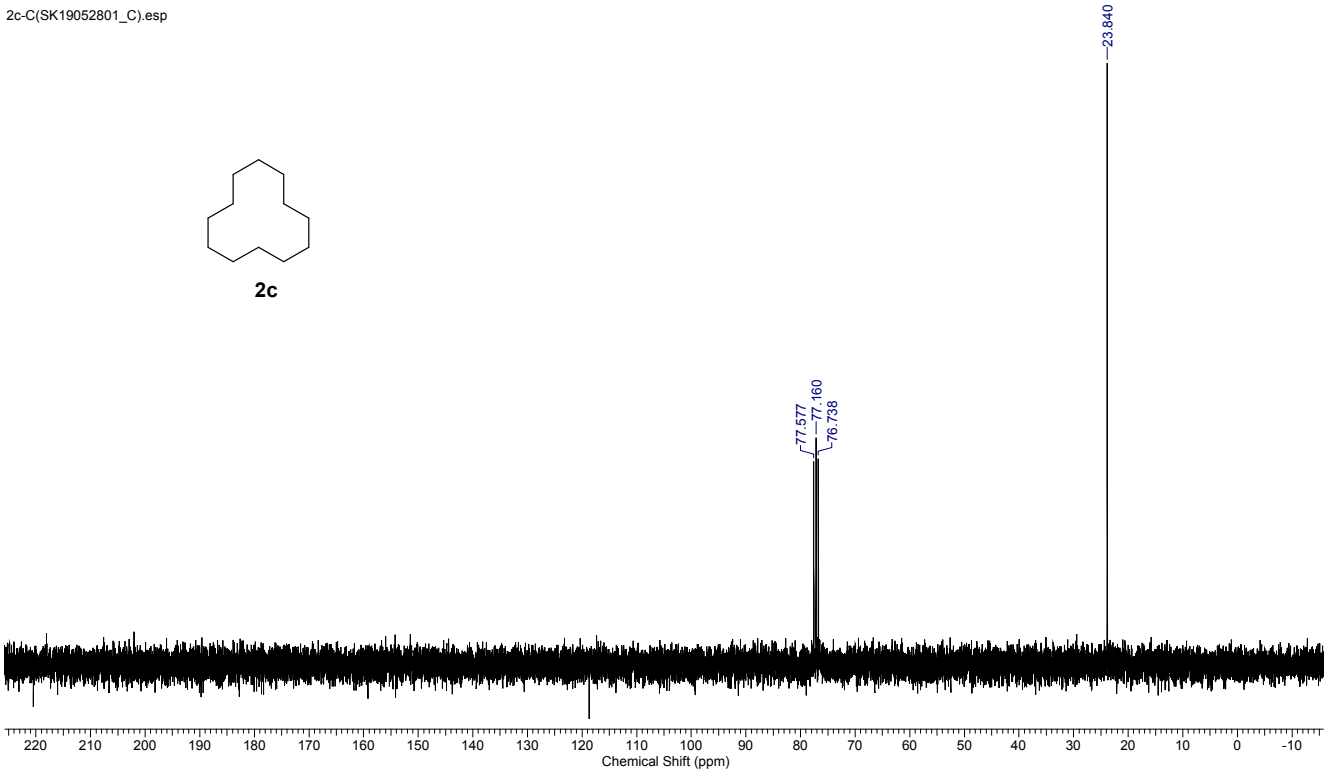


2019/05/28 19:47:53

Acquisition Time (sec)	0.8527	***Comment***	c13-NMR	***Date***	May 28 2019	***Date Stamp***	May 28 2019
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2019NMR K¥2019NMR(agilent)¥koba¥SK19052801_C.fid¥fid					***Frequency (MHz)***	75.46
Nucleus	13C	***Number of Transients***	32	***Original Points Count***	19335	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	8957.2949
Spectrum Type	STANDARD	***Sweep Width (Hz)***	22675.74	***Temperature (degree C)***	AMBIENT TEMPERATURE		

2c-C(SK19052801_C).esp

2c

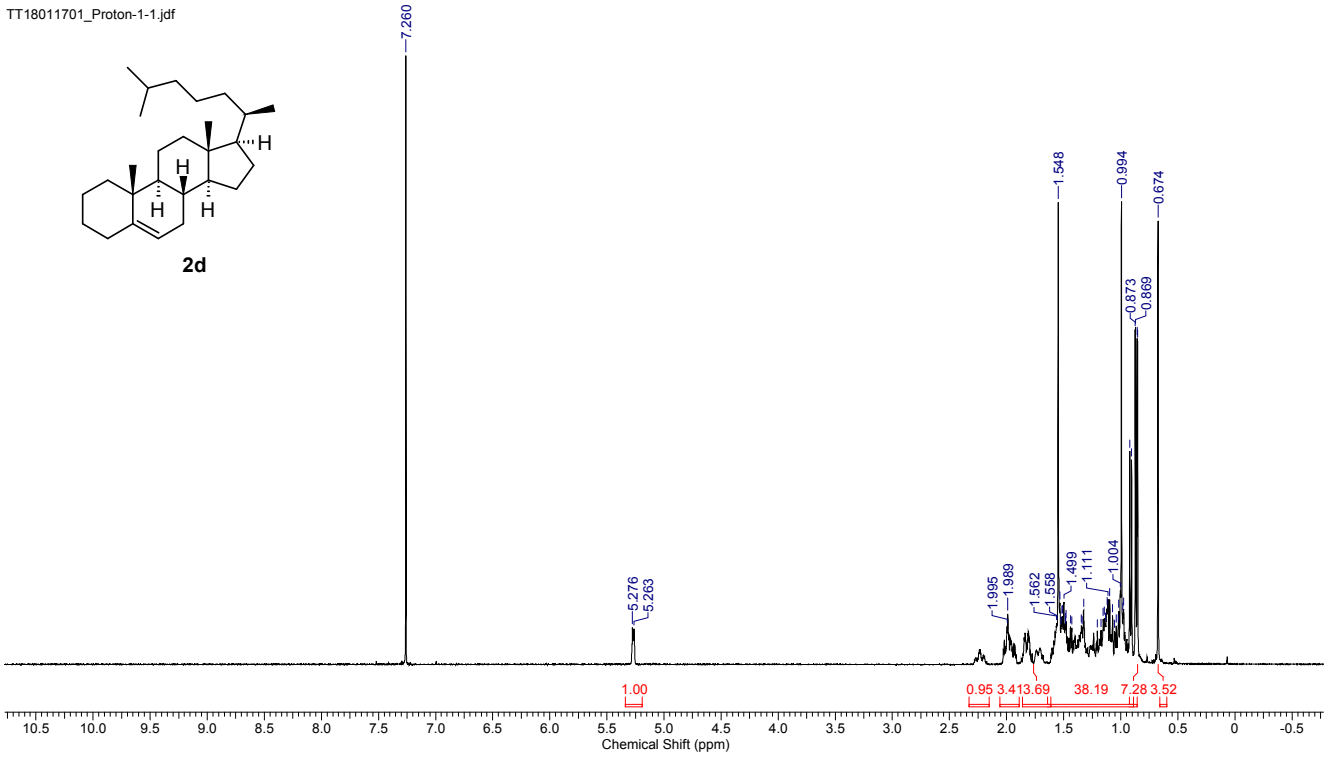


2019/03/01 14:24:18

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	17 Jan 2018 10:40:49		
Date Stamp	17 Jan 2018 10:39:58						
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2017NMR K¥2017NMR(JEOL)¥[redacted]TT18011701 Proton-1-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	20.800		

TT18011701_Proton-1-1.jdf

2d

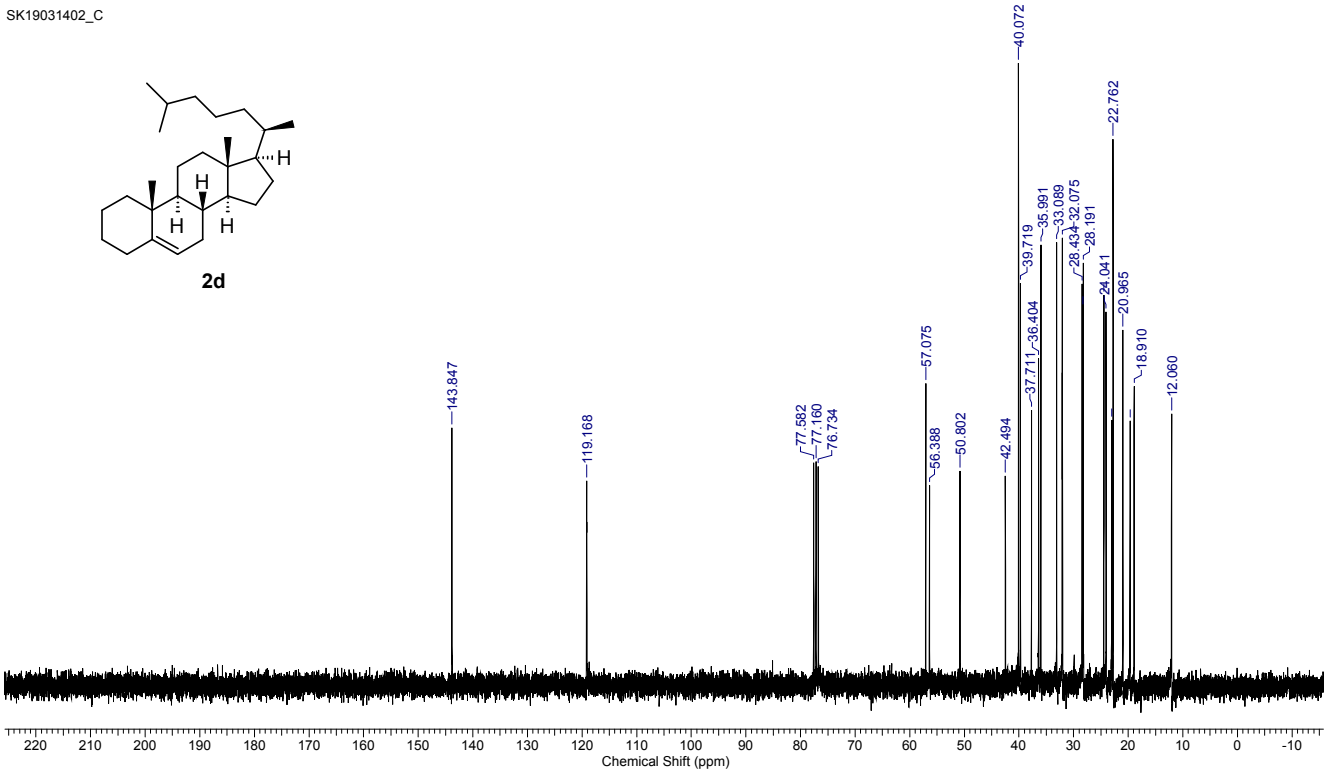


2019/03/14 17:39:06

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Mar 14 2019	*Date Stamp*	Mar 14 2019		
File Name	¥¥Mac¥iCloud¥[redacted]NMR[redacted]¥2019NMR K¥koba¥SK19031402_C.fid¥fid					*Frequency (MHz)*	75.46	*Nucleus*	13C
Number of Transients	128	*Original Points Count*	19335	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	30.00
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	8957.2949	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74
Temperature (degree C)	AMBIENT TEMPERATURE								

SK19031402_C

2d

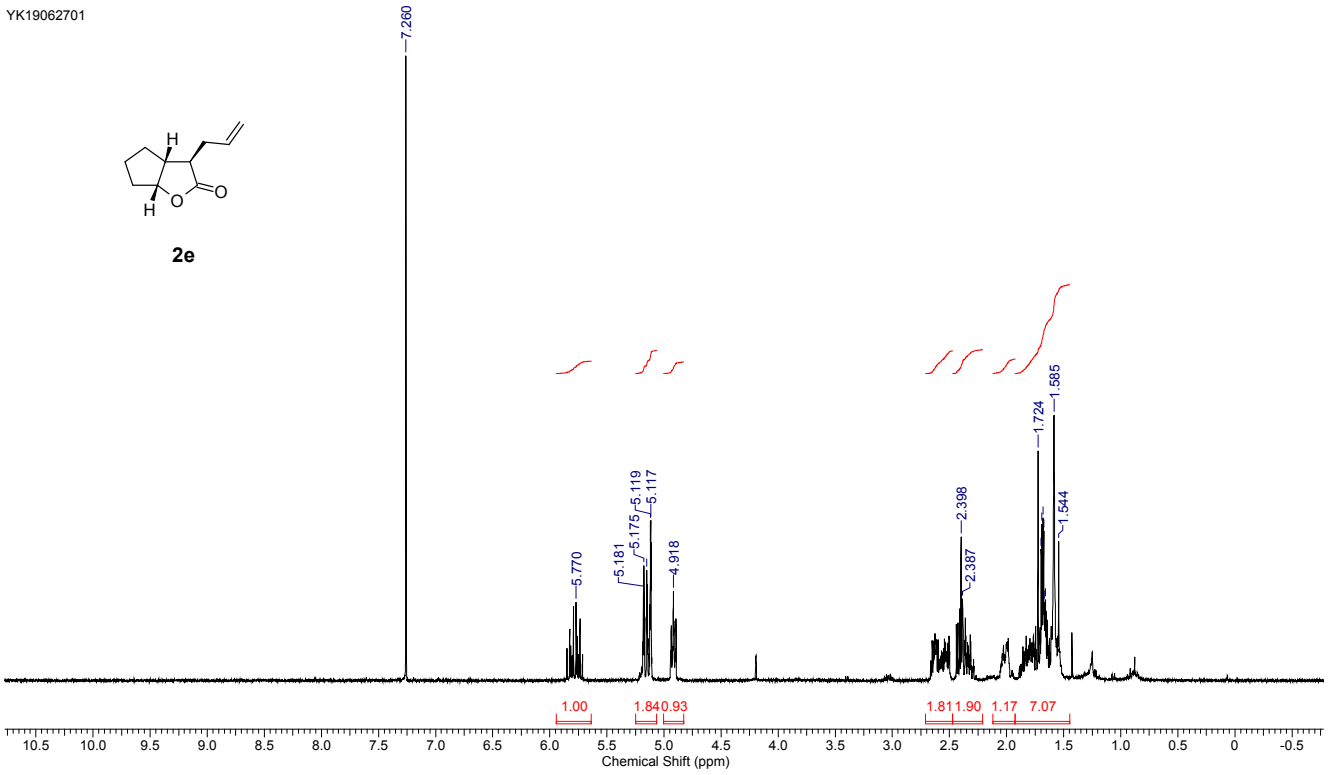


2019/06/27 16:18:55

Acquisition Time (sec)	3.5561	Comment	STANDARD 1H OBSERVE			Date	Jun 27 2019
Date Stamp	Jun 27 2019	File Name	¥¥Mac¥iCloud¥[redacted]NMR¥[redacted]¥2019NMR K¥2019NMR(agilent)¥kuroda¥YK19062701.fid¥fid				
Frequency (MHz)	300.05	Nucleus	1H	Number of Transients	16	Original Points Count	17080
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	28.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1698.7449	Spectrum Type	STANDARD	Sweep Width (Hz)	4803.07	Temperature (degree C)	AMBIENT TEMPERATURE

YK19062701

2e

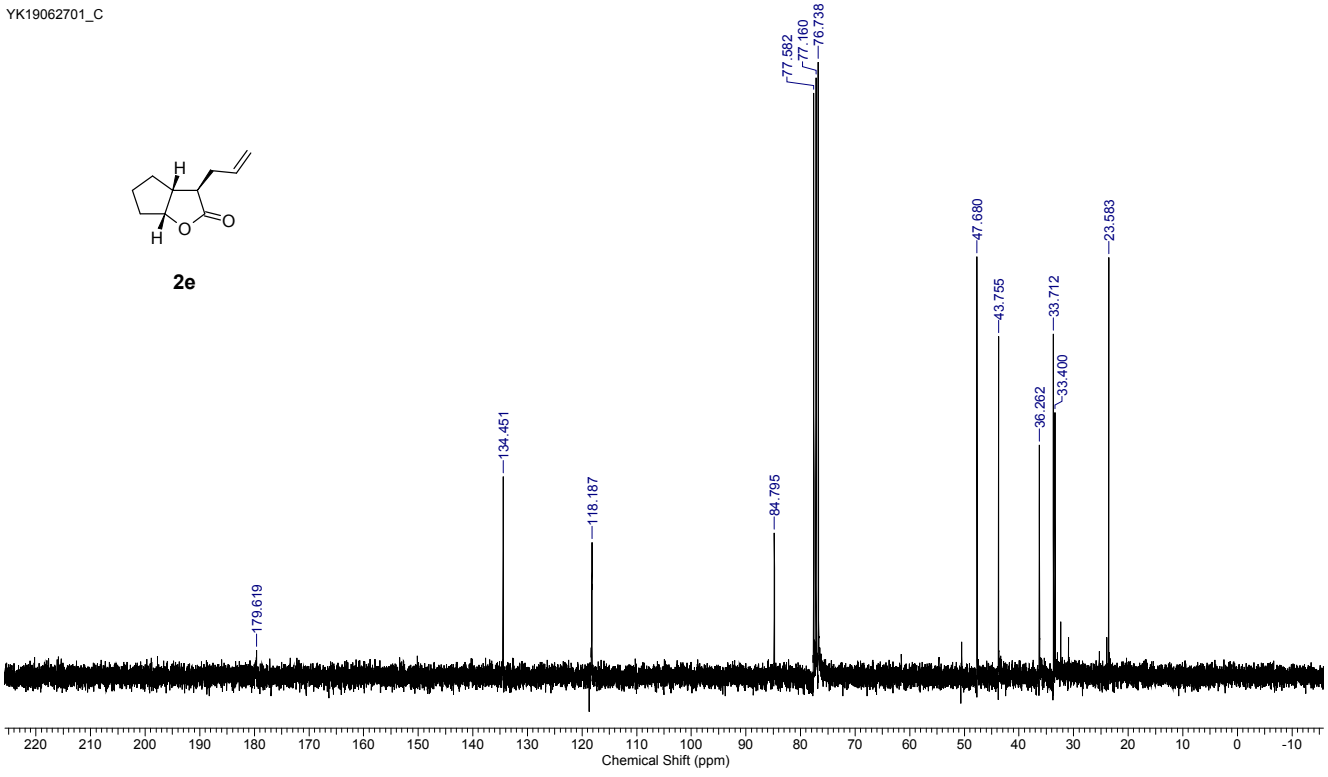


2019/06/27 16:37:17

Acquisition Time (sec)	0.8527	Comment	c13-NMR	Date	Jun 27 2019	Date Stamp	Jun 27 2019
File Name	¥¥Mac¥iCloud¥[redacted]NMR¥[redacted]¥2019NMR K¥2019NMR(agilent)¥kuroda¥YK19062701_C.fid¥fid					Frequency (MHz)	75.46
Nucleus	13C	Number of Transients	1024	Original Points Count	19335	Points Count	65536
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	8957.2959
Spectrum Type	STANDARD	Sweep Width (Hz)	22675.74	Temperature (degree C)	AMBIENT TEMPERATURE		

YK19062701_C

2e

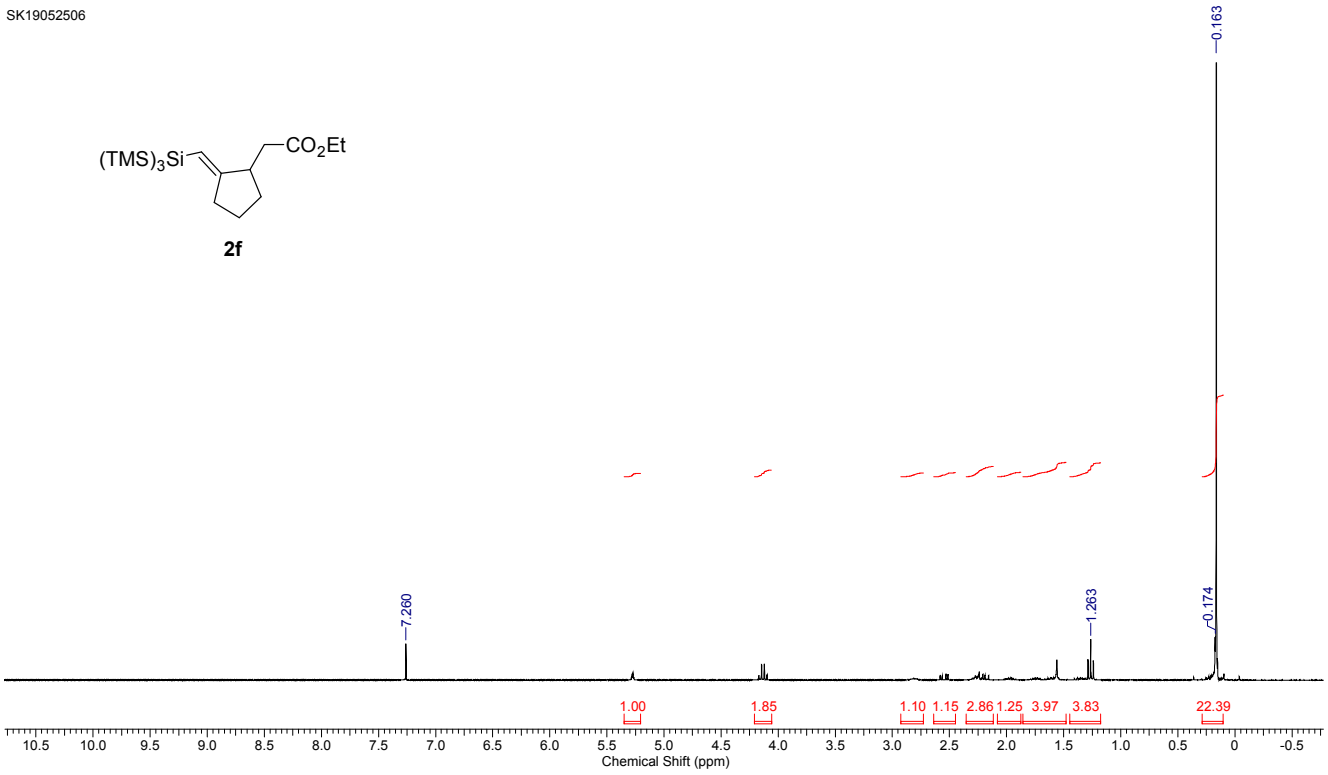


2019/05/28 14:23:29

Acquisition Time (sec)	3.5561	***Comment***	STANDARD 1H OBSERVE			***Date***	May 25 2019
Date Stamp	May 25 2019	***File Name***	¥¥Mac¥iCloud¥[redacted]NMR¥[redacted]¥2019NMR K¥2019NMR(agilent)¥koba¥SK19052506.fid¥fid				
Frequency (MHz)	300.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	17080
Points Count	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1698.7450	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4803.07	***Temperature (degree C)***	AMBIENT TEMPERATURE

SK19052506

2f

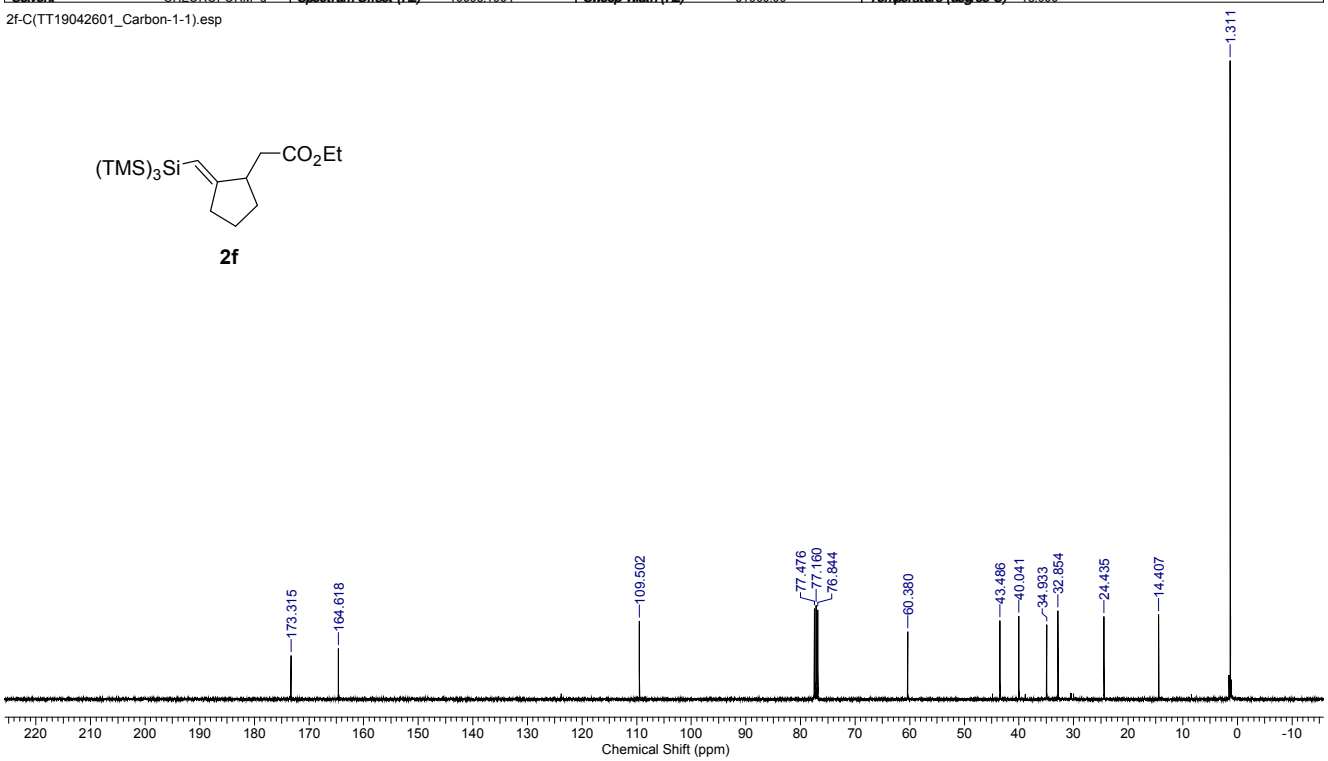


2019/05/28 14:42:54

Acquisition Time (sec)	1.0381	***Comment***	single pulse decoupled gated NOE			***Date***	26 Apr 2019 13:16:47
Date Stamp	26 Apr 2019 12:37:16						
File Name	¥¥Mac¥iCloud¥[redacted]NMR¥[redacted]¥2019NMR K¥2019NMR(JEOL)¥[redacted]NMR2019¥TT19042601_Carbon-1-1.jdf						
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1024	***Origin***	ECA
Original Points Count	32768	***Owner***	delta	***Points Count***	65536	***Pulse Sequence***	carbon.jxp
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	10058.1504	***Sweep Width (Hz)***	31565.66	***Temperature (degree C)***	18.600

2f-C(TT19042601_Carbon-1-1).esp

2f

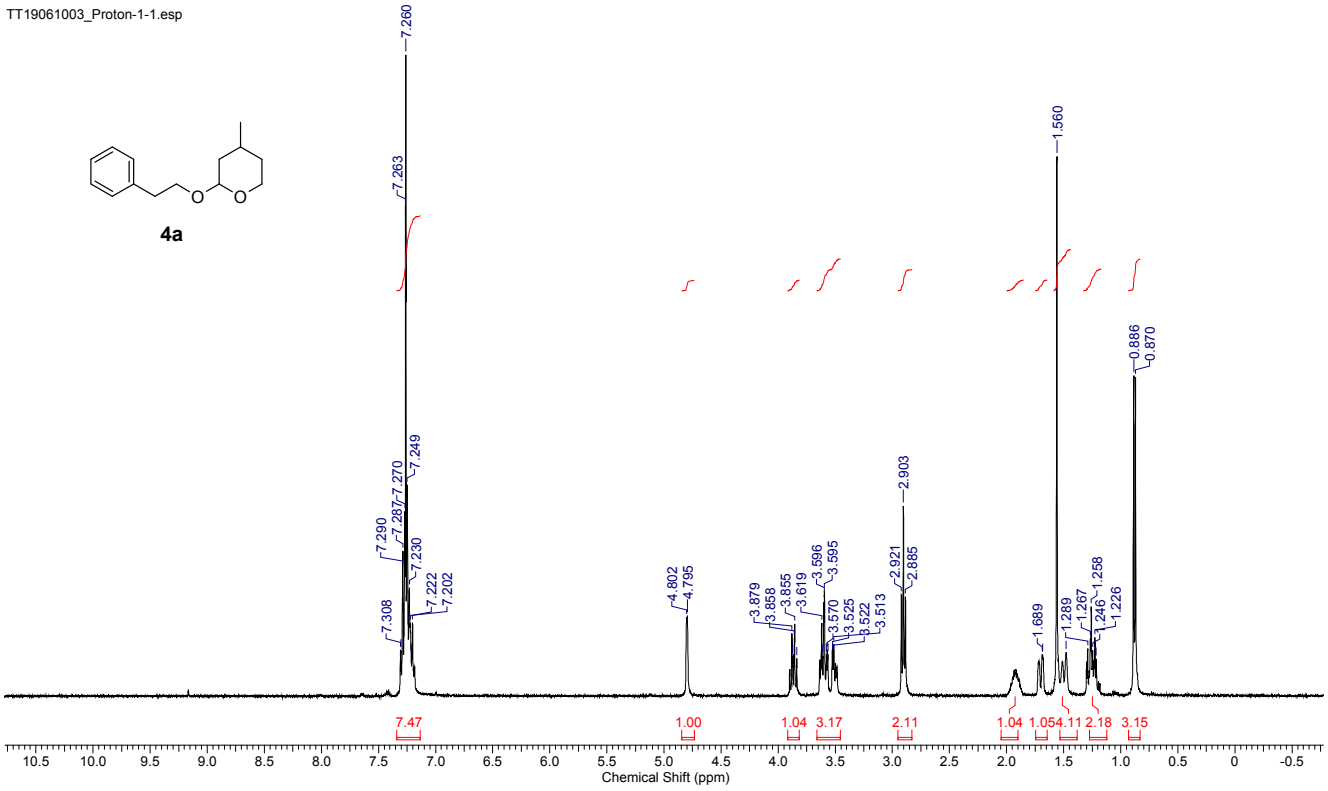


2019/06/25 12:36:12

Acquisition Time (sec)	2.1863	*Comment*	single pulse	*Date*	10 Jun 2019 13:42:09			*Date Stamp*	10 Jun 2019 13:41:18
File Name	¥¥WS¥data¥▒▒▒▒▒▒TT19061003 Proton-1-1.jdf			*Frequency (MHz)*	399.78	*Nucleus*	1H	*Number of Transients*	8
Origin	ECA	*Original Points Count*	16384	*Owner*	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	2003.9476	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	19.800

TT19061003_Proton-1-1.esp

4a

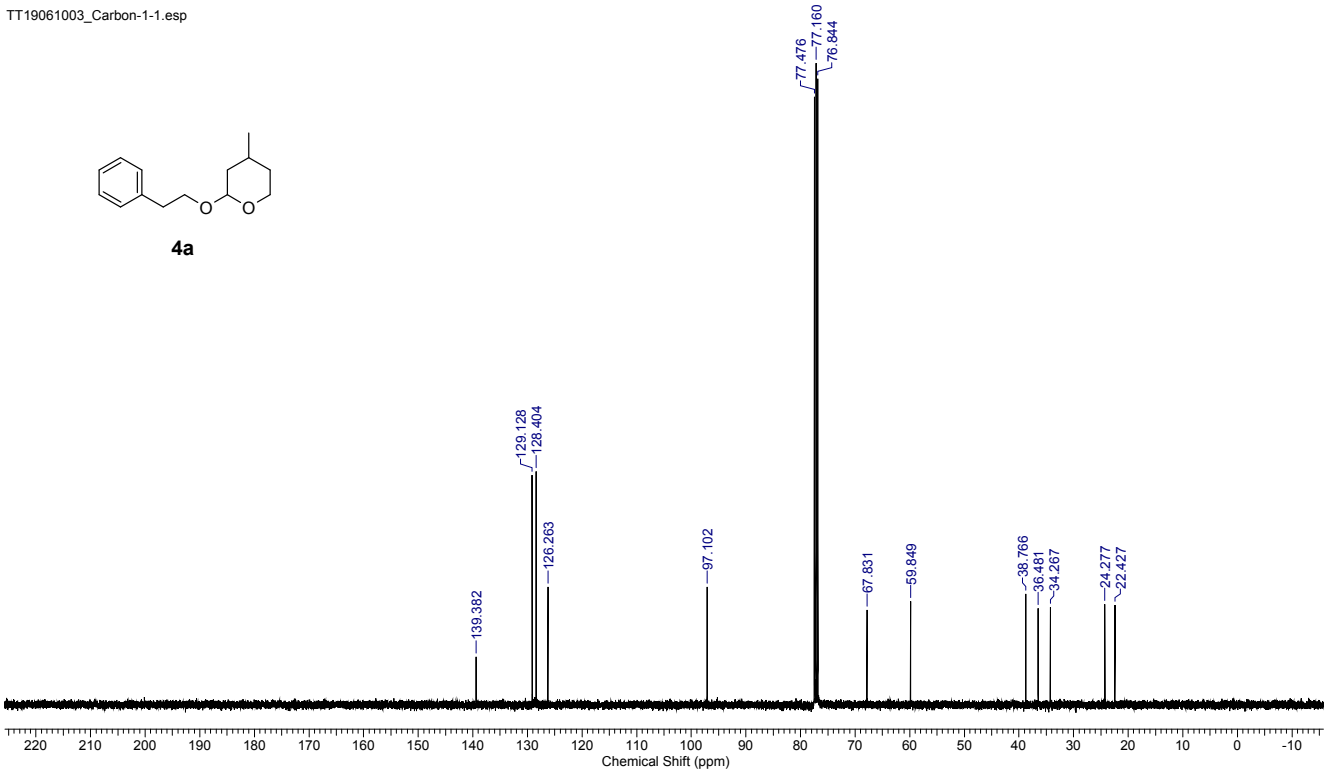


2019/06/25 12:38:25

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	14 Jun 2019 08:52:38		
Date Stamp	14 Jun 2019 08:13:06			*File Name*	¥¥WS¥data¥▒▒▒▒▒▒TT19061003 Carbon-1-1.jdf			*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	1024	*Origin*	ECA	*Original Points Count*	32768	*Owner*	delta
Points Count	65536	*Pulse Sequence*	carbon.jxp	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	10058.1504
Sweep Width (Hz)	31565.66	*Temperature (degree C)*	21.100						

TT19061003_Carbon-1-1.esp

4a

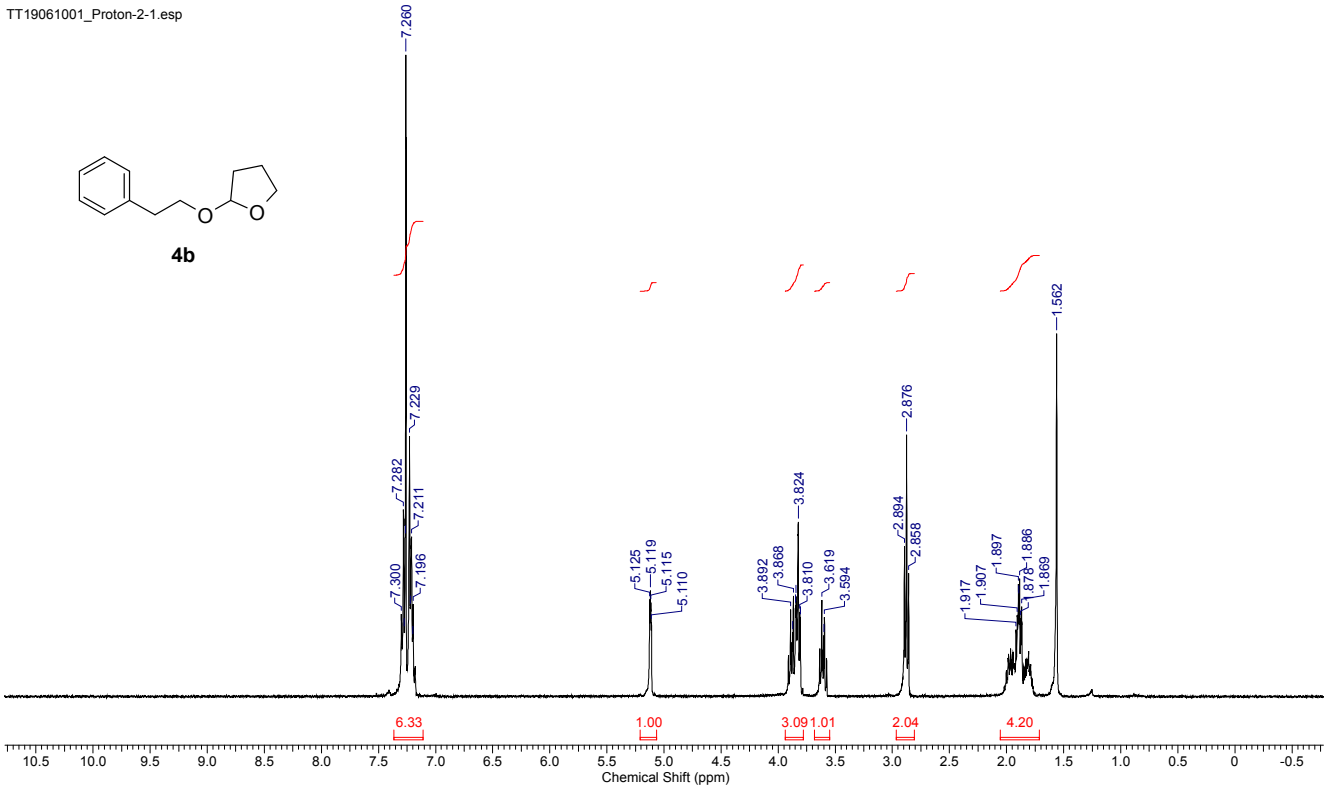


2019/06/25 12:40:24

Acquisition Time (sec)	2.1863	*Comment*	single pulse	*Date*	10 Jun 2019 13:30:16			*Date Stamp*	10 Jun 2019 13:29:24
File Name	¥¥WS¥data¥▒▒▒▒▒▒TT19061001 Proton-2-1.jdf			*Frequency (MHz)*	399.78	*Nucleus*	1H	*Number of Transients*	8
Origin	ECA	*Original Points Count*	16384	*Owner*	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	2003.2618	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	20.000

TT19061001_Proton-2-1.esp

4b

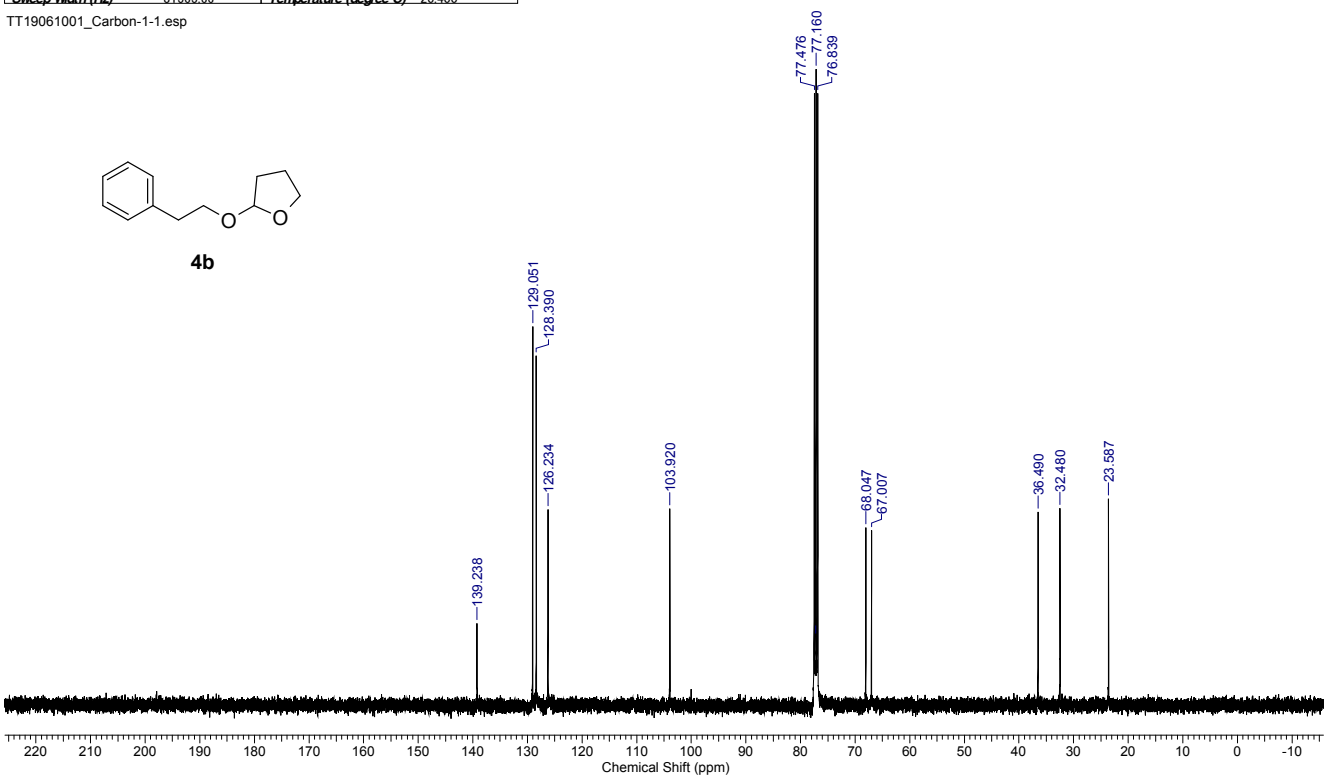


2019/06/25 12:41:24

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	14 Jun 2019 13:24:13		
Date Stamp	14 Jun 2019 12:44:42			*File Name*	¥¥WS¥data¥▒▒▒▒▒▒TT19061001 Carbon-1-1.jdf			*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	1024	*Origin*	ECA	*Original Points Count*	32768	*Owner*	delta
Points Count	65536	*Pulse Sequence*	carbon.jxp	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	10056.7051
Sweep Width (Hz)	31565.66	*Temperature (degree C)*	20.400						

TT19061001_Carbon-1-1.esp

4b

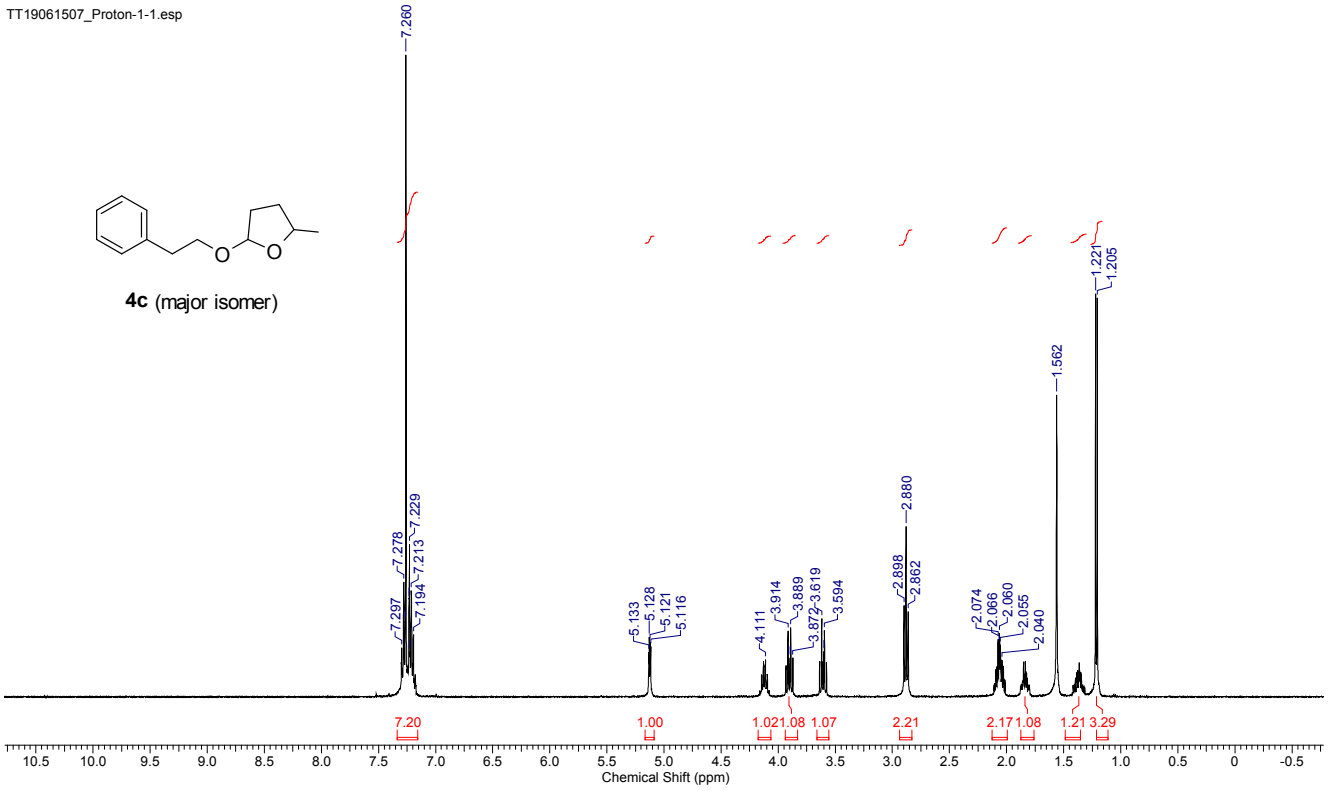


2019/06/25 12:44:12

Acquisition Time (sec)	2.1863	*Comment*	single pulse	*Date*	15 Jun 2019 11:56:09			*Date Stamp*	15 Jun 2019 11:55:18
File Name	¥¥WS¥data¥▒▒▒▒▒▒TT19061507 Proton-1-1.jdf			*Frequency (MHz)*	399.78	*Nucleus*	1H	*Number of Transients*	8
Origin	ECA	*Original Points Count*	16384	*Owner*	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	20.500

TT19061507_Proton-1-1.esp

4c (major isomer)

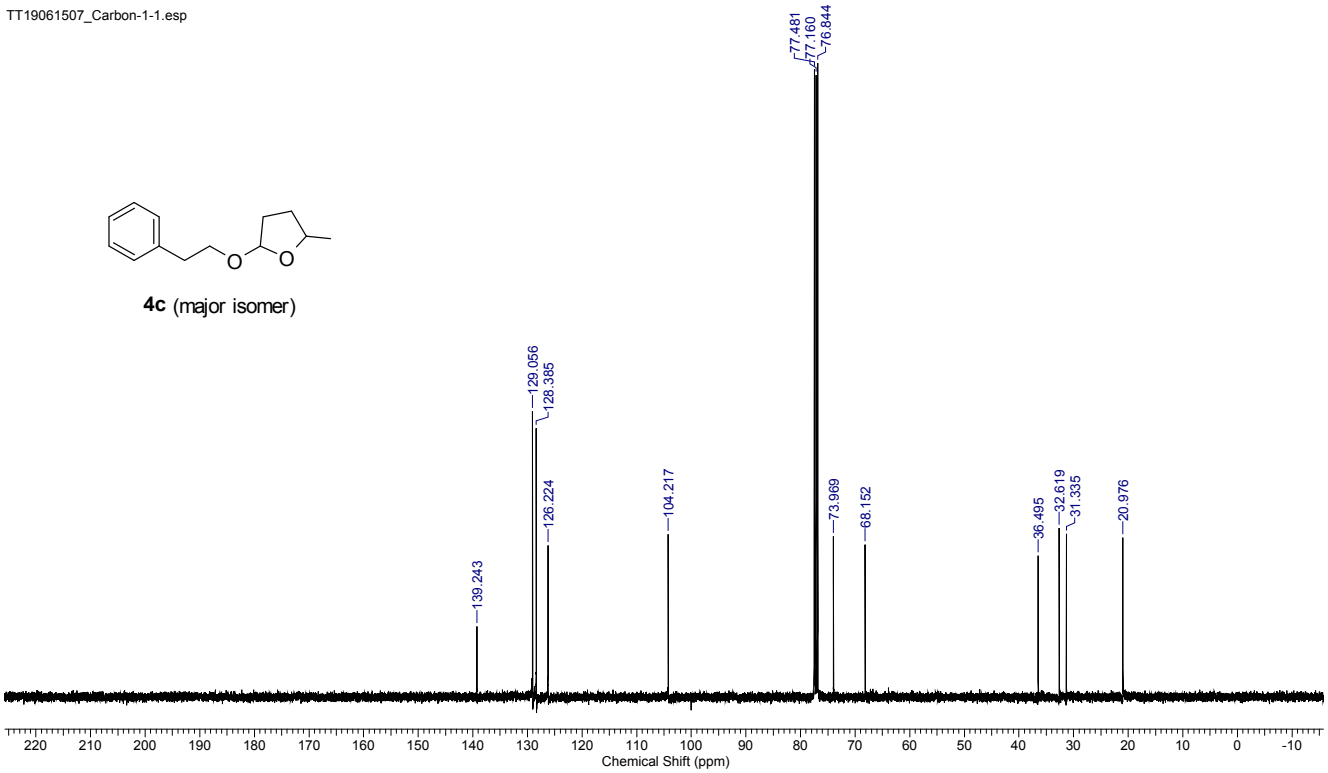


2019/06/25 12:46:31

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	17 Jun 2019 08:12:18		
Date Stamp	17 Jun 2019 07:32:47			*File Name*	¥¥WS¥data¥▒▒▒▒▒▒TT19061507 Carbon-1-1.jdf			*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	1024	*Origin*	ECA	*Original Points Count*	32768	*Owner*	delta
Points Count	65536	*Pulse Sequence*	carbon.jxp	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	10056.7051
Sweep Width (Hz)	31565.66	*Temperature (degree C)*	18.700						

TT19061507_Carbon-1-1.esp

4c (major isomer)

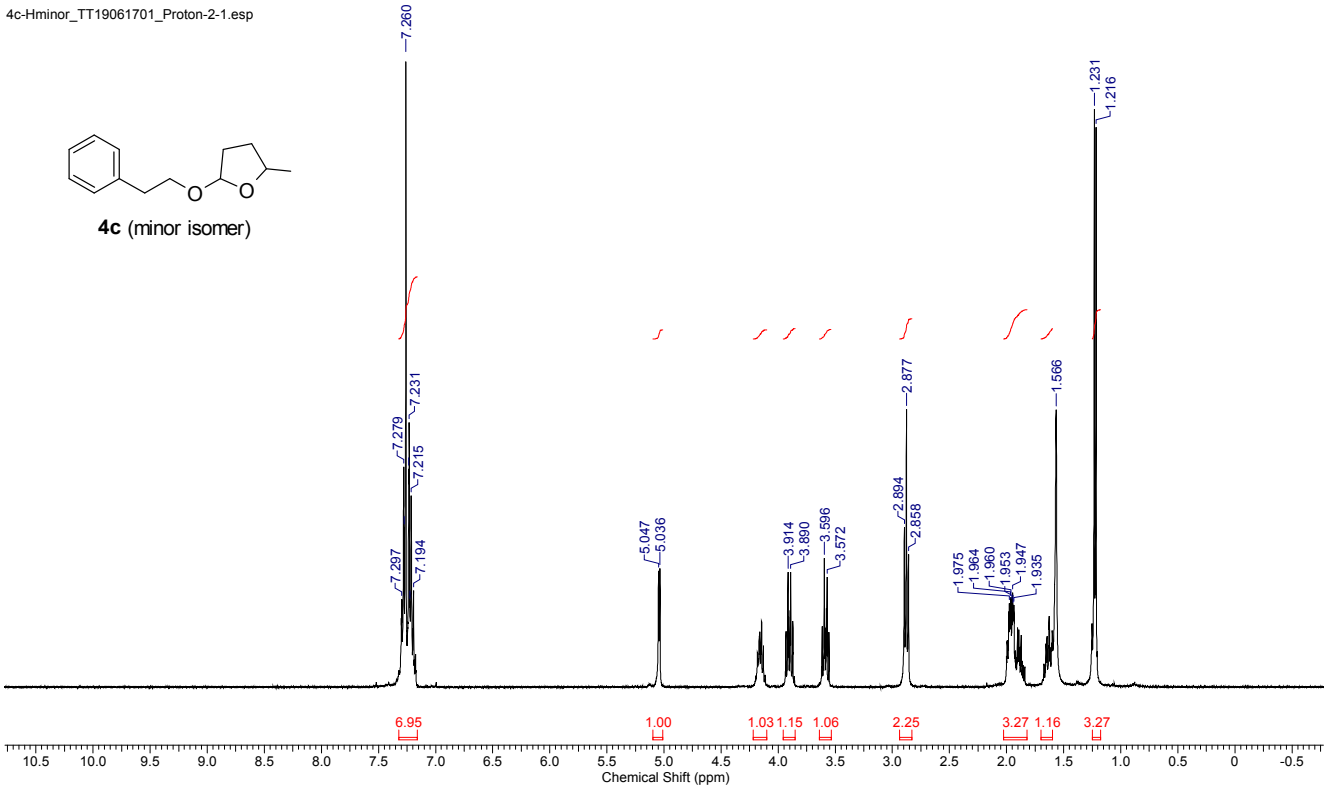


2019/06/25 15:11:46

Acquisition Time (sec)	2.1863	*Comment*	single pulse	*Date*	17 Jun 2019 13:07:34			*Date Stamp*	17 Jun 2019 13:06:43
File Name	¥¥WS¥data¥▒▒▒▒▒▒TT19061701 Proton-2-1.jdf			*Frequency (MHz)*	399.78	*Nucleus*	1H	*Number of Transients*	8
Origin	ECA	*Original Points Count*	16384	*Owner*	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	2003.7192	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	20.400

4c-Hminor_TT19061701_Proton-2-1.esp

4c (minor isomer)

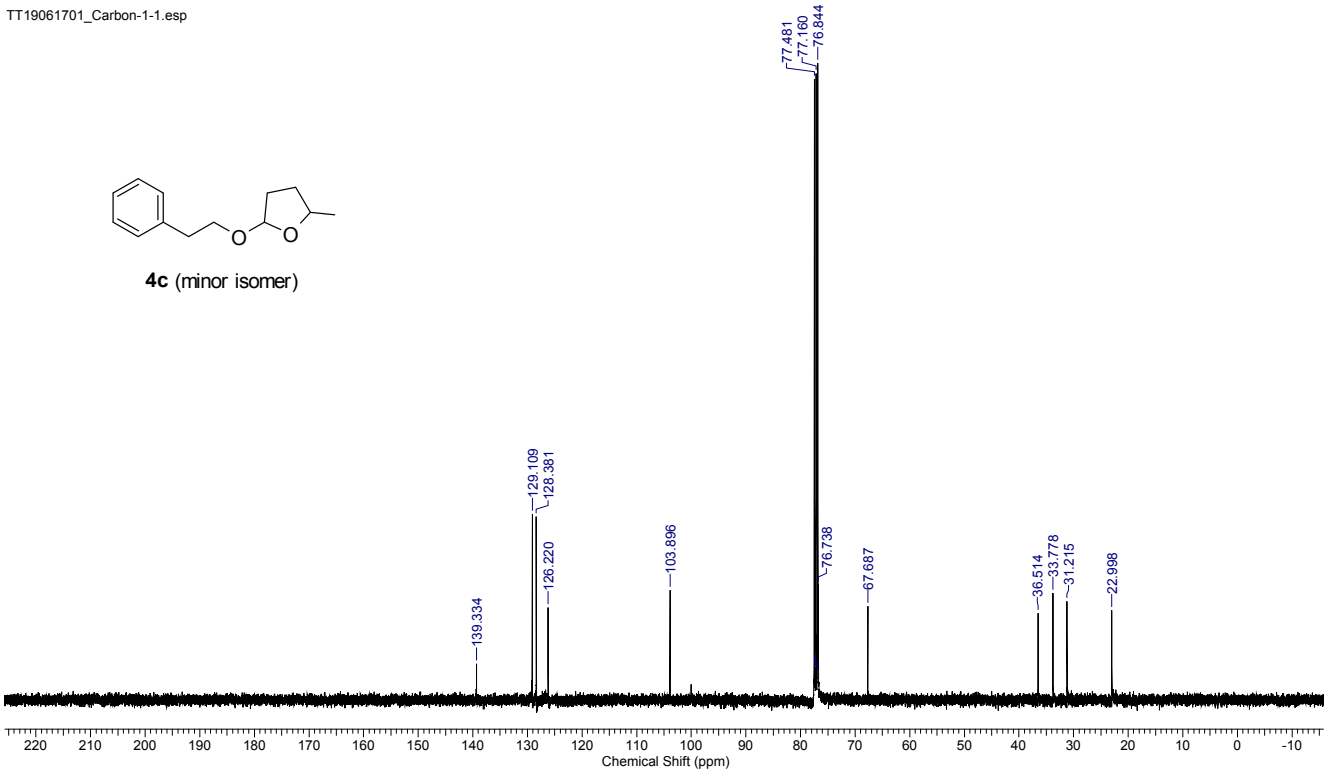


2019/06/25 12:53:13

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	17 Jun 2019 11:17:36		
Date Stamp	17 Jun 2019 11:01:27			*File Name*	¥¥WS¥data¥▒▒▒▒▒▒TT19061701 Carbon-1-1.jdf			*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	756	*Origin*	ECA	*Original Points Count*	32768	*Owner*	delta
Points Count	65536	*Pulse Sequence*	carbon.jxp	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	10057.6689
Sweep Width (Hz)	31565.66	*Temperature (degree C)*	19.600						

TT19061701_Carbon-1-1.esp

4c (minor isomer)

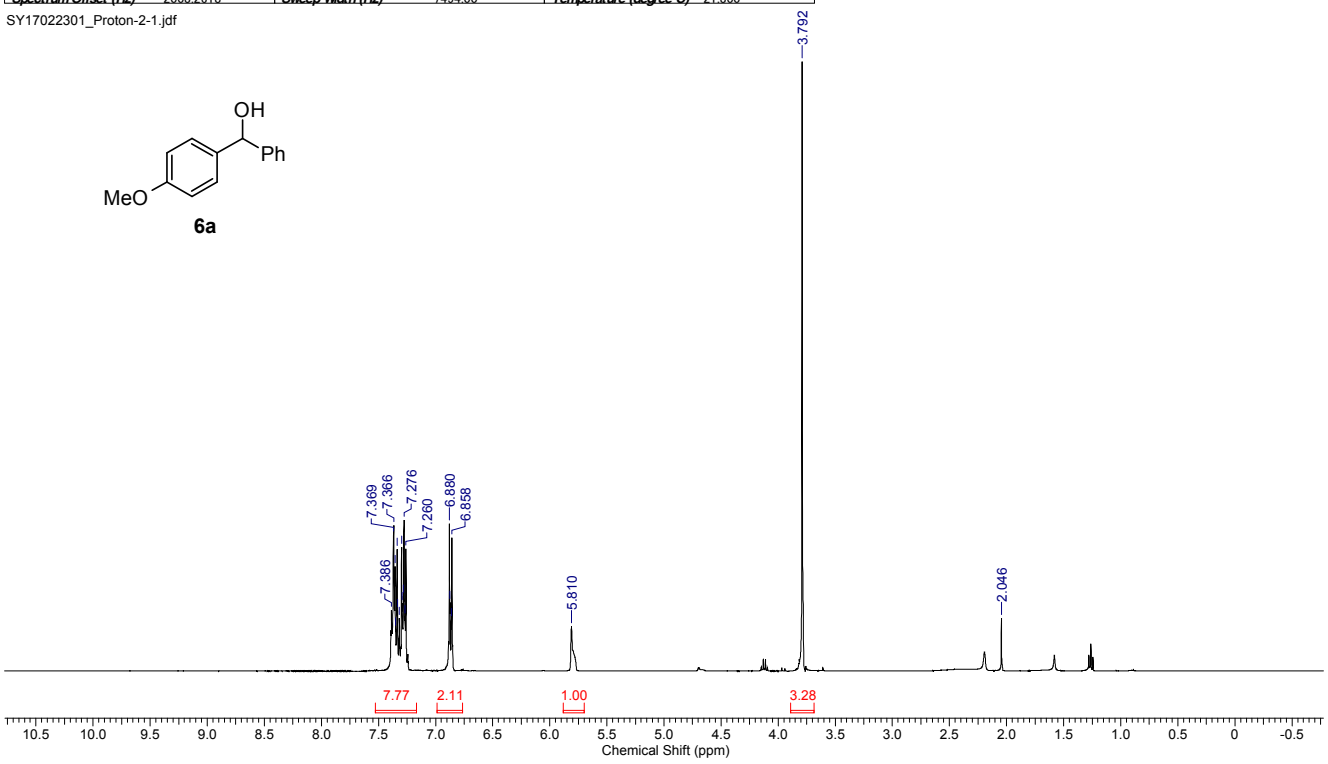


2019/03/02 14:09:19

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	23 Feb 2017 13:05:05		
Date Stamp	23 Feb 2017 13:04:14						
File Name	¥¥Mac¥iCloud¥[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY17022301 Proton-2-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.2618	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	21.300		

SY17022301_Proton-2-1.jdf

6a

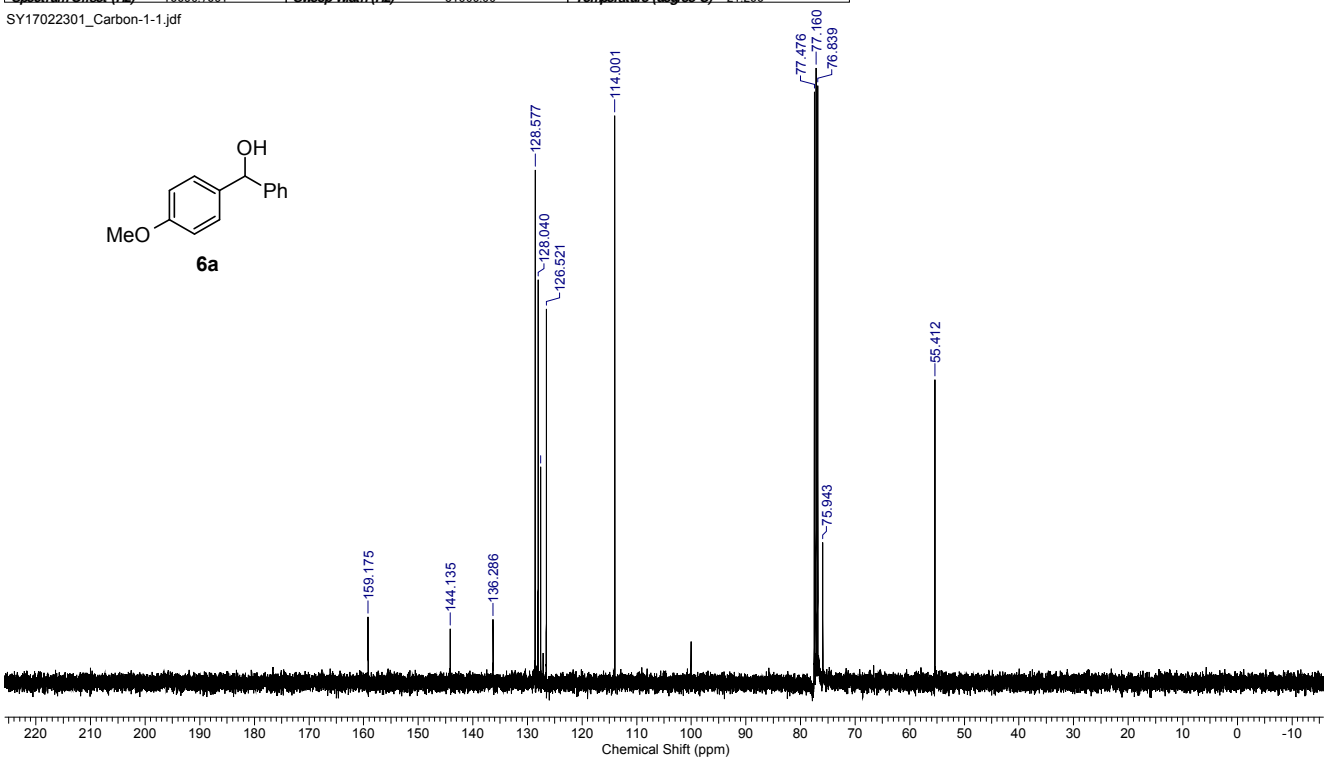


2019/03/02 14:15:45

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	23 Feb 2017 13:17:03
Date Stamp	23 Feb 2017 13:07:01						
File Name	¥¥Mac¥iCloud¥[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY17022301 Carbon-1-1.jdf					*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	256	*Origin*	ECA	*Original Points Count*	32768
Owner	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	10056.7051	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	21.200		

SY17022301_Carbon-1-1.jdf

6a

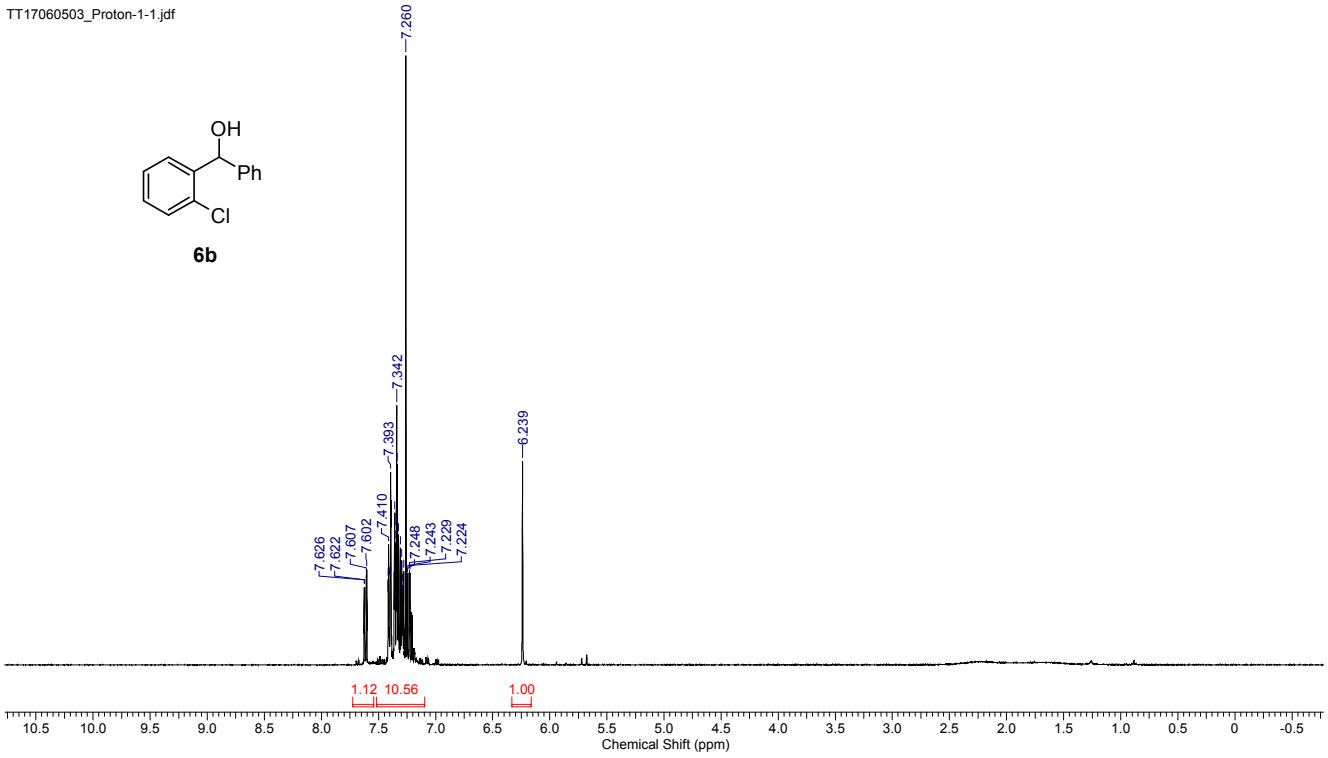


2019/03/02 14:46:39

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	05 Jun 2017 12:10:22
Date Stamp	05 Jun 2017 12:09:31				
File Name	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2017NMR K¥2017NMR(JEOL)¥[illegible]¥TT17060503 Proton-1-1.jdf			*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Spectrum Offset (Hz)	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	20.500

TT17060503_Proton-1-1.jdf

6b

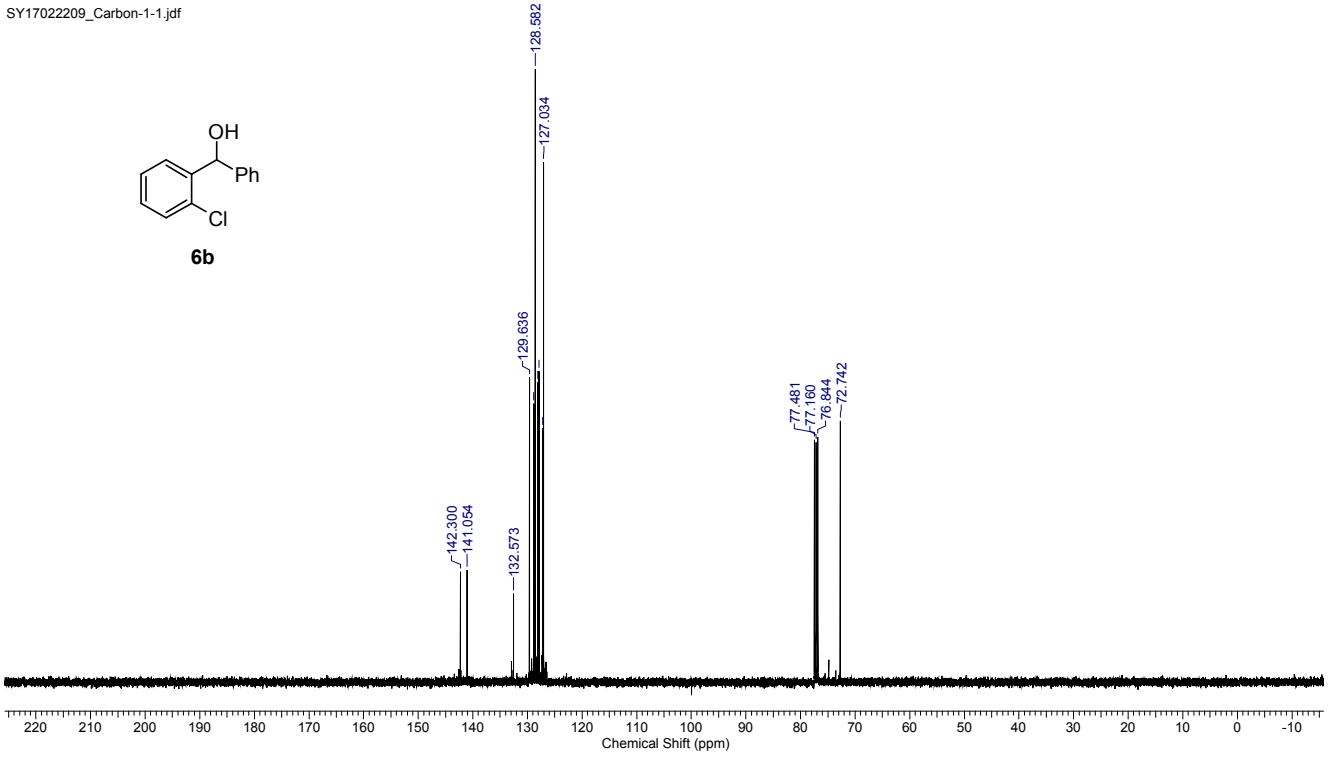


2019/03/02 14:53:35

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE	*Date*	22 Feb 2017 14:27:47
Date Stamp	22 Feb 2017 14:22:40				
File Name	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY17022209 Carbon-1-1.jdf			*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	128	*Origin*	ECA
Owner	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp
Spectrum Offset (Hz)	10049.9629	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	19.400

SY17022209_Carbon-1-1.jdf

6b

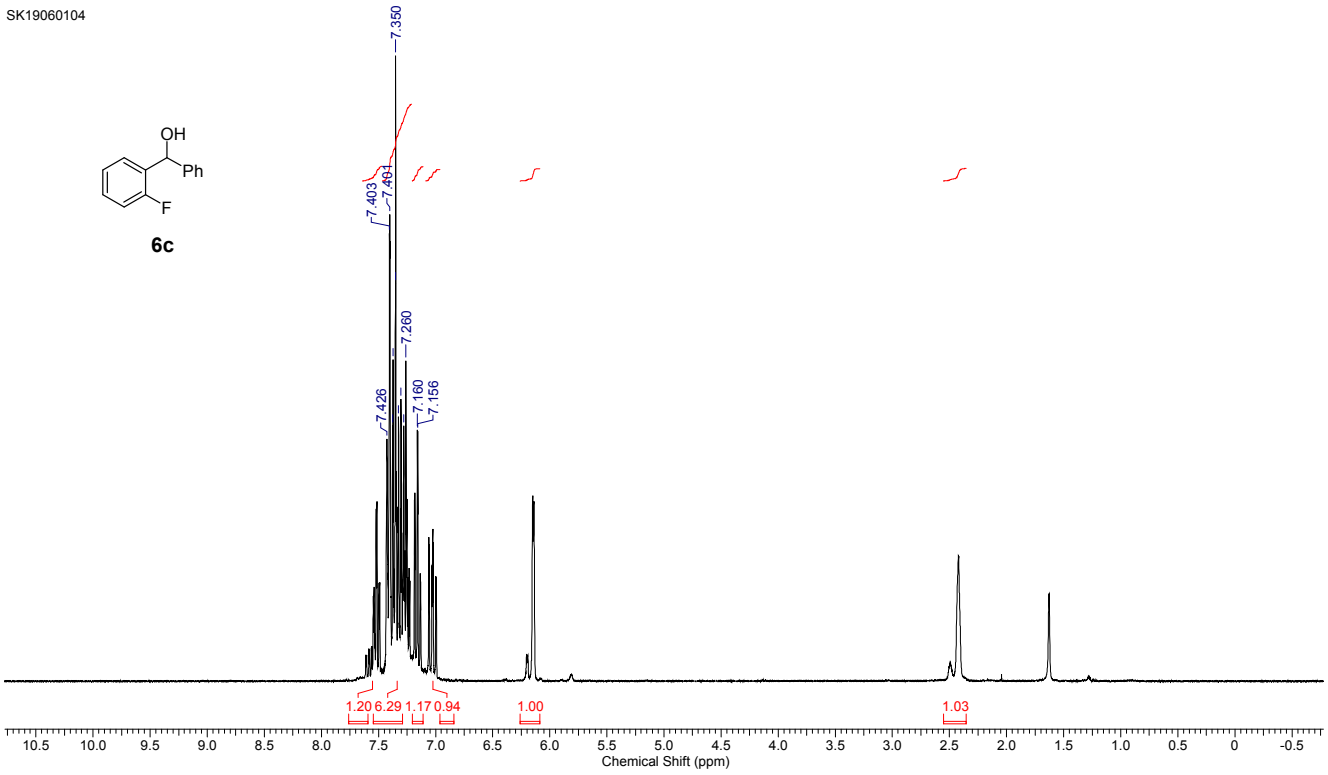


2019/06/03 10:19:52

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jun 1 2019
Date Stamp	Jun 1 2019	*File Name*	¥¥Mac¥iCloud¥[illegible]2019NMR K¥2019NMR(agilent)¥koba¥SK19060104.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	24.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1698.8915	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

SK19060104

6c

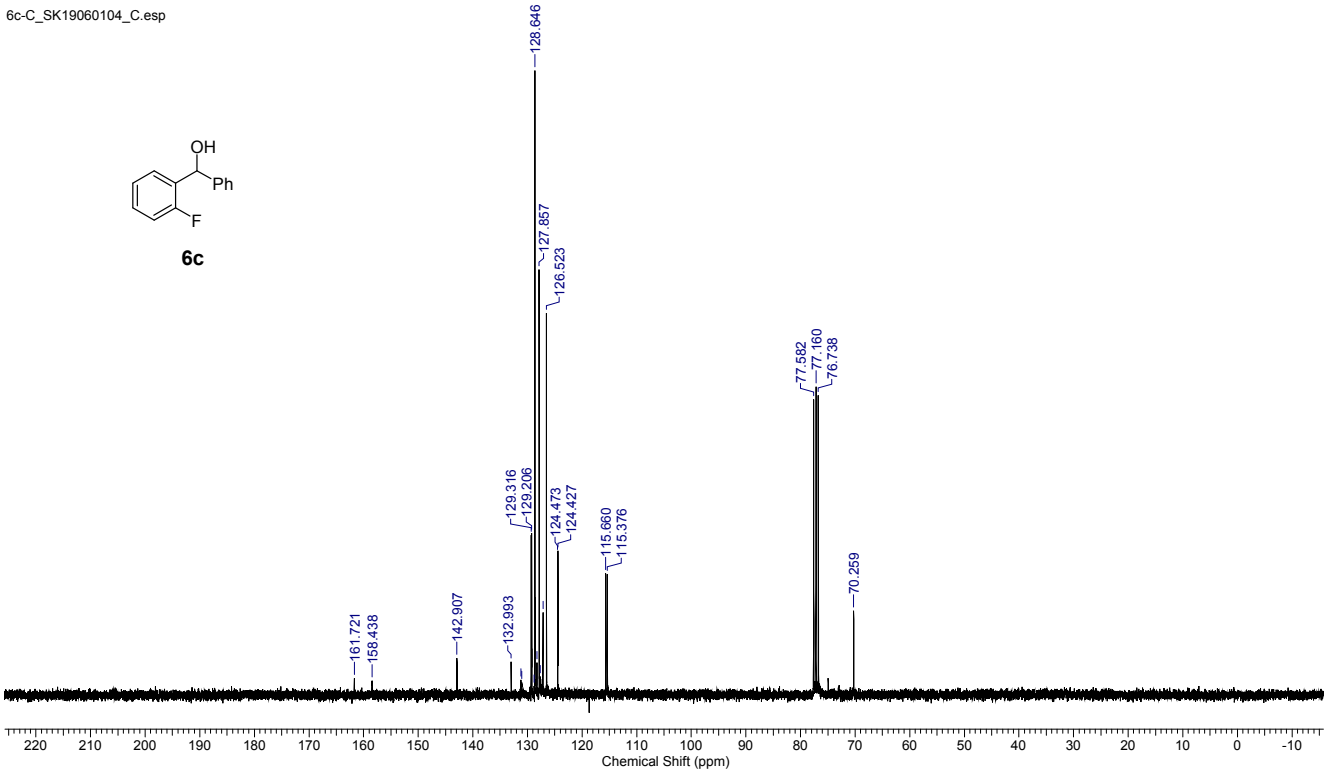


2019/06/03 13:14:37

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Jun 1 2019	*Date Stamp*	Jun 1 2019
File Name	¥¥Mac¥iCloud¥[illegible]2019NMR K¥2019NMR(agilent)¥koba¥SK19060104_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	1024	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8955.5654
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

6c-C_SK19060104_C.esp

6c

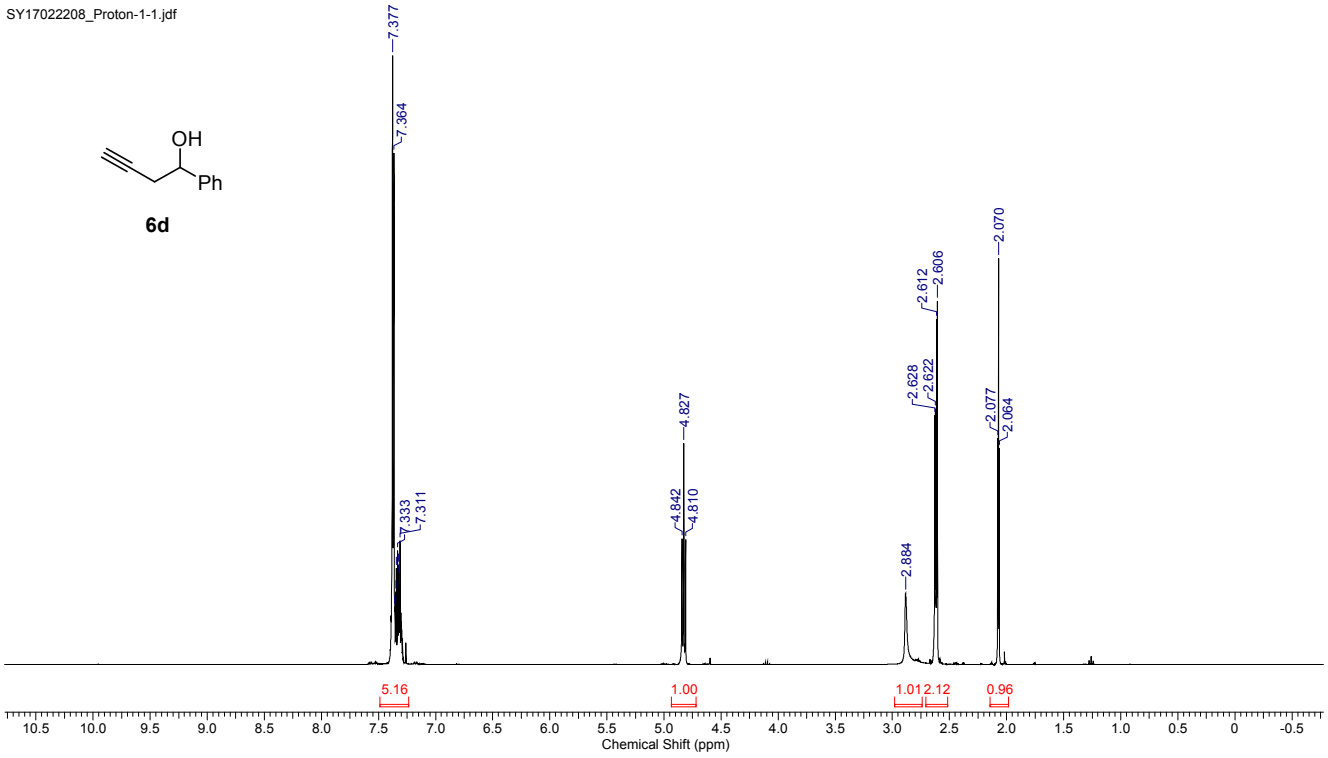


2019/03/02 15:40:19

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	22 Feb 2017 14:10:24		
Date Stamp	22 Feb 2017 14:09:33						
File Name	¥¥Mac¥iCloud¥[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY17022208 Proton-1-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.9476	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	19.300		

SY17022208_Proton-1-1.jdf

6d

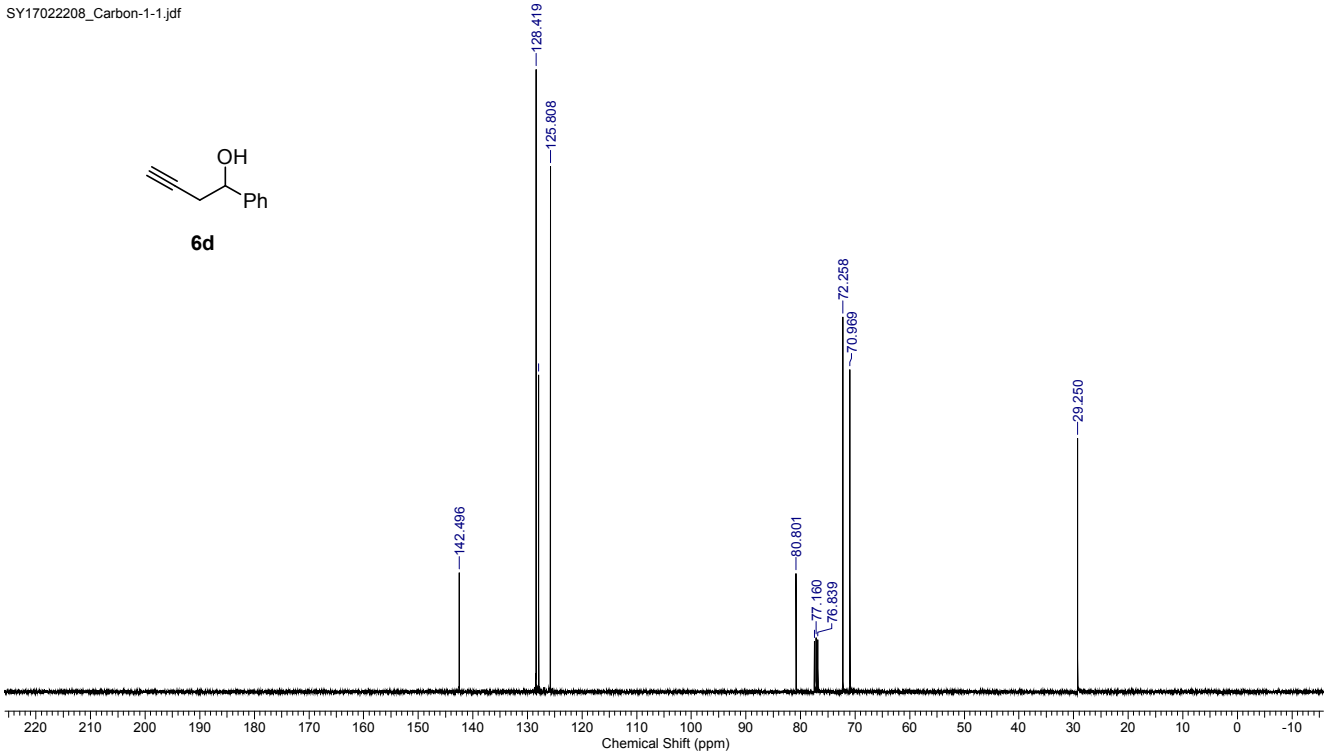


2019/03/02 15:43:06

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	22 Feb 2017 14:17:31
Date Stamp	22 Feb 2017 14:12:24						
File Name	¥¥Mac¥iCloud¥[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY17022208 Carbon-1-1.jdf					*Frequency (MHz)*	100.53
Nucleus	13C	*Number of Transients*	128	*Origin*	ECA	*Original Points Count*	32768
Owner	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	10036.4756	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	19.300		

SY17022208_Carbon-1-1.jdf

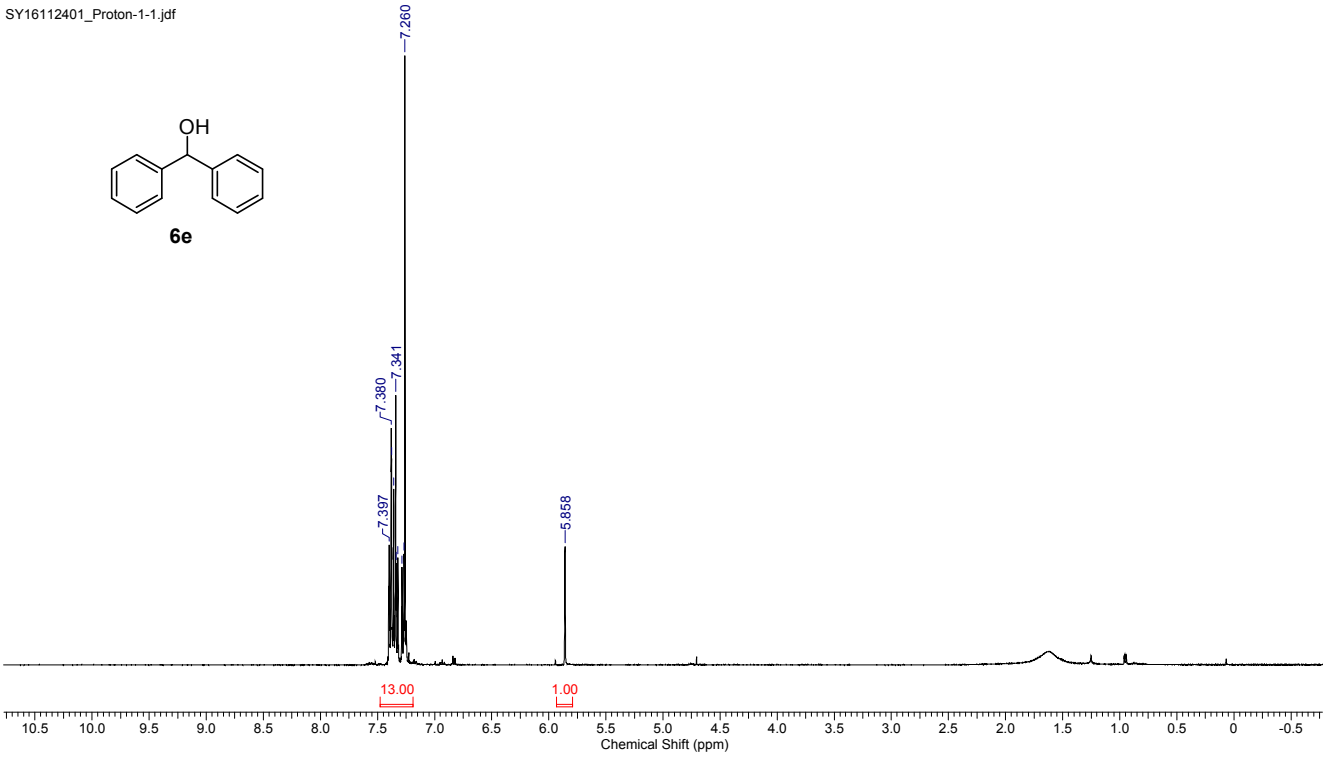
6d



2019/03/02 16:00:03

Acquisition Time (sec)	2.1863	***Comment***	single_pulse	***Date***	24 Nov 2016 08:16:25		
Date Stamp	24 Nov 2016 08:15:34						
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY16112401 Proton-1-1.jdf					***Frequency (MHz)***	399.78
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA	***Original Points Count***	16384
Owner	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2003.2618	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	17.200		

SY16112401_Proton-1-1.jdf

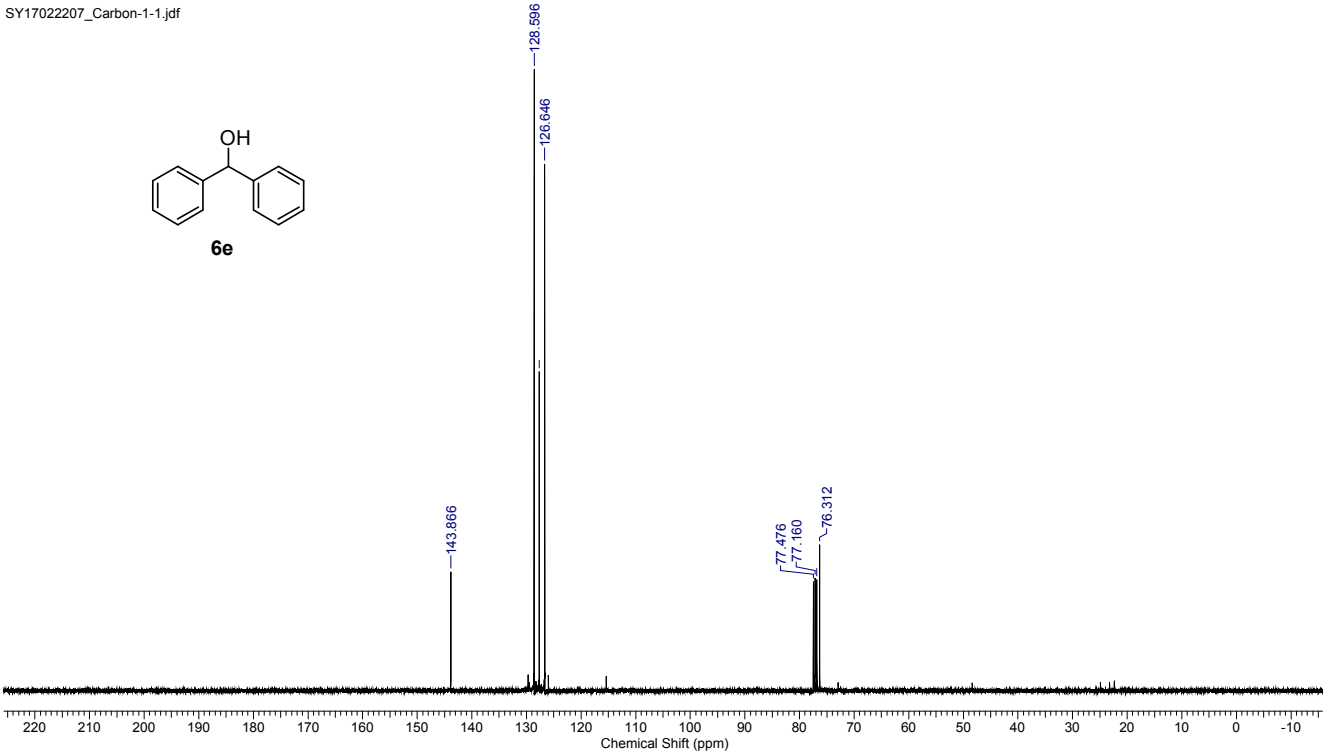


6e

2019/03/02 16:09:08

Acquisition Time (sec)	1.0381	***Comment***	single pulse decoupled gated NOE			***Date***	22 Feb 2017 13:10:04
Date Stamp	22 Feb 2017 13:04:52						
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]¥SY17022207 Carbon-1-1.jdf					***Frequency (MHz)***	100.53
Nucleus	13C	***Number of Transients***	130	***Origin***	ECA	***Original Points Count***	32768
Owner	delta	***Points Count***	65536	***Pulse Sequence***	carbon.jxp	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10049.4805	***Sweep Width (Hz)***	31565.66	***Temperature (degree C)***	19.100		

SY17022207_Carbon-1-1.jdf



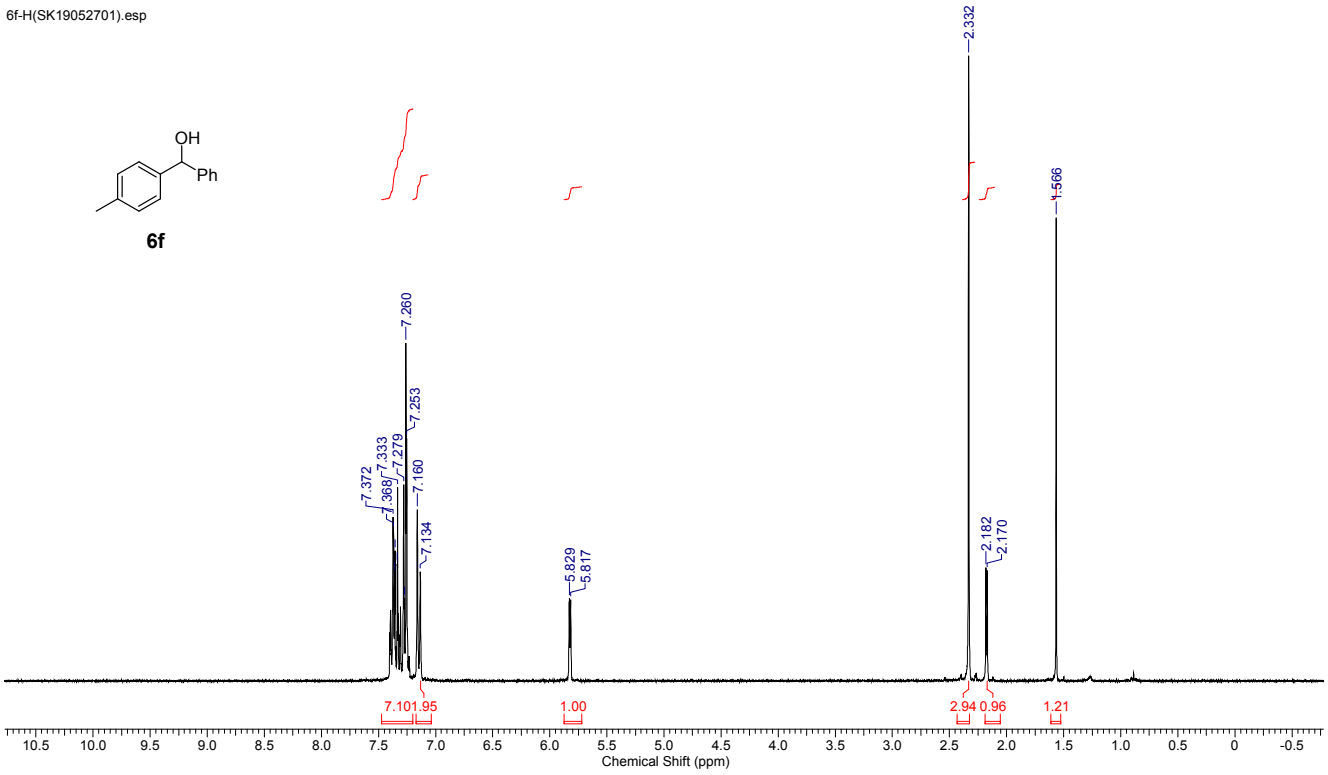
6e

2019/05/27 11:34:09

Acquisition Time (sec)	3.5561	***Comment***	STANDARD 1H OBSERVE			***Date***	May 27 2019
Date Stamp	May 27 2019	***File Name***	¥¥Mac¥iCloud¥[illegible]¥2019NMR K¥2019NMR(agilent)¥koba¥SK19052701.fid¥fid				
Frequency (MHz)	300.05	***Nucleus***	1H	***Number of Transients***	16	***Original Points Count***	17080
Points Count	65536	***Pulse Sequence***	s2pul	***Receiver Gain***	34.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1698.8181	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4803.07	***Temperature (degree C)***	AMBIENT TEMPERATURE

6f-H(SK19052701).esp

6f

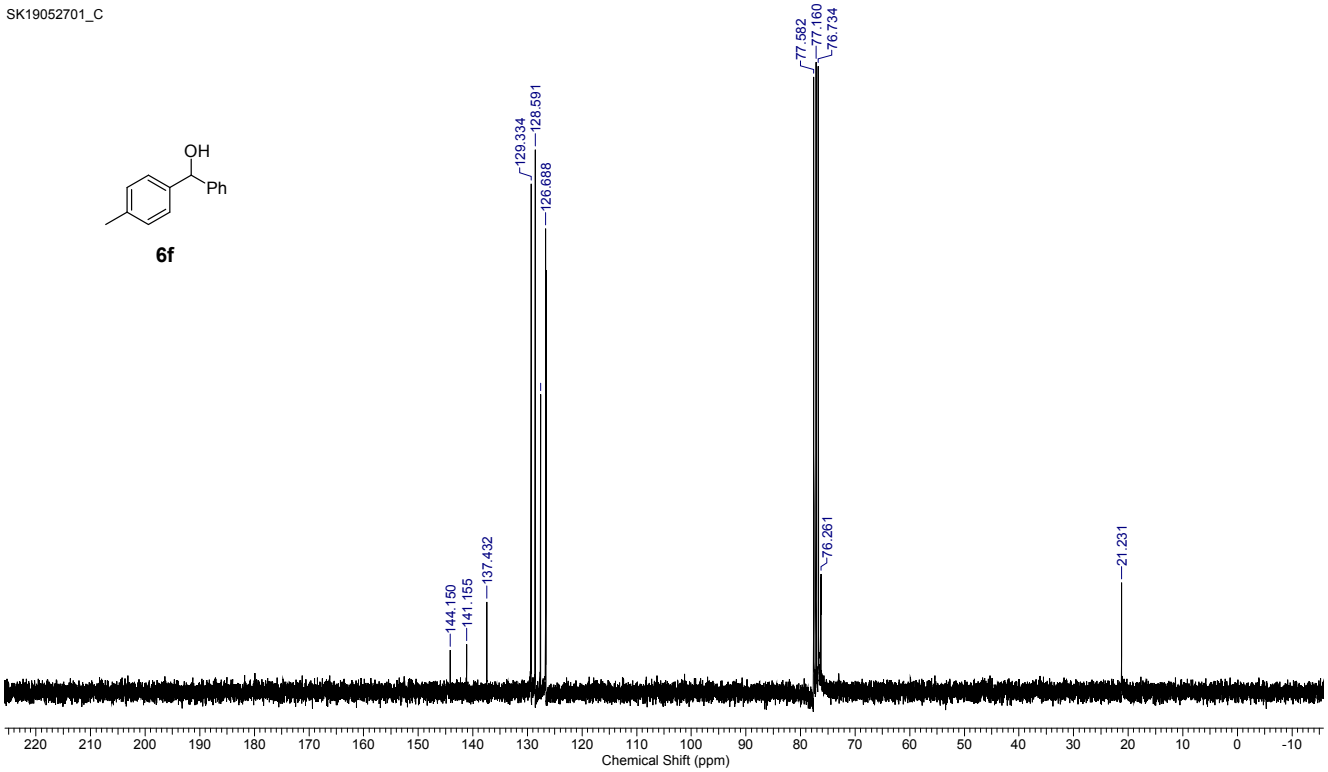


2019/05/27 11:50:14

Acquisition Time (sec)	0.8527	***Comment***	c13-NMR	***Date***	May 27 2019	***Date Stamp***	May 27 2019
File Name	¥¥Mac¥iCloud¥[illegible]¥2019NMR K¥2019NMR(agilent)¥koba¥SK19052701_C.fid¥fid					***Frequency (MHz)***	75.46
Nucleus	13C	***Number of Transients***	1024	***Original Points Count***	19335	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	8957.2959
Spectrum Type	STANDARD	***Sweep Width (Hz)***	22675.74	***Temperature (degree C)***	AMBIENT TEMPERATURE		

SK19052701_C

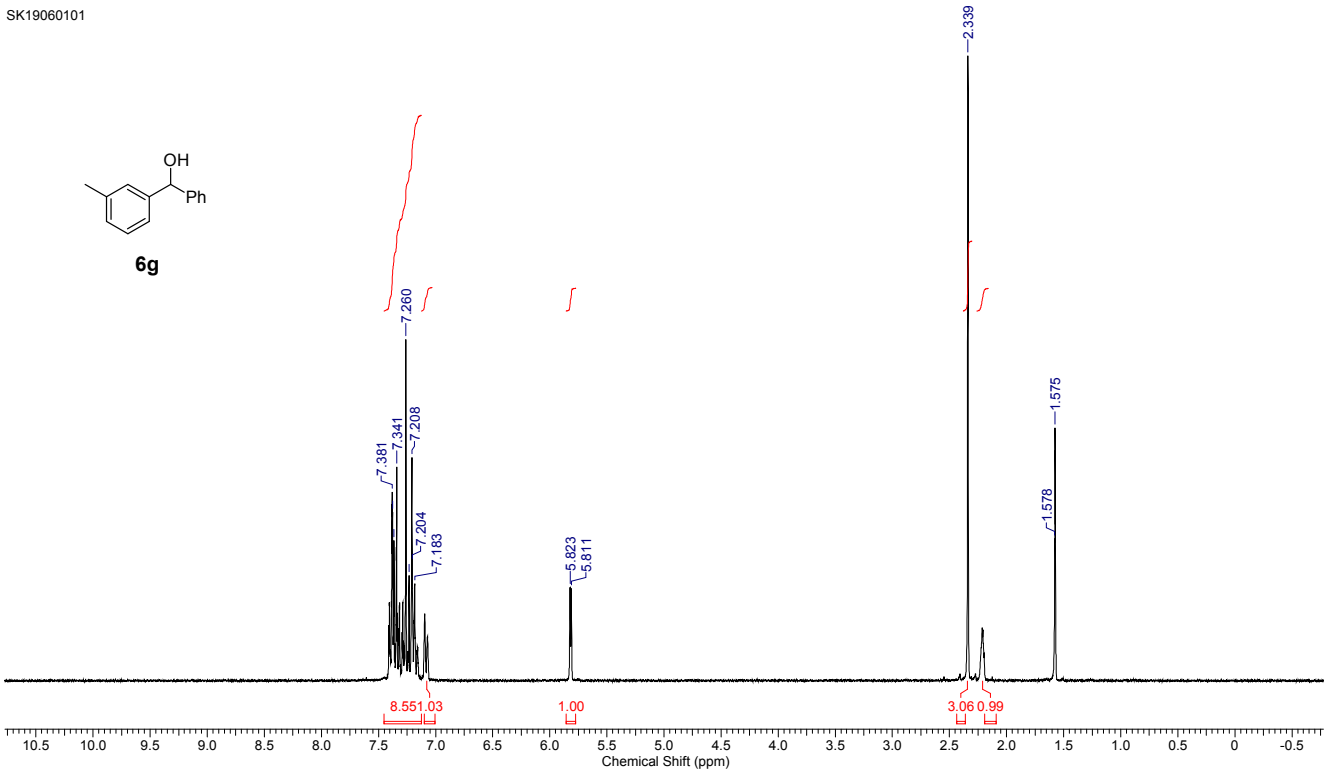
6f



2019/06/04 8:51:12

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jun 1 2019
Date Stamp	Jun 1 2019	*File Name*	¥¥Mac¥iCloud¥[illegible]2019NMR K¥2019NMR(agilent)¥koba¥SK19060101.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	34.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1698.8915	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

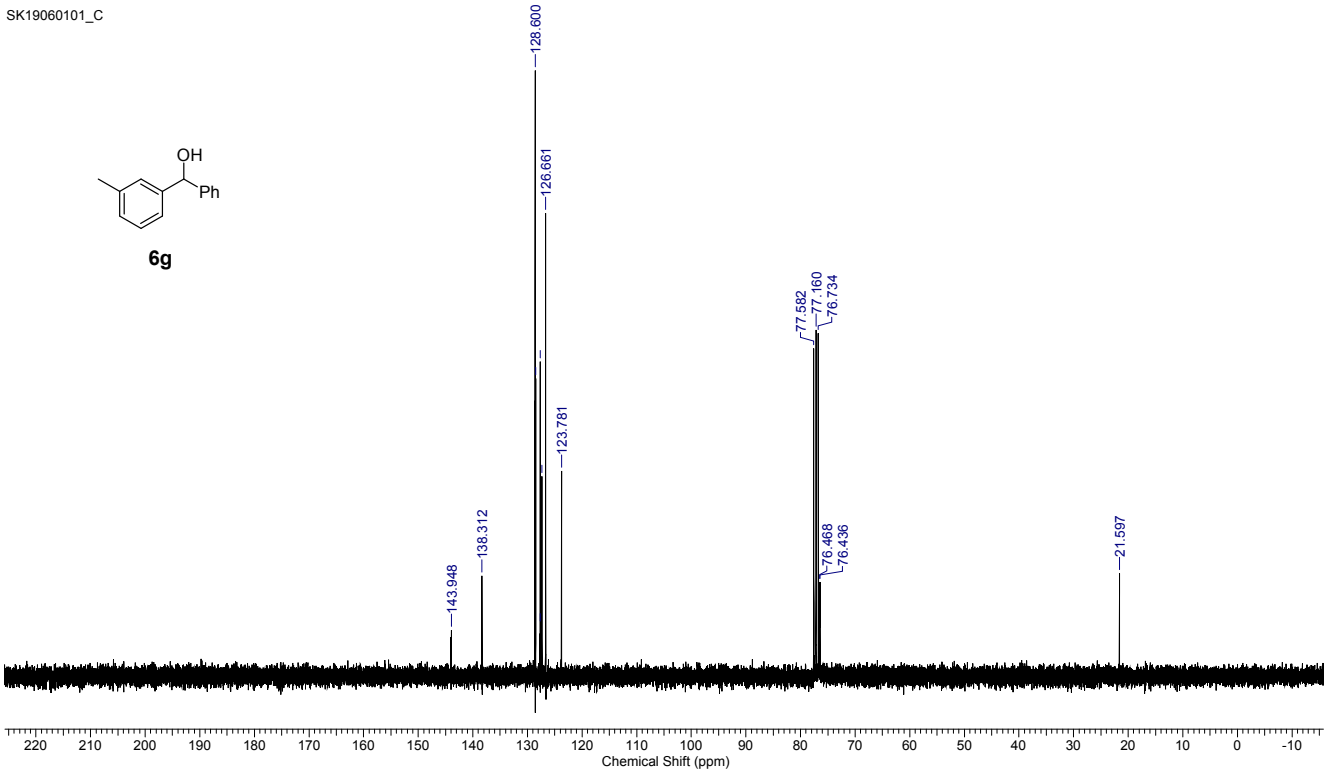
SK19060101



2019/06/04 8:58:21

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Jun 1 2019	*Date Stamp*	Jun 1 2019
File Name	¥¥Mac¥iCloud¥[illegible]2019NMR K¥2019NMR(agilent)¥koba¥SK19060101_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	512	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8955.9121
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

SK19060101_C

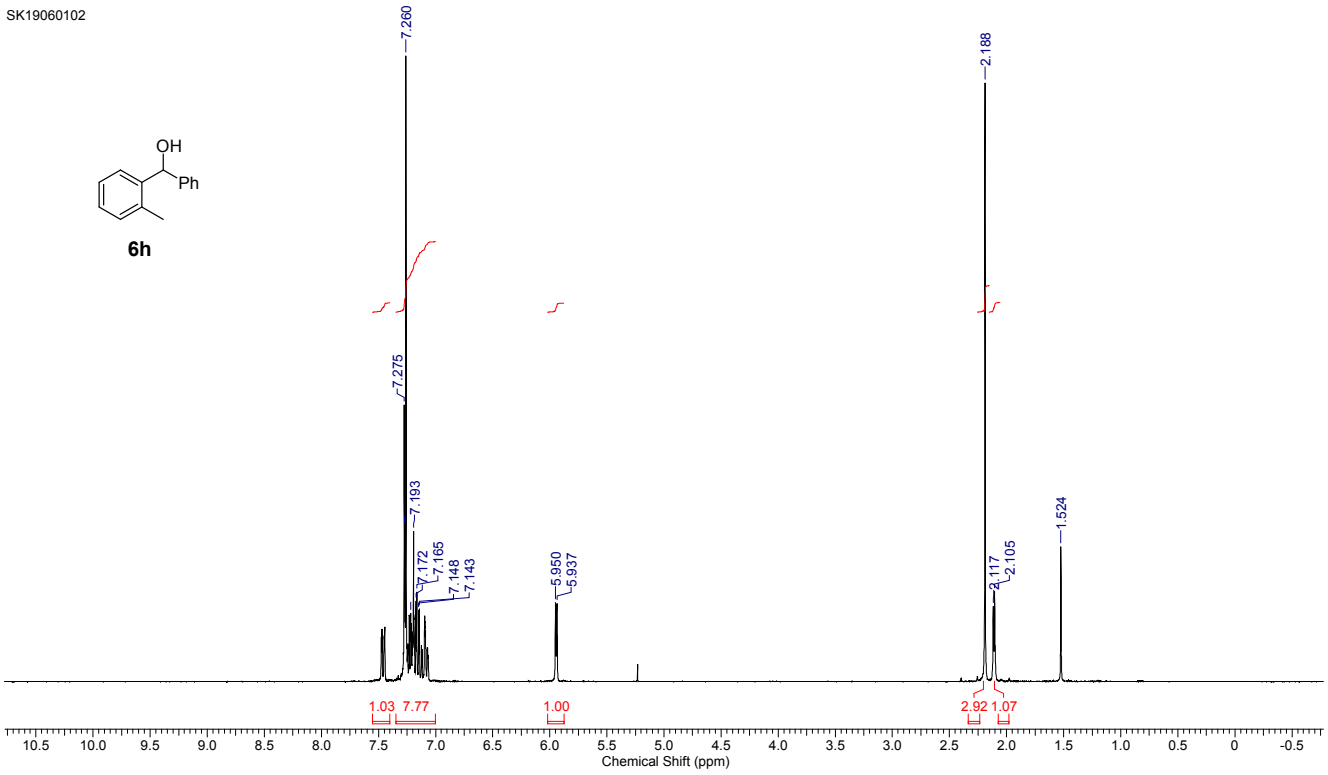


2019/06/04 9:17:20

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jun 1 2019
Date Stamp	Jun 1 2019	*File Name*	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2019NMR K¥2019NMR(agilent)¥koba¥SK19060102.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	24.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1678.7367	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

SK19060102

6h

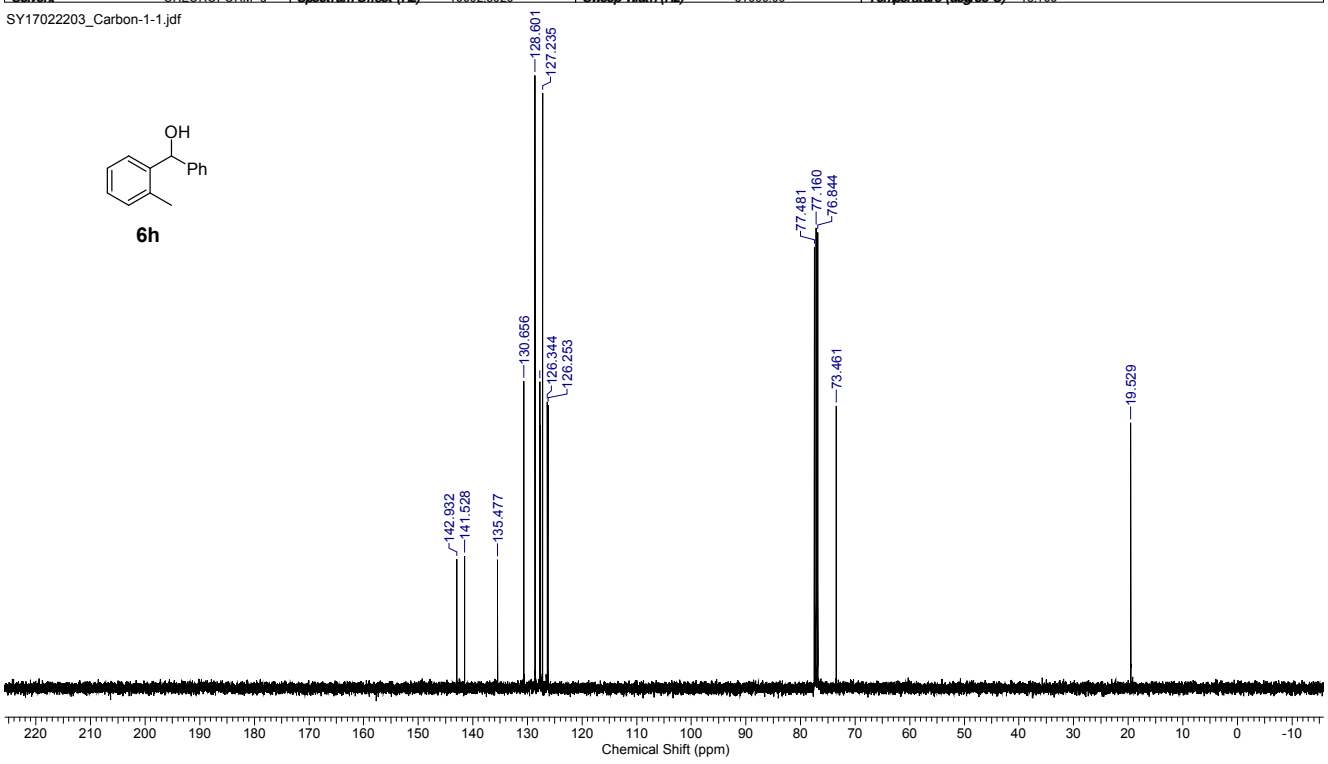


2019/06/04 9:28:56

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	22 Feb 2017 10:18:29
Date Stamp	22 Feb 2017 10:11:22						
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2016NMR K¥2016NMR(JEOL)¥[illegible]NMR2016¥SY17022203_Carbon-1-1.jdf						
Frequency (MHz)	100.53	*Nucleus*	13C	*Number of Transients*	180	*Origin*	ECA
Original Points Count	32768	*Owner*	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp
Solvent	CHLOROFORM-d	*Spectrum Offset (Hz)*	10052.8525	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	18.100

SY17022203_Carbon-1-1.jdf

6h

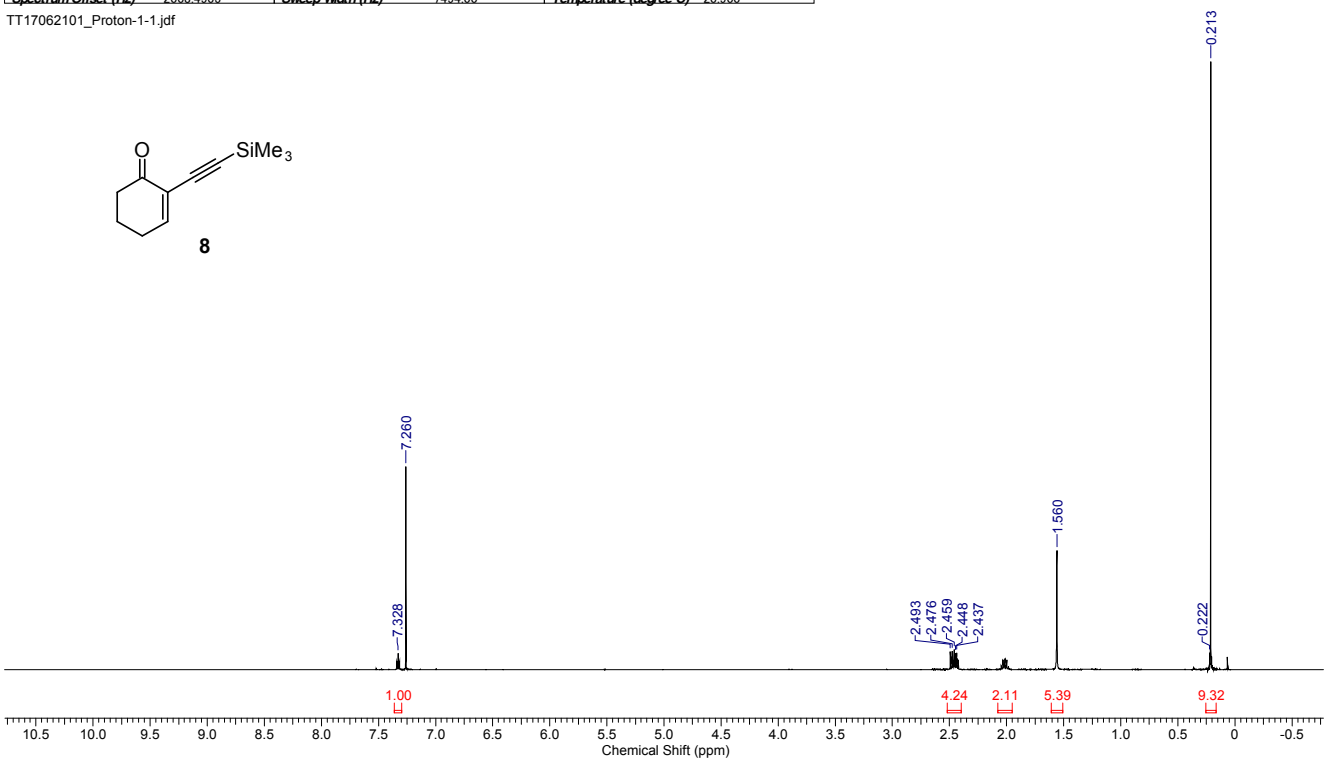


2019/03/02 16:52:32

Acquisition Time (sec)	2.1863	***Comment***	single_pulse	***Date***	21 Jun 2017 13:01:19
Date Stamp	21 Jun 2017 13:00:28				
File Name	¥¥Mac¥iCloud¥[illegible]¥2017NMR K¥2017NMR(JEOL)¥[illegible]¥TT17062101 Proton-1-1.jdf			***Frequency (MHz)***	399.78
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA
Original Points Count	16384	***Owner***	delta	***Points Count***	32768
Pulse Sequence	proton.jxp	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2003.4905
Sweep Width (Hz)	7494.00	***Temperature (degree C)***	20.900		

TT17062101_Proton-1-1.jdf

8

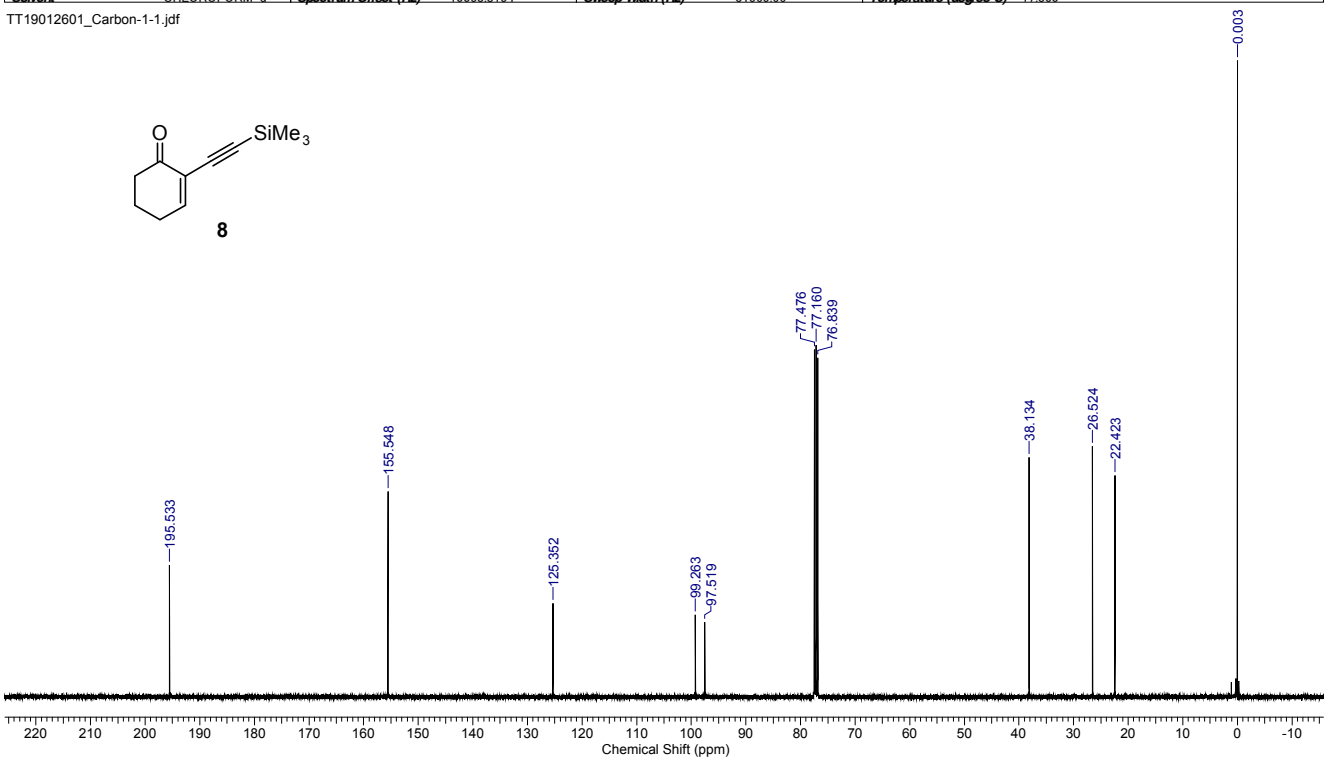


2019/03/07 19:44:44

Acquisition Time (sec)	1.0381	***Comment***	single pulse decoupled gated NOE	***Date***	26 Jan 2019 09:34:46
Date Stamp	26 Jan 2019 08:55:14				
File Name	¥¥Mac¥iCloud¥[illegible]¥2018NMR K¥2018NMR(JEOL)¥[illegible]¥NMR2018¥TT19012601 Carbon-1-1.jdf				
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1024
Origin	ECA	***Original Points Count***	32768	***Owner***	delta
Points Count	65536	***Pulse Sequence***	carbon.jxp	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	10053.8154	***Sweep Width (Hz)***	31565.66	***Temperature (degree C)***	17.300

TT19012601_Carbon-1-1.jdf

8

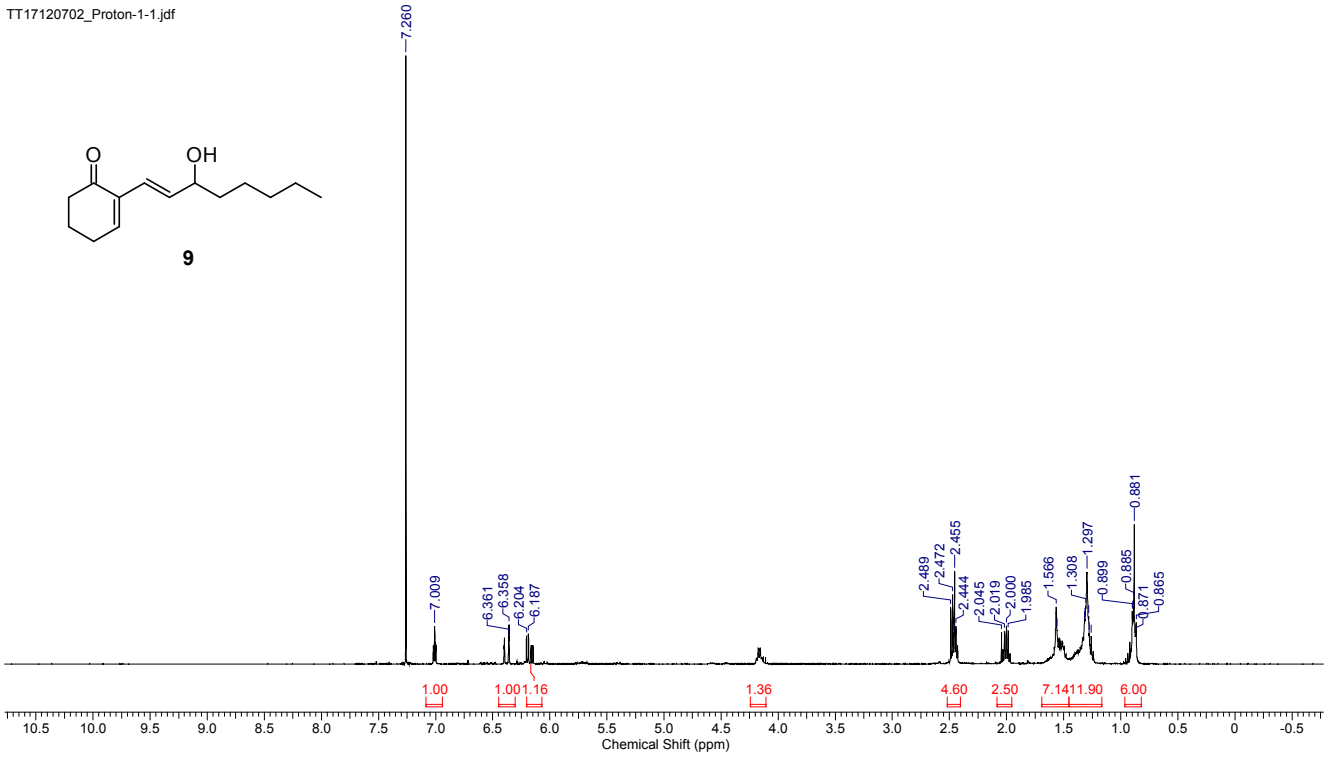


2019/03/04 10:16:00

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	07 Dec 2017 11:41:15		
Date Stamp	07 Dec 2017 11:40:24						
File Name	¥¥Mac¥iCloud¥[illegible]¥2017NMR K¥2017NMR(JEOL)¥[illegible]¥TT17120702_Proton-1-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	20.500		

TT17120702_Proton-1-1.jdf

9

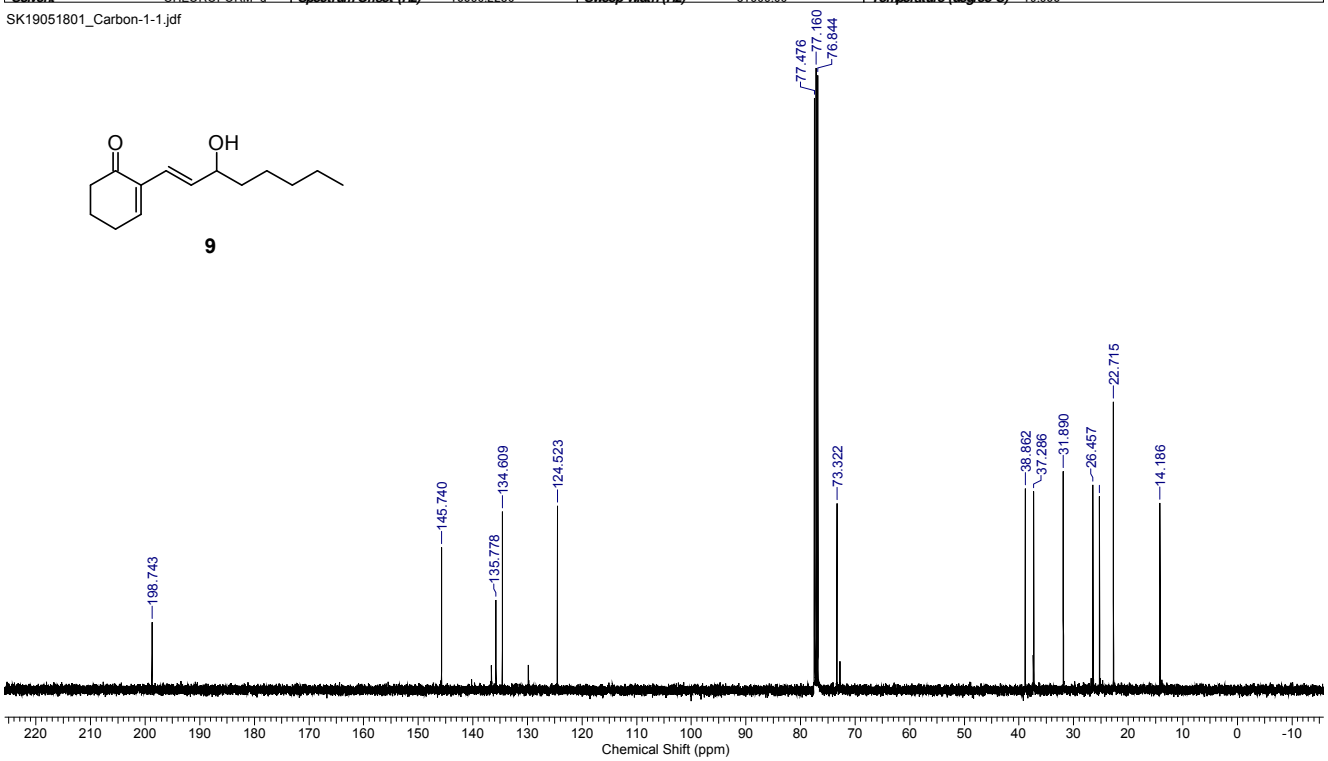


2019/05/18 14:12:29

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	18 May 2019 09:41:10
Date Stamp	18 May 2019 09:01:38						
File Name	¥¥Mac¥iCloud¥[illegible]¥2019NMR K¥2019NMR(JEOL)¥[illegible]NMR2019¥SK19051801_Carbon-1-1.jdf						
Frequency (MHz)	100.53	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	ECA
Original Points Count	32768	*Owner*	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp
Solvent	CHLOROFORM-d	*Spectrum Offset (Hz)*	10056.2236	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	19.500

SK19051801_Carbon-1-1.jdf

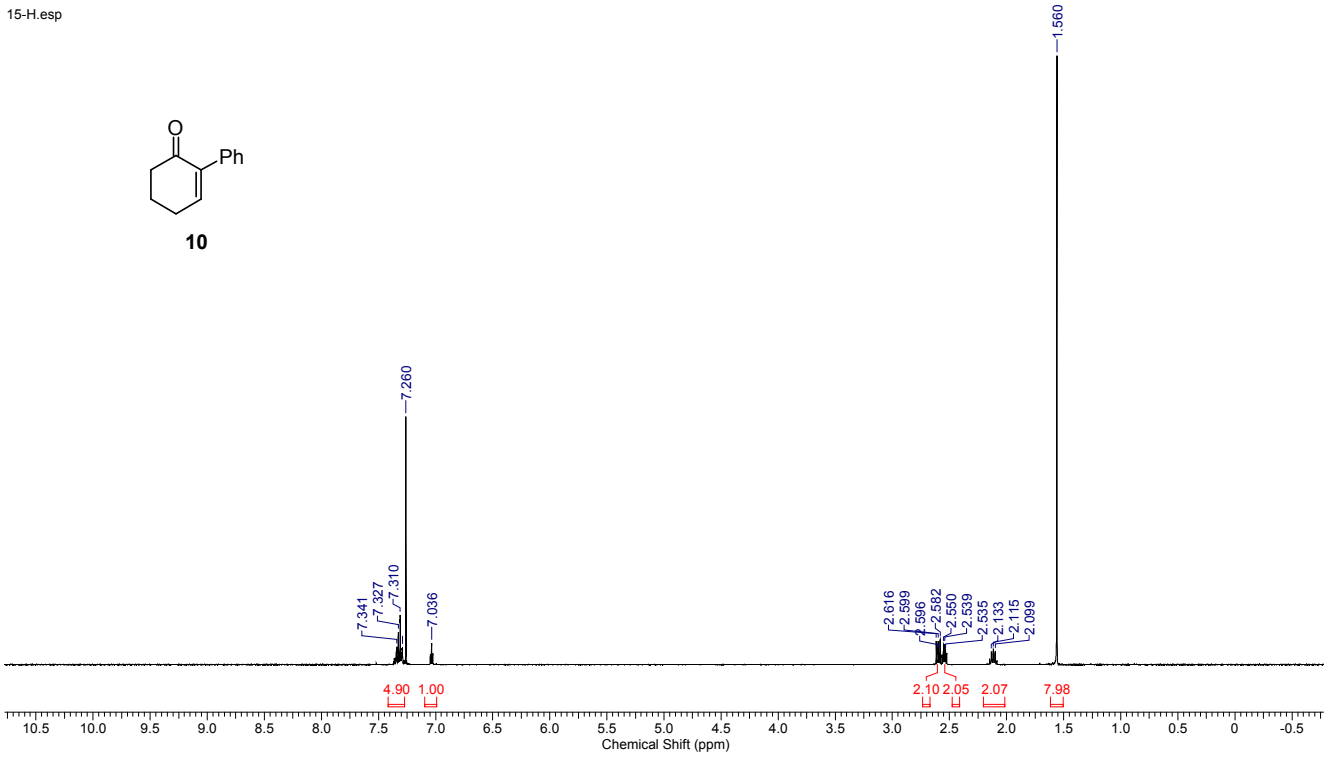
9



2019/03/04 11:47:02

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	13 Sep 2017 12:04:48		
Date Stamp	13 Sep 2017 12:03:57						
File Name	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2017NMR K¥2017NMR(JEOL)¥[illegible]¥TT17091301 Proton-1-1.jdf					*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	16384
Owner	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	22.900		

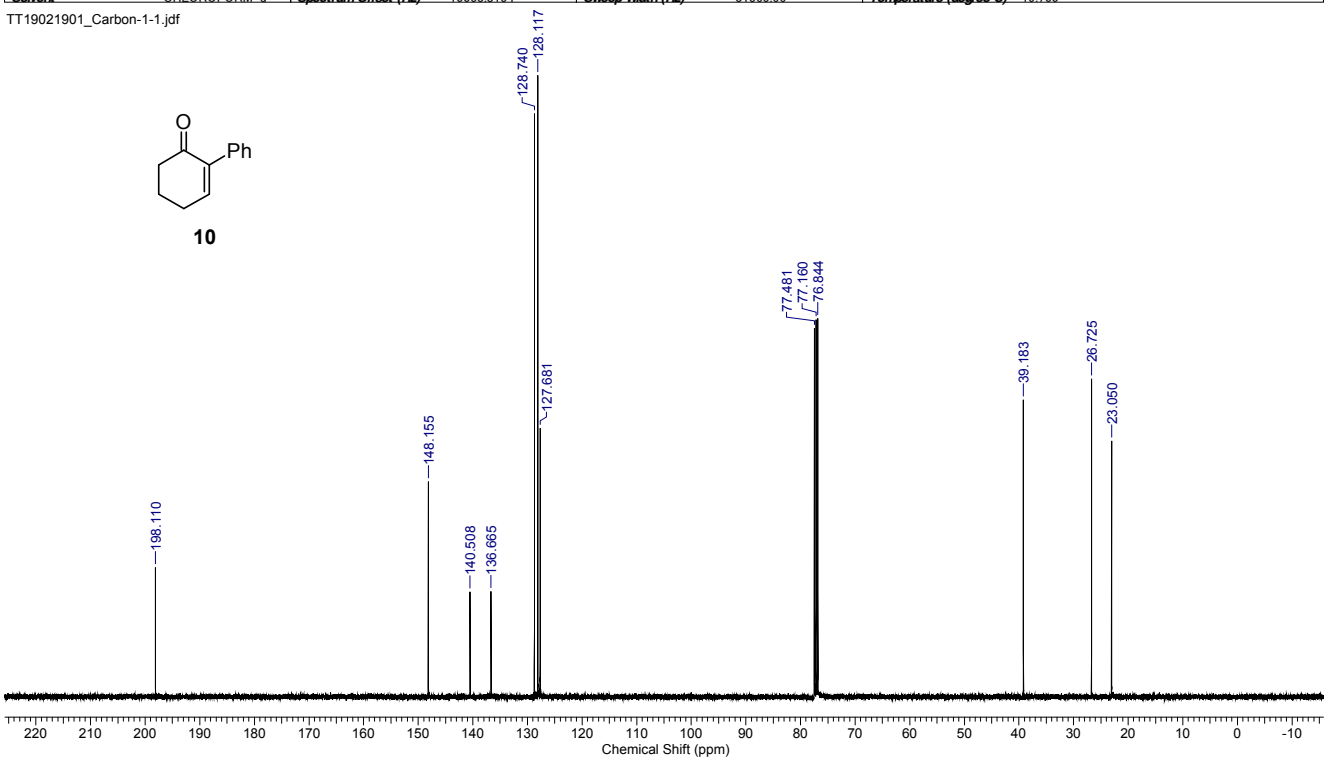
15-H.esp



2019/03/07 19:49:19

Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE			*Date*	19 Feb 2019 11:26:54
Date Stamp	19 Feb 2019 10:47:22						
File Name	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2018NMR K¥2018NMR(JEOL)¥[illegible]NMR2018¥TT19021901 Carbon-1-1.jdf						
Frequency (MHz)	100.53	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	ECA
Original Points Count	32768	*Owner*	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp
Solvent	CHLOROFORM-d	*Spectrum Offset (Hz)*	10053.8154	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	19.700

TT19021901_Carbon-1-1.jdf

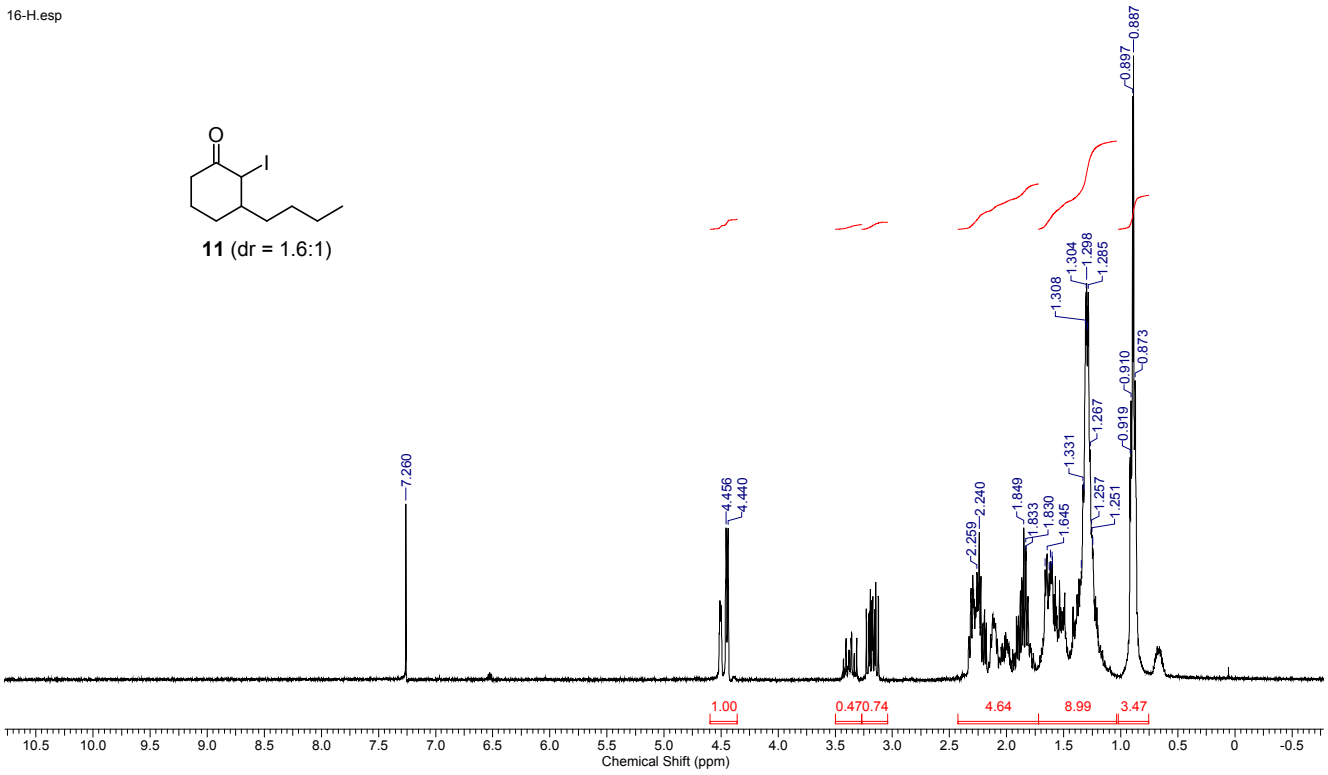


2019/03/04 13:05:30

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jun 30 2017
Date Stamp	Jun 30 2017	*File Name*	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2017NMR K¥2017NMR(agilent)¥tamura¥TT17063002.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	4	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	18.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1698.5983	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

16-H.esp

11 (dr = 1.6:1)

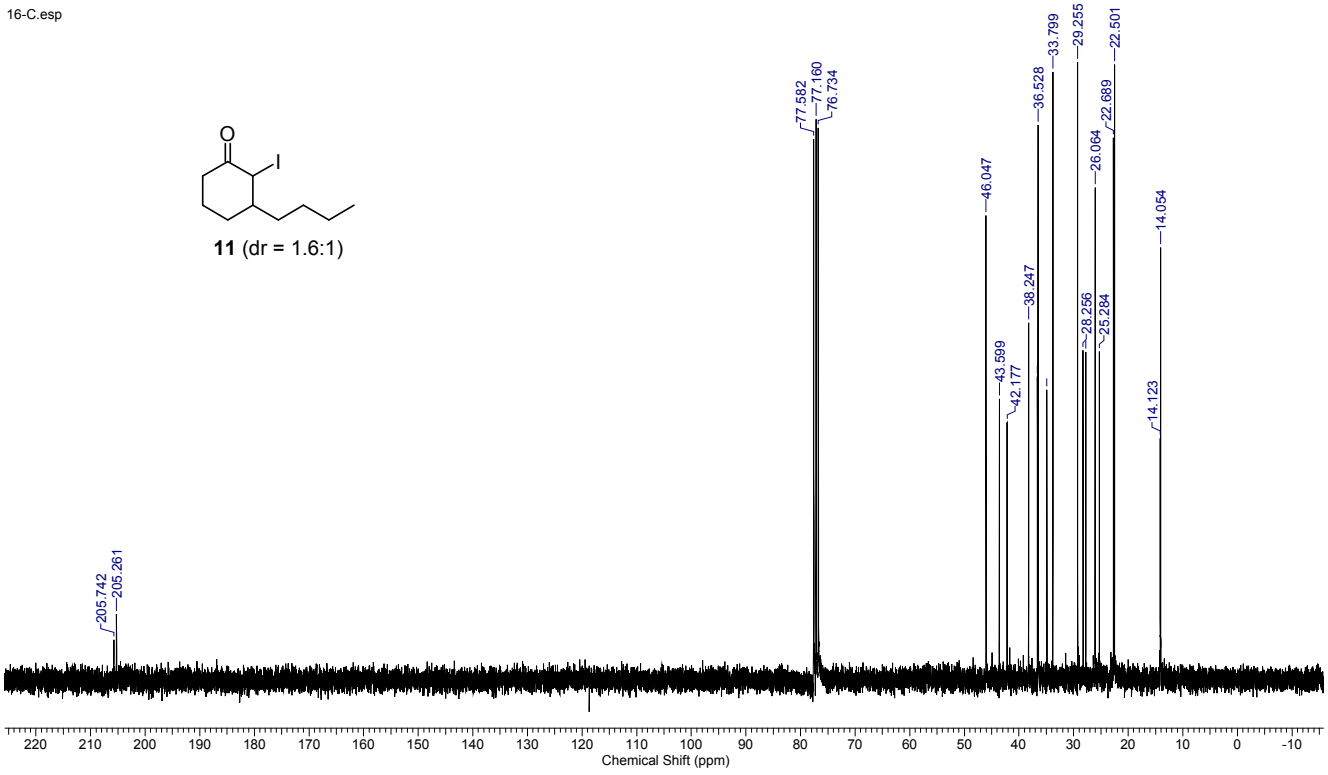


2019/03/04 12:38:13

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Jun 30 2017	*Date Stamp*	Jun 30 2017
File Name	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2017NMR K¥2017NMR(agilent)¥tamura¥TT17063002_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	672	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8954.8730
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

16-C.esp

11 (dr = 1.6:1)

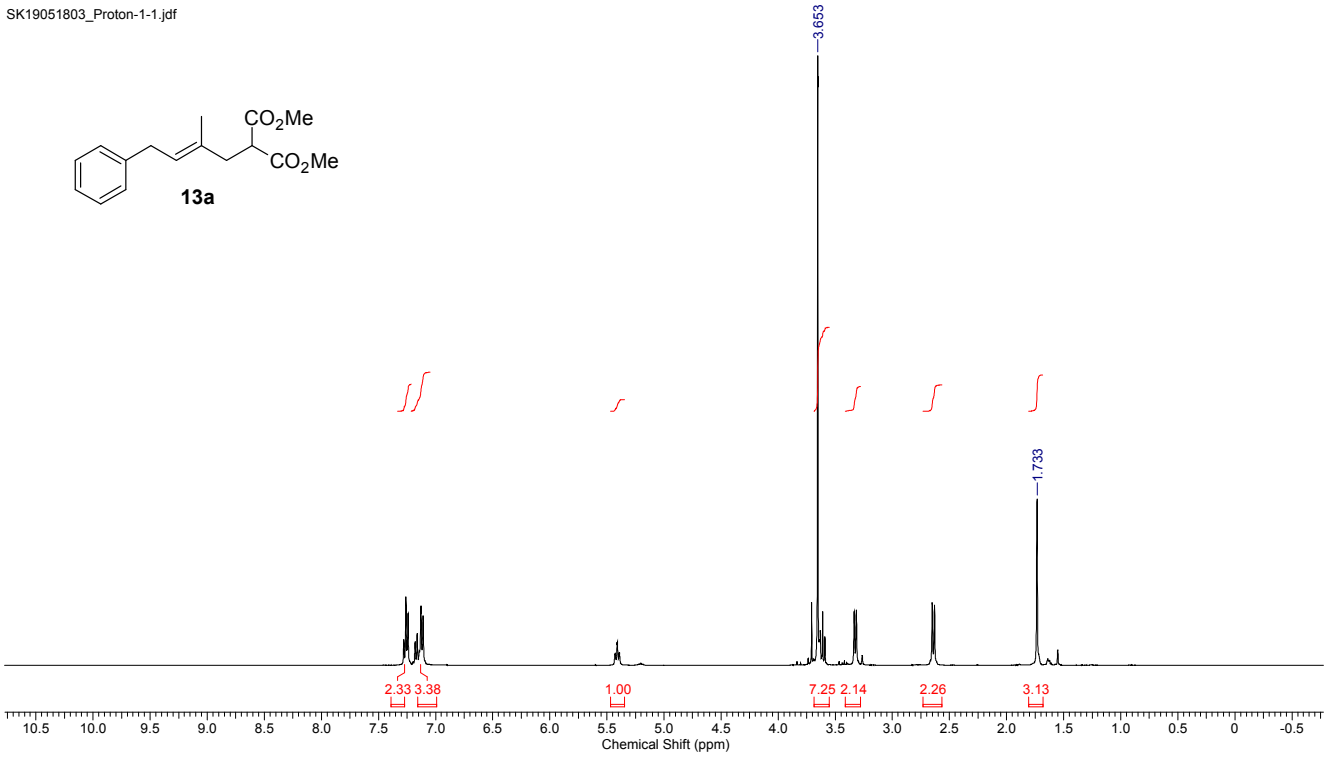


2019/05/18 16:59:14

Acquisition Time (sec)	2.1863	***Comment***	single pulse	***Date***	18 May 2019 12:01:26		
Date Stamp	18 May 2019 12:00:35						
File Name	¥¥Mac¥iCloud¥ｱﾌﾟﾘｹｰｼｮﾝ¥NMRｱﾌﾟﾘｹｰｼｮﾝ¥2019NMR K¥2019NMR(JEOL)¥ﾃﾞｰﾀNMR2019¥SK19051803 Proton-1-1.jdf						
Frequency (MHz)	399.78	***Nucleus***	1H	***Number of Transients***	8	***Origin***	ECA
Original Points Count	16384	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	1999.8311	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	19.800

SK19051803_Proton-1-1.jdf

13a

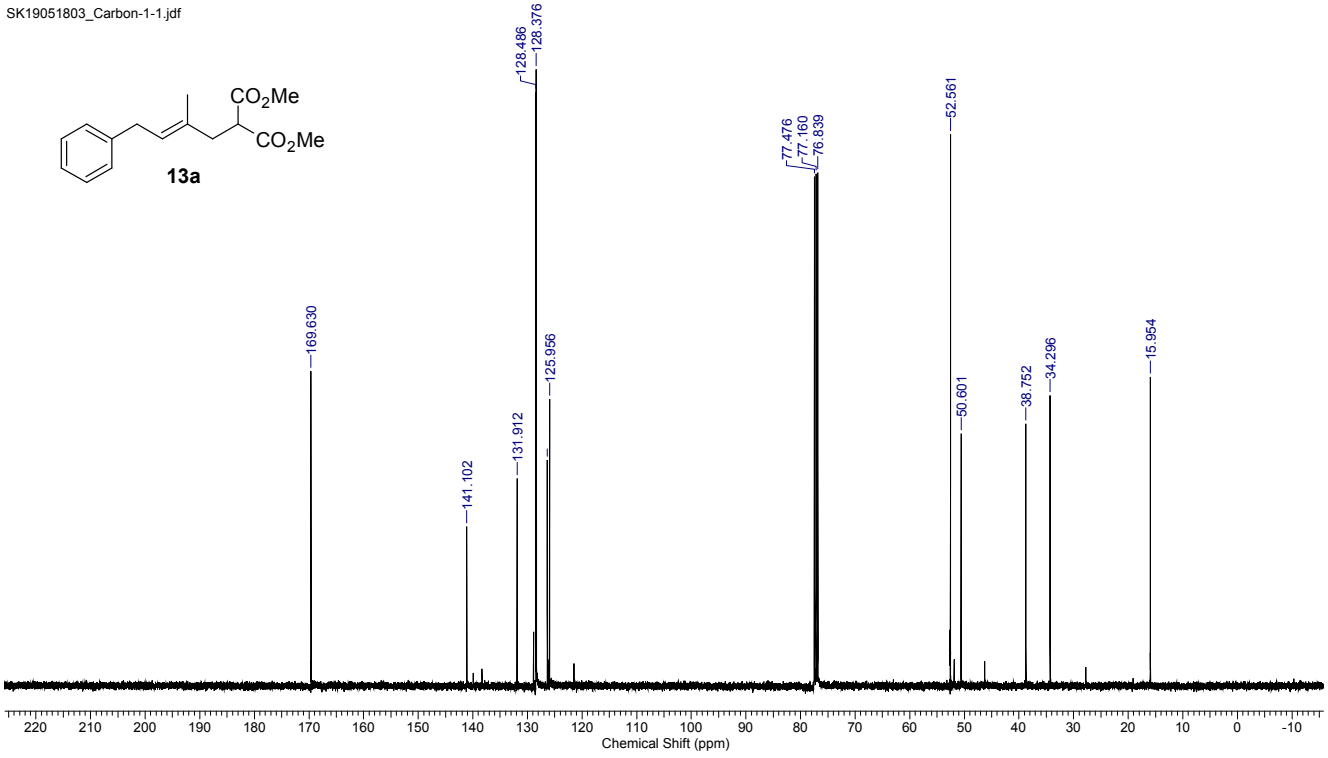


2019/05/18 17:10:38

Acquisition Time (sec)	1.0381	***Comment***	single pulse decoupled gated NOE			***Date***	18 May 2019 12:43:20
Date Stamp	18 May 2019 12:03:48						
File Name	¥¥Mac¥iCloud¥ｱﾌﾟﾘｹｰｼｮﾝ¥NMRｱﾌﾟﾘｹｰｼｮﾝ¥2019NMR K¥2019NMR(JEOL)¥ﾃﾞｰﾀNMR2019¥SK19051803 Carbon-1-1.jdf						
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1024	***Origin***	ECA
Original Points Count	32768	***Owner***	delta	***Points Count***	65536	***Pulse Sequence***	carbon.jxp
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	10053.8154	***Sweep Width (Hz)***	31565.66	***Temperature (degree C)***	19.600

SK19051803_Carbon-1-1.jdf

13a

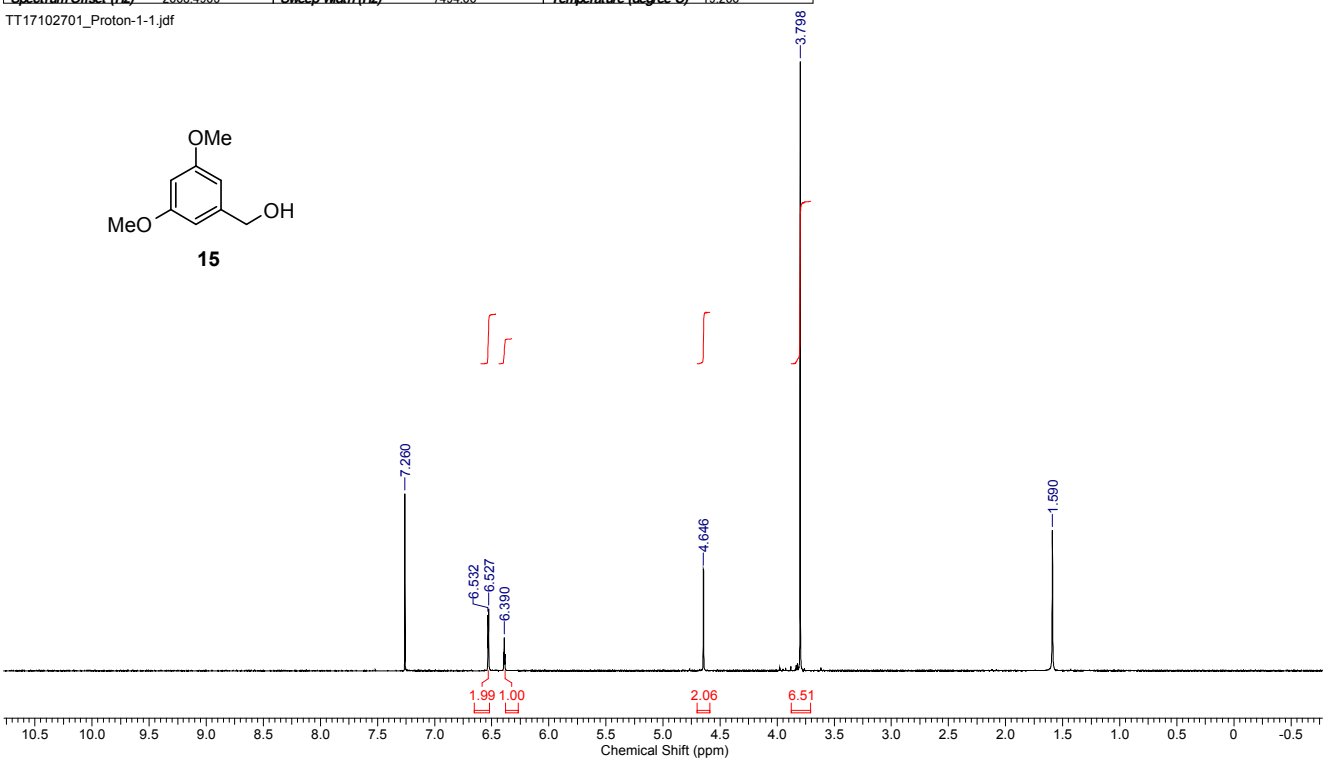


2019/03/04 15:03:16

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	27 Oct 2017 13:42:46
Date Stamp	27 Oct 2017 13:41:55				
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2017NMR K¥2017NMR(JEOL)¥[illegible]TT17102701 Proton-1-1.jdf			*Frequency (MHz)*	399.78
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA
Original Points Count	16384	*Owner*	delta	*Points Count*	32768
Pulse Sequence	proton.jxp	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	2003.4905
Sweep Width (Hz)	7494.00	*Temperature (degree C)*	19.200		

TT17102701_Proton-1-1.jdf

15

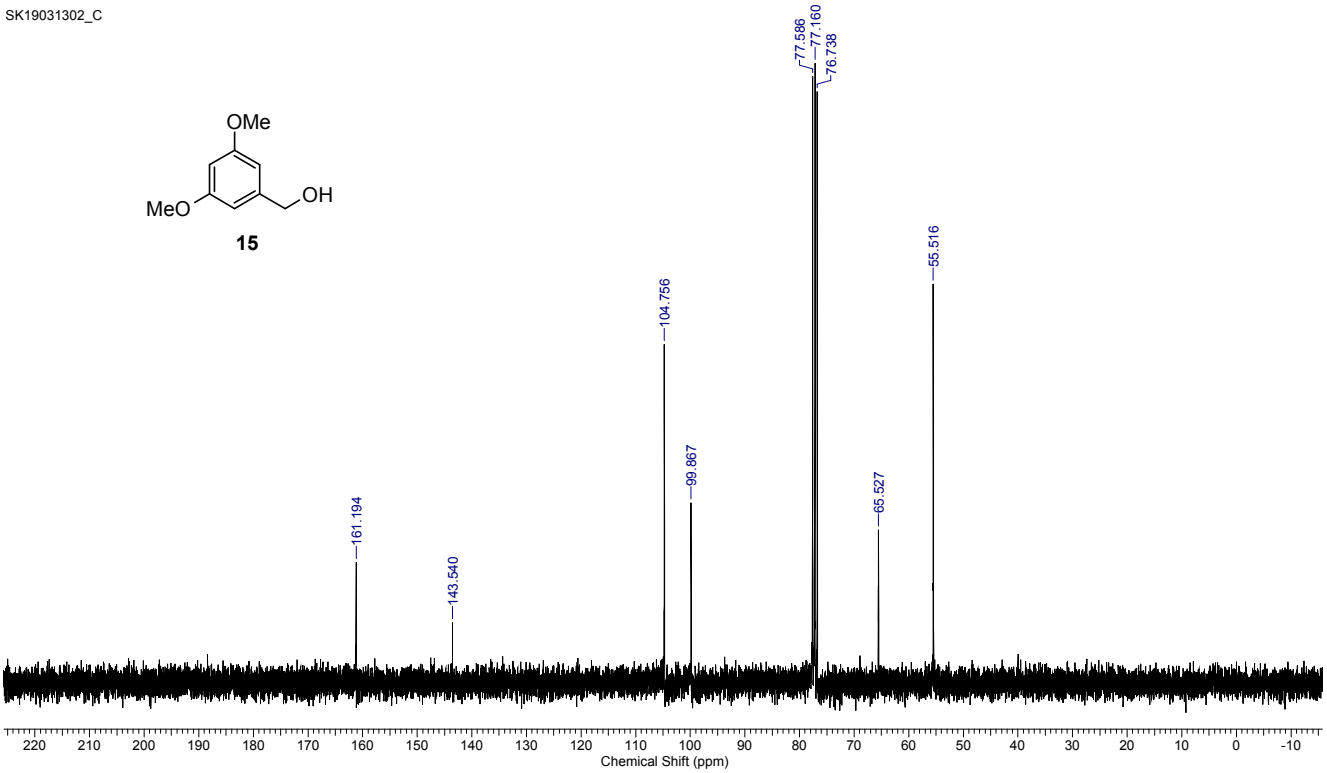


2019/03/13 20:07:24

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Mar 13 2019	*Date Stamp*	Mar 13 2019
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2019NMR K¥koba¥SK19031302 C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	512	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8956.6035
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

SK19031302_C

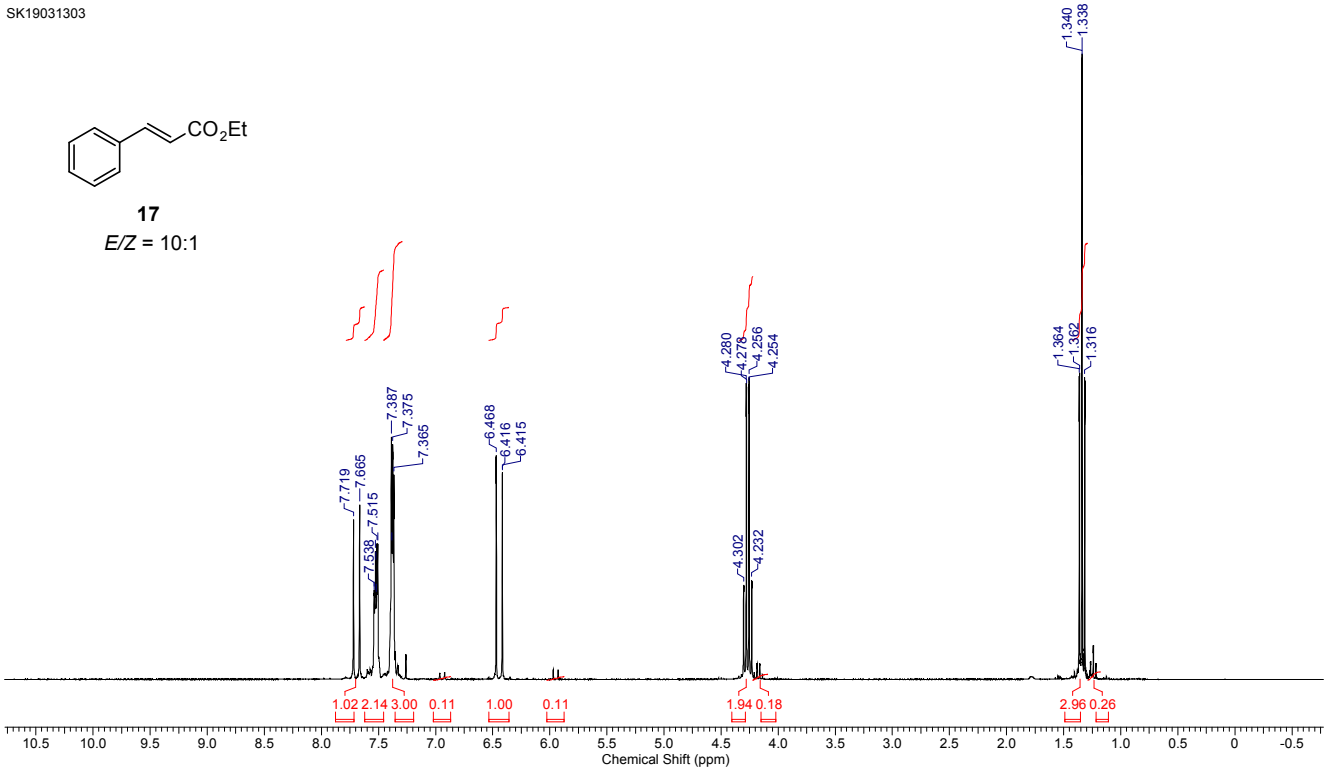
15



2019/03/13 16:53:34

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Mar 13 2019
Date Stamp	Mar 13 2019	*File Name*	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2019NMR K¥koba¥SK19031303.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	16.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1699.2579	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

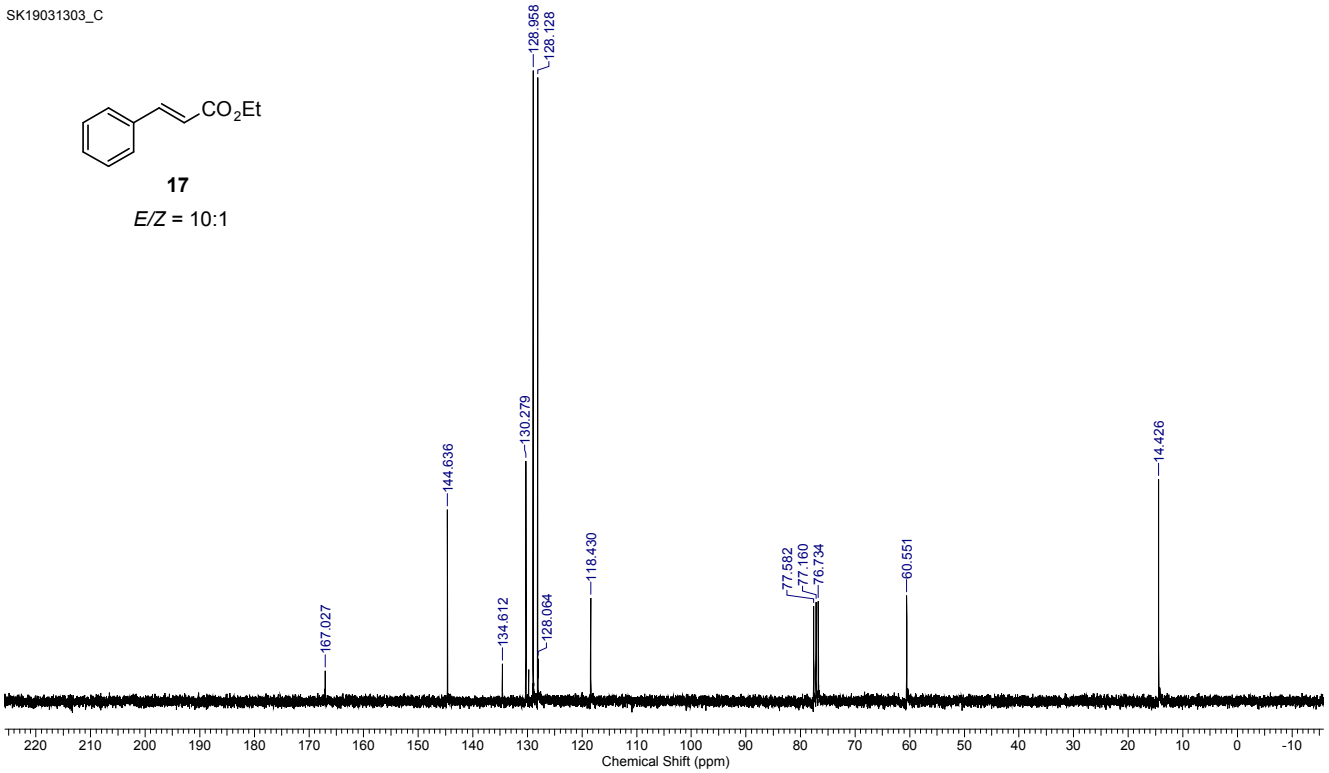
SK19031303



2019/03/13 17:28:42

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Mar 13 2019	*Date Stamp*	Mar 13 2019		
File Name	¥¥Mac¥iCloud¥[illegible]NMR¥[illegible]¥2019NMR K¥koba¥SK19031303_C.fid¥fid					*Frequency (MHz)*	75.46	*Nucleus*	13C
Number of Transients	128	*Original Points Count*	19335	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	30.00
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	8952.7979	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74
Temperature (degree C)	AMBIENT TEMPERATURE								

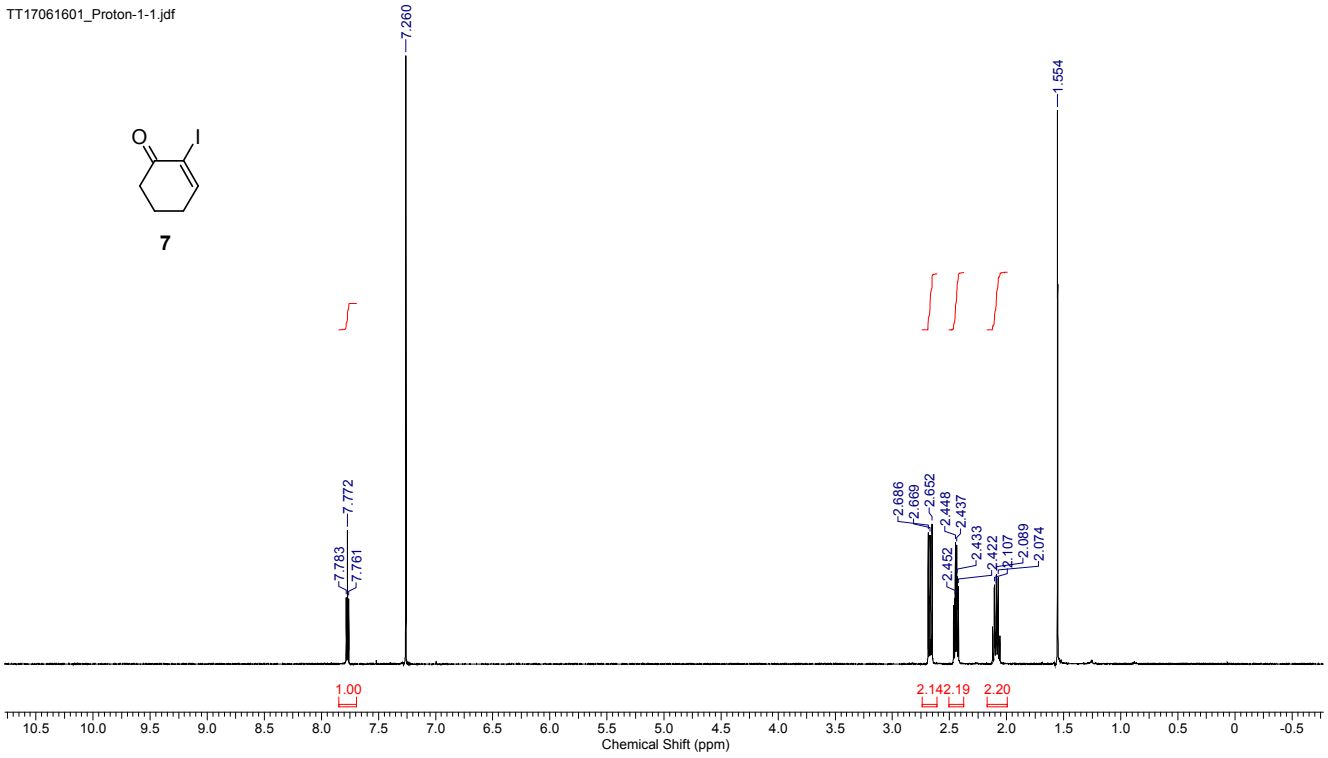
SK19031303_C



2019/03/04 16:06:39

Acquisition Time (sec)	2.1863	***Comment***	single_pulse	***Date***	16 Jun 2017 09:17:57		
Date Stamp	16 Jun 2017 09:17:05						
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2017NMR K¥2017NMR(JEOL)¥[illegible]¥TT17061601 Proton-1-1.jdf					***Frequency (MHz)***	399.78
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA	***Original Points Count***	16384
Owner	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	2003.4905	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	21.300		

TT17061601_Proton-1-1.jdf

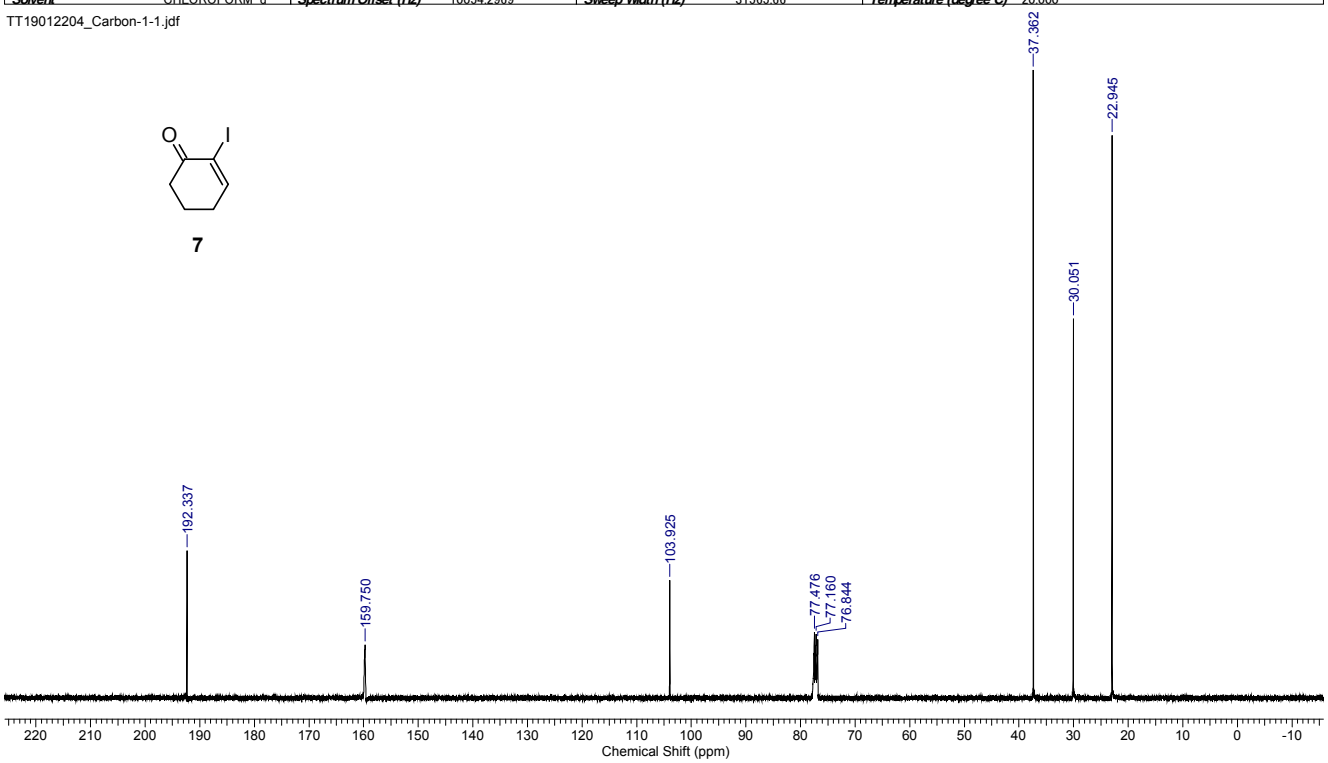


7

2019/03/07 19:55:27

Acquisition Time (sec)	1.0381	***Comment***	single pulse decoupled gated NOE			***Date***	22 Jan 2019 12:38:09
Date Stamp	22 Jan 2019 11:58:38						
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2018NMR K¥2018NMR(JEOL)¥[illegible]NMR2018¥TT19012204 Carbon-1-1.jdf						
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1024	***Origin***	ECA
Original Points Count	32768	***Owner***	delta	***Points Count***	65536	***Pulse Sequence***	carbon.jxp
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	10054.2969	***Sweep Width (Hz)***	31565.66	***Temperature (degree C)***	20.000

TT19012204_Carbon-1-1.jdf

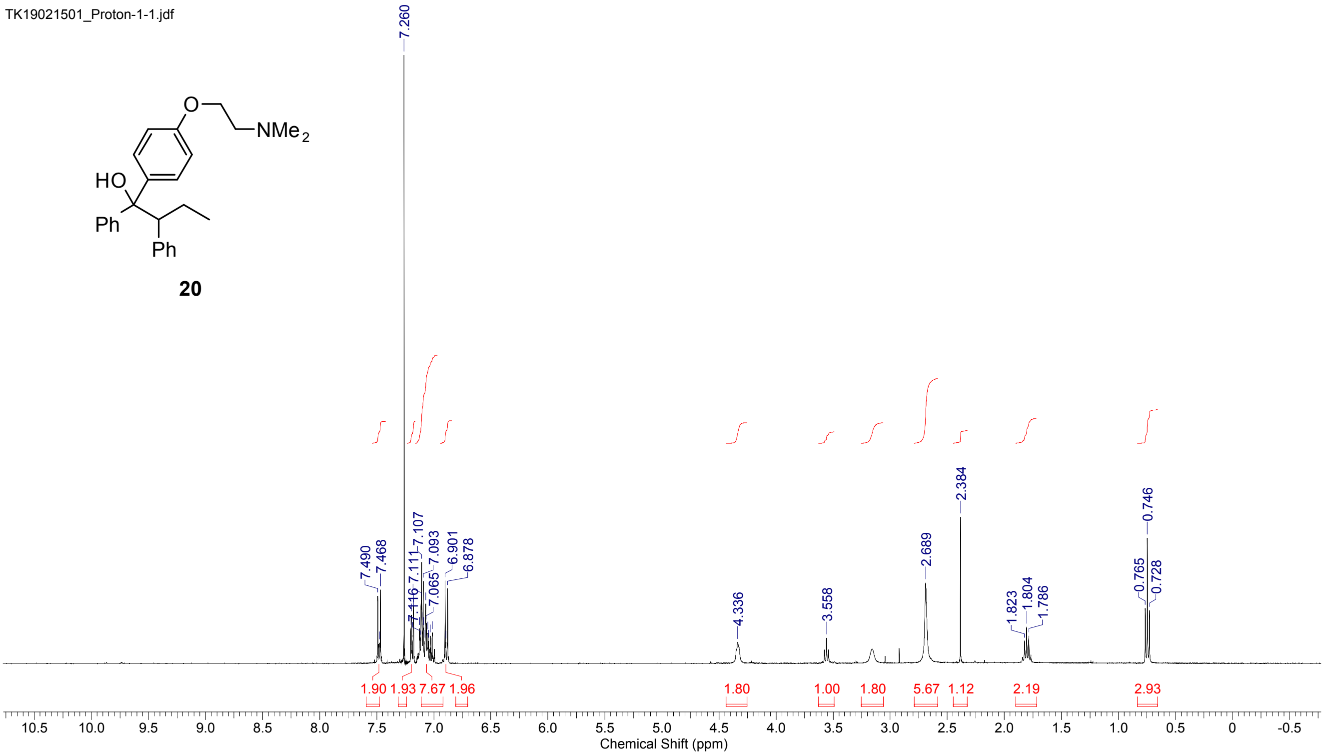


7

2019/03/06 18:12:27

Acquisition Time (sec)	2.1863	Comment	single pulse	Date	15 Feb 2019 08:46:58		
Date Stamp	15 Feb 2019 08:46:07						
File Name	¥¥Mac¥iCloud¥_[illegible]NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK19021501_Proton-1-1.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8	Origin	ECA
Original Points Count	16384	Owner	delta	Points Count	32768	Pulse Sequence	proton.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2003.2618	Sweep Width (Hz)	7494.00	Temperature (degree C)	16.700

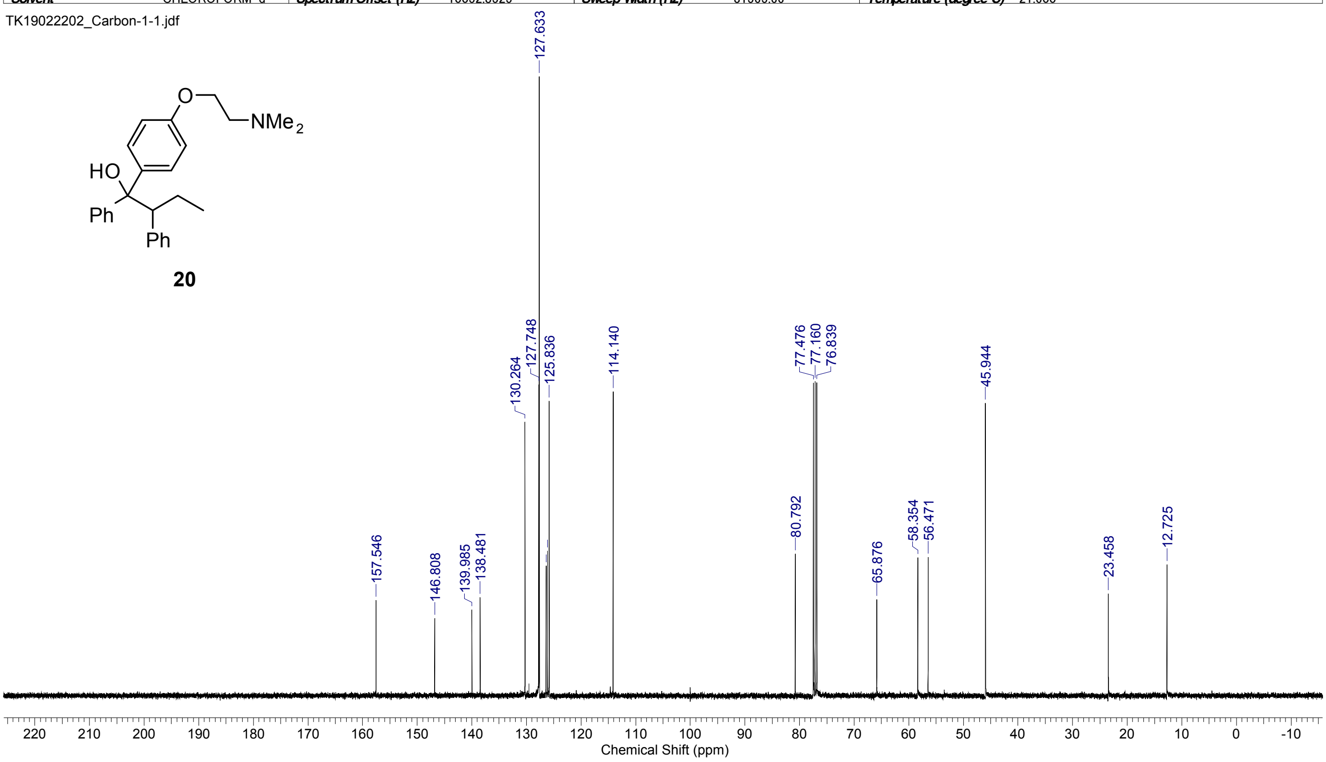
TK19021501_Proton-1-1.jdf



2019/03/06 18:34:43

Acquisition Time (sec)	1.0381	Comment	single pulse decoupled gated NOE	Date	22 Feb 2019 11:32:42		
Date Stamp	22 Feb 2019 11:12:50						
File Name	¥¥Mac¥iCloud¥_[illegible]NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK19022202_Carbon-1-1.jdf						
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	512	Origin	ECA
Original Points Count	32768	Owner	delta	Points Count	65536	Pulse Sequence	carbon.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10052.8525	Sweep Width (Hz)	31565.66	Temperature (degree C)	21.600

TK19022202_Carbon-1-1.jdf

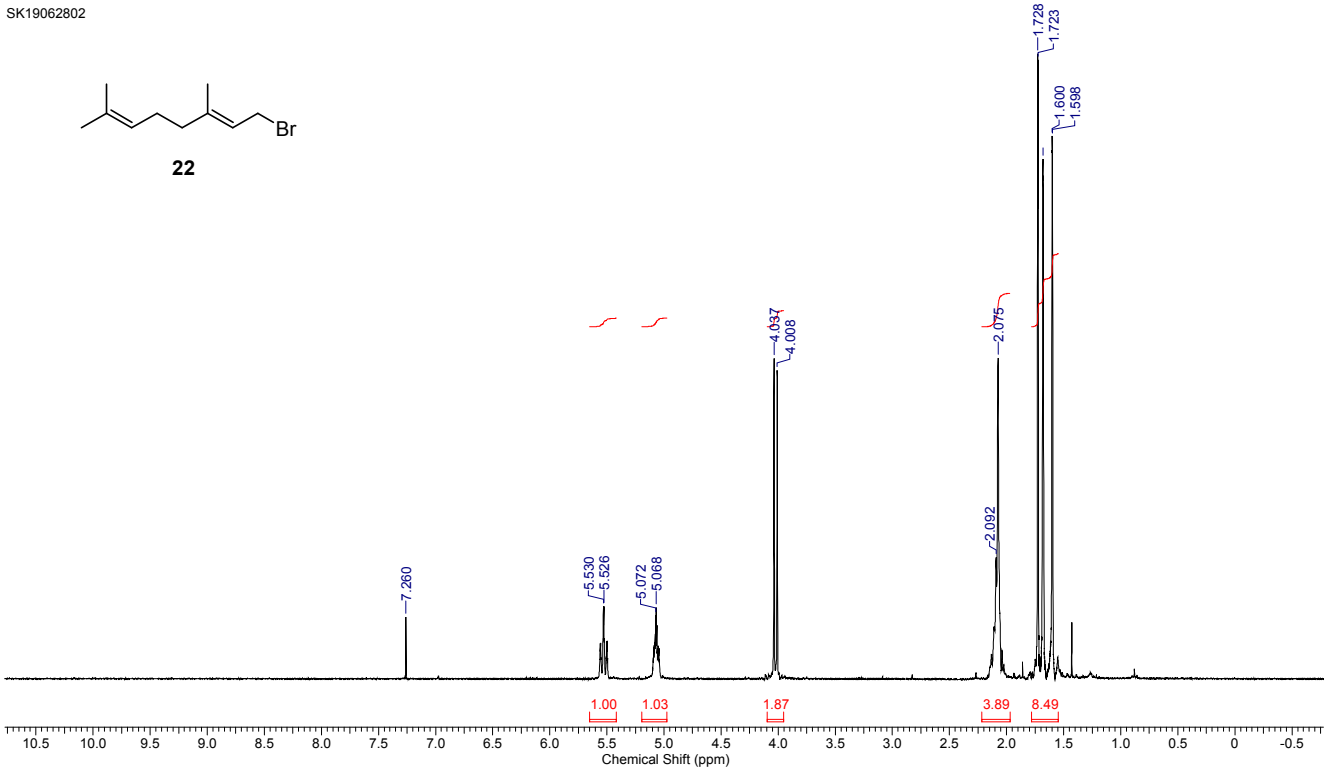


2019/06/28 15:42:33

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jun 28 2019
Date Stamp	Jun 28 2019	*File Name*	¥¥Mac¥iCloud¥ [illegible] ¥2019NMR K¥2019NMR(agilent)¥koba¥SK19062802.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	2	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	16.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1698.8182	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

SK19062802

22

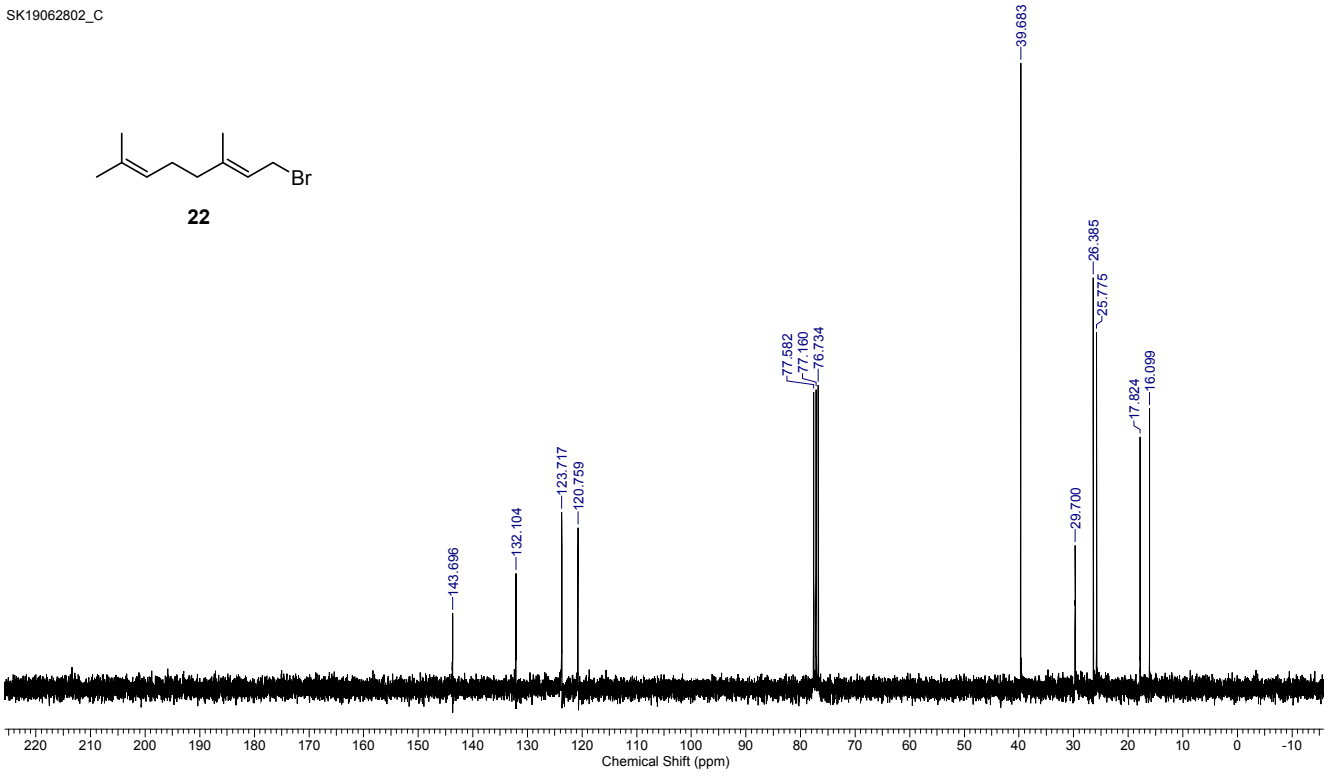


2019/06/28 15:45:50

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Jun 28 2019	*Date Stamp*	Jun 28 2019
File Name	¥¥Mac¥iCloud¥ [illegible] ¥2019NMR K¥2019NMR(agilent)¥koba¥SK19062802_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	256	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8957.2949
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

SK19062802_C

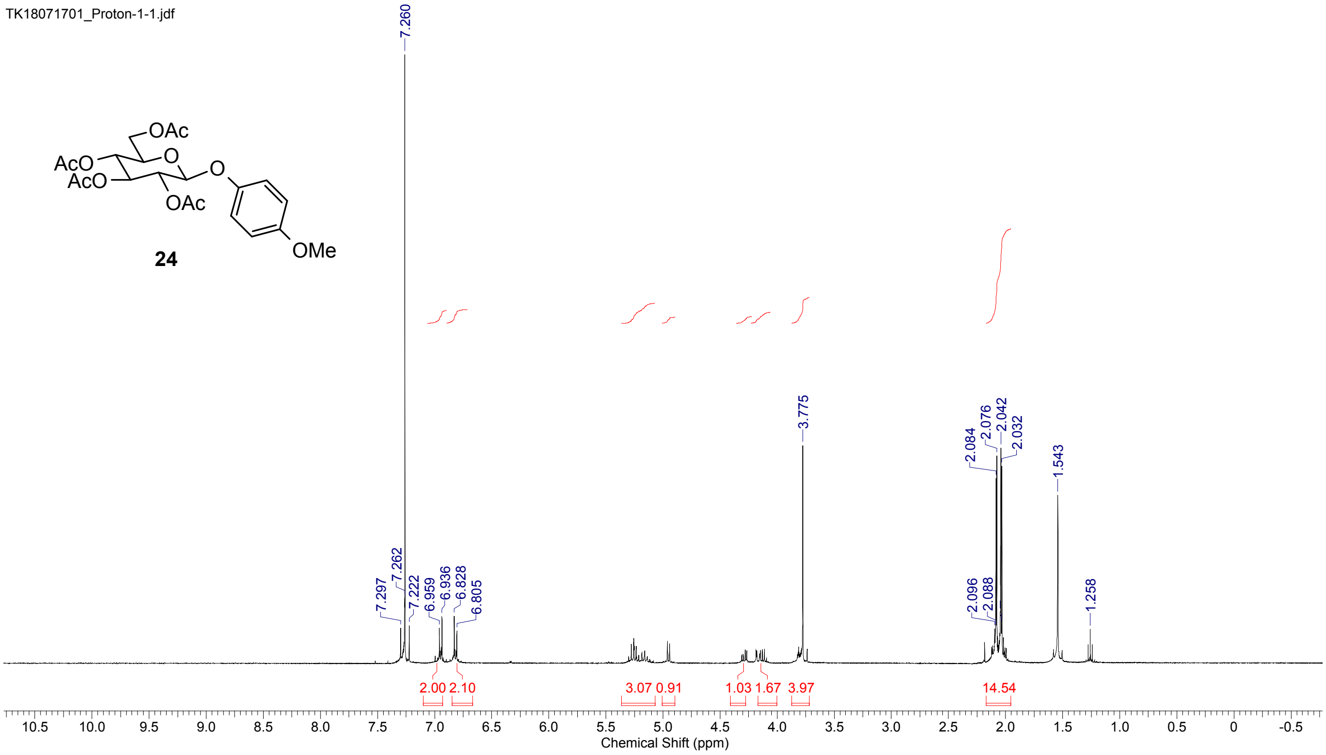
22



2019/03/06 19:08:41

Acquisition Time (sec)	2.1863	Comment	single_pulse	Date	17 Jul 2018 08:14:45		
Date Stamp	17 Jul 2018 08:13:54						
File Name	¥¥Mac¥iCloud¥_ĦĦĦĦĦĦ¥NMR_ĦĦĦĦĦĦĦĦĦĦ¥2018NMR_K¥2018NMR(JEOL)¥_ĦĦNMR2018¥TK18071701_Proton-1-1.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8	Origin	ECA
Original Points Count	16384	Owner	delta	Points Count	32768	Pulse Sequence	proton.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2003.7192	Sweep Width (Hz)	7494.00	Temperature (degree C)	24.300

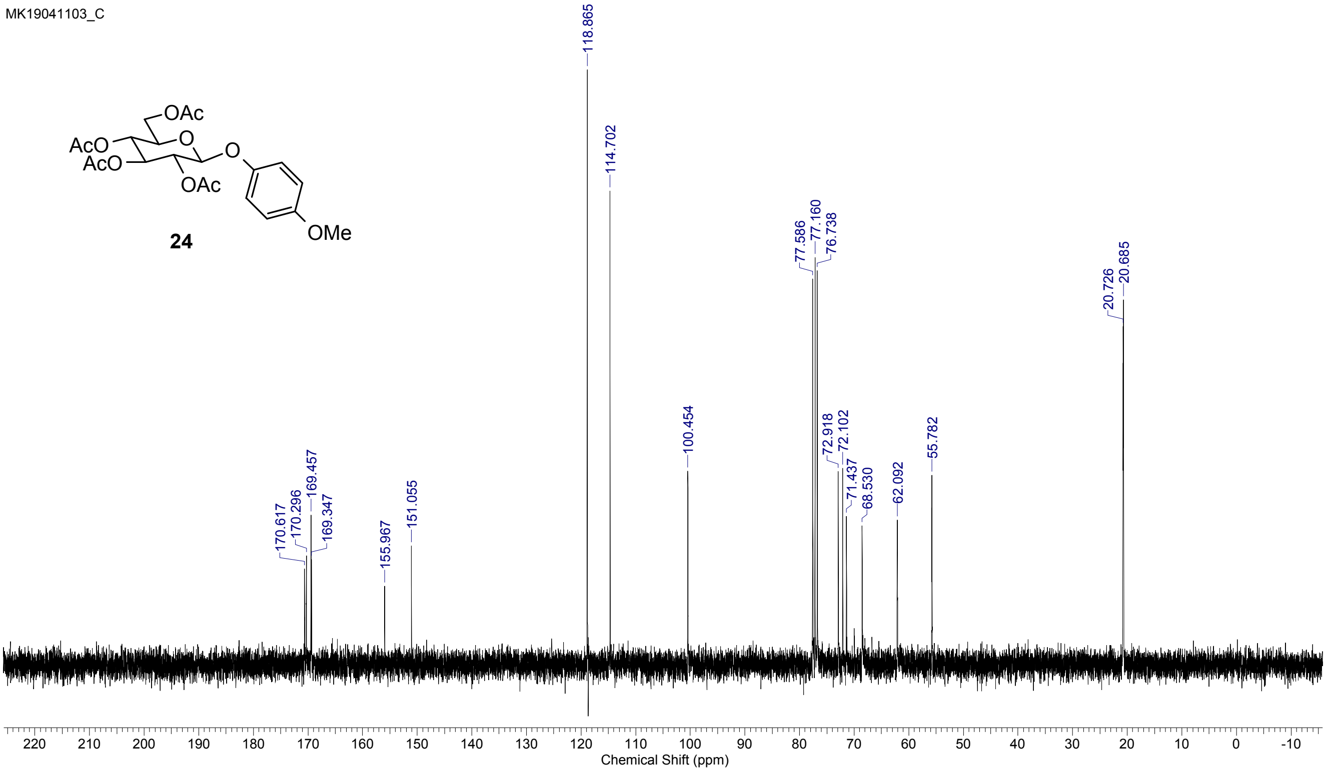
TK18071701_Proton-1-1.jdf



2019/05/14 17:09:50

Acquisition Time (sec)	0.8527	Comment	c13-NMR	Date	May 14 2019	Date Stamp	May 14 2019
File Name	¥¥Mac¥iCloud¥_ĦĦĦĦĦĦ¥NMR_ĦĦĦĦĦĦĦĦĦĦ¥2019NMR_K¥2019NMR(agilent)¥koshishiba¥MK19041103_C.fid¥fid					Frequency (MHz)	75.46
Nucleus	13C	Number of Transients	256	Original Points Count	19335	Points Count	65536
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	8954.8730
Spectrum Type	STANDARD	Sweep Width (Hz)	22675.74	Temperature (degree C)	AMBIENT TEMPERATURE		

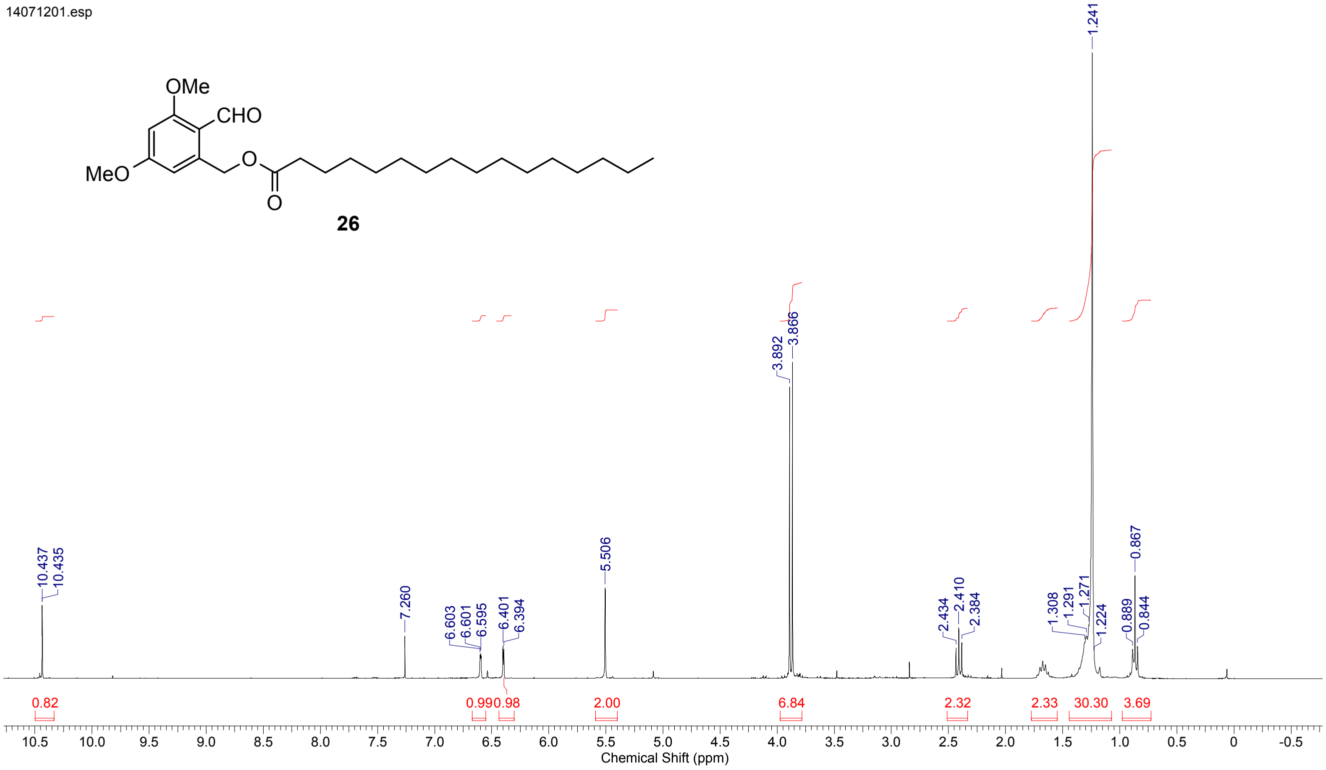
MK19041103_C



2019/03/04 19:50:01

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jul 12 2014
Date Stamp	Jul 12 2014	*File Name*	¥¥PSF¥Home¥Documents¥[illegible]NMR[illegible]¥2014NMR¥yasumoto¥14071201.fid¥fid				
Frequency (MHz)	300.06	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	16.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1698.6199	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

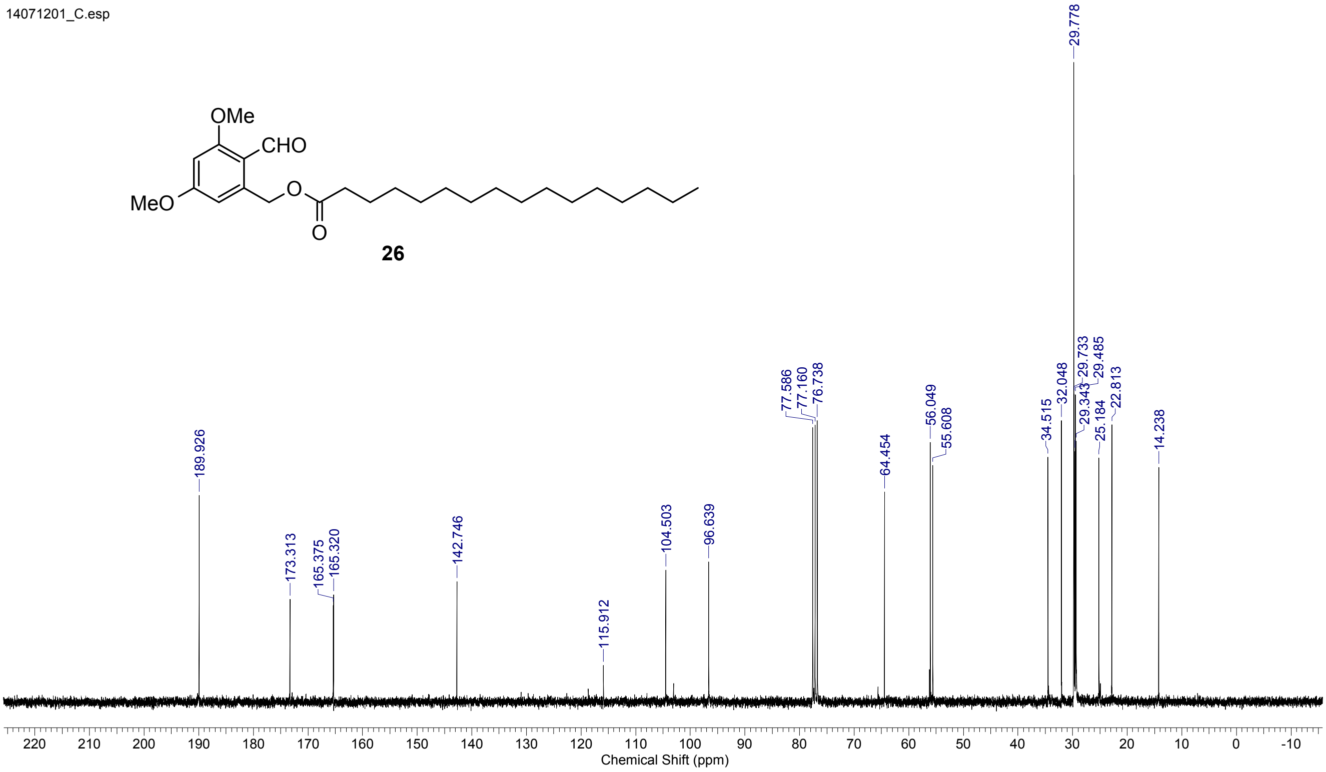
14071201.esp



2019/03/04 19:54:04

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Jul 12 2014	*Date Stamp*	Jul 12 2014
File Name	¥¥PSF¥Home¥Documents¥[illegible]NMR[illegible]¥2014NMR¥yasumoto¥14071201_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	736	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	8954.5850	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE

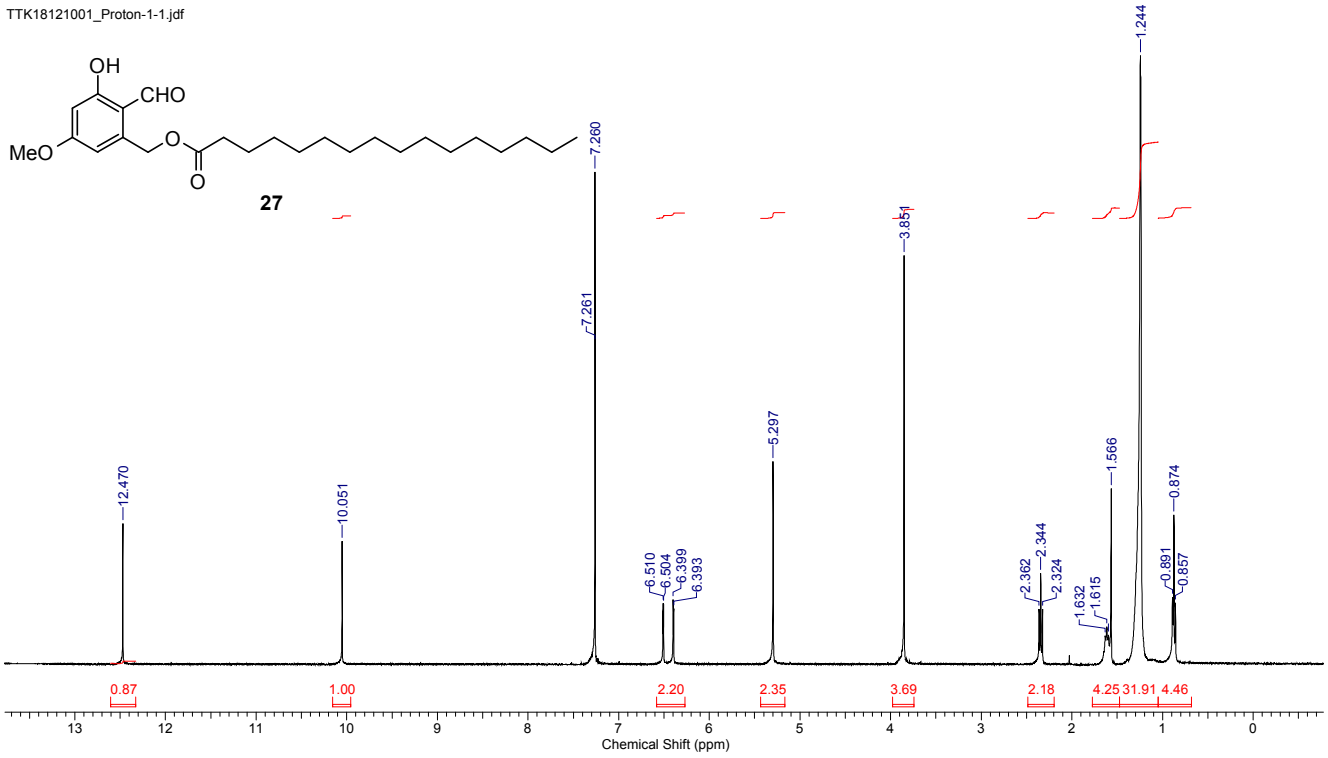
14071201_C.esp



2019/03/06 20:14:04

Acquisition Time (sec)	2.1863	***Comment***	single_pulse	***Date***	10 Dec 2018 08:00:26		
Date Stamp	10 Dec 2018 07:59:35						
File Name	¥¥Mac¥iCloud¥ [illegible]NMR [illegible]¥2018NMR K¥2018NMR(JEOL)¥ [illegible]NMR2018¥TTK18121001 Proton-1-1.jdf						
Frequency (MHz)	399.78	***Nucleus***	1H	***Number of Transients***	8	***Origin***	ECA
Original Points Count	16384	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	2003.9476	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	13.800

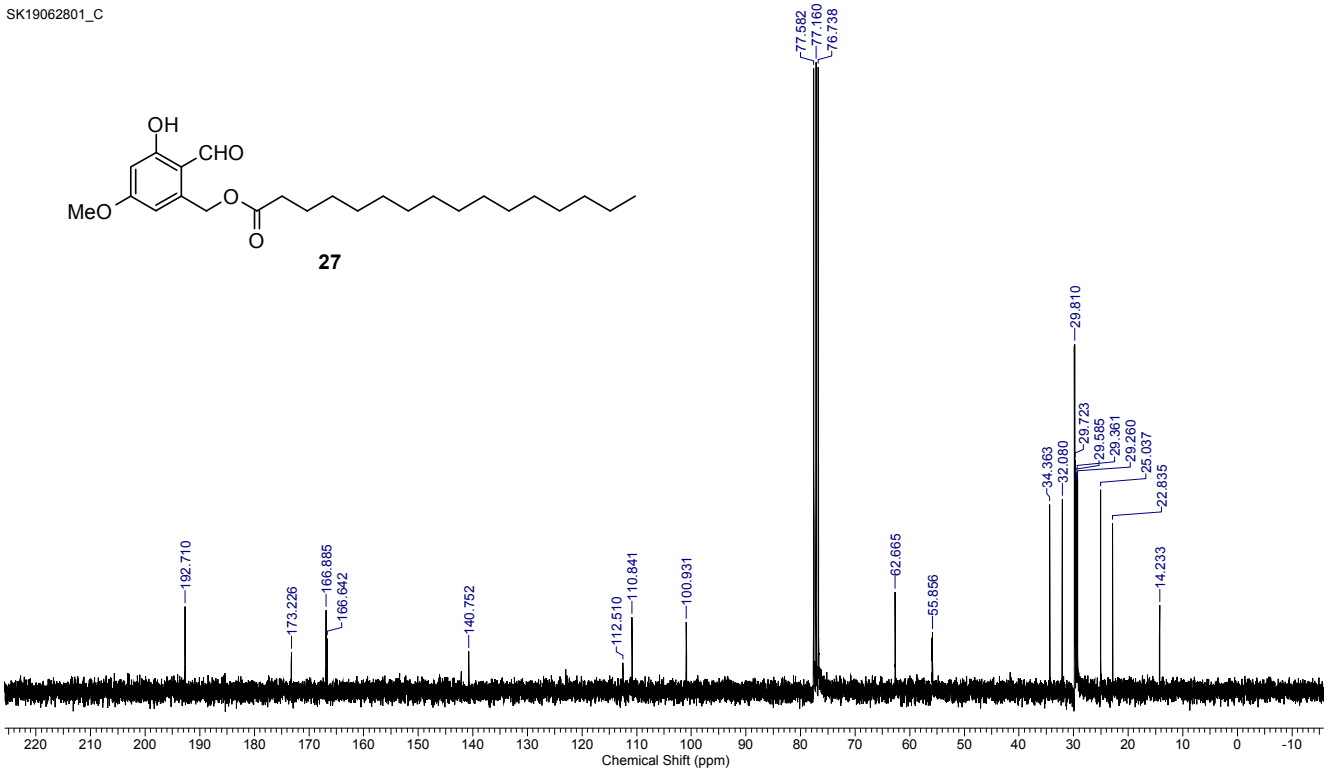
TTK18121001_Proton-1-1.jdf



2019/06/28 15:52:20

Acquisition Time (sec)	0.8527	***Comment***	c13-NMR	***Date***	Jun 28 2019	***Date Stamp***	Jun 28 2019
File Name	¥¥Mac¥iCloud¥ [illegible]NMR [illegible]¥2019NMR K¥2019NMR(agilent)¥koba¥SK19062801_C.fid¥fid					***Frequency (MHz)***	75.46
Nucleus	13C	***Number of Transients***	832	***Original Points Count***	19335	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	8958.3340
Spectrum Type	STANDARD	***Sweep Width (Hz)***	22675.74	***Temperature (degree C)***	AMBIENT TEMPERATURE		

SK19062801_C

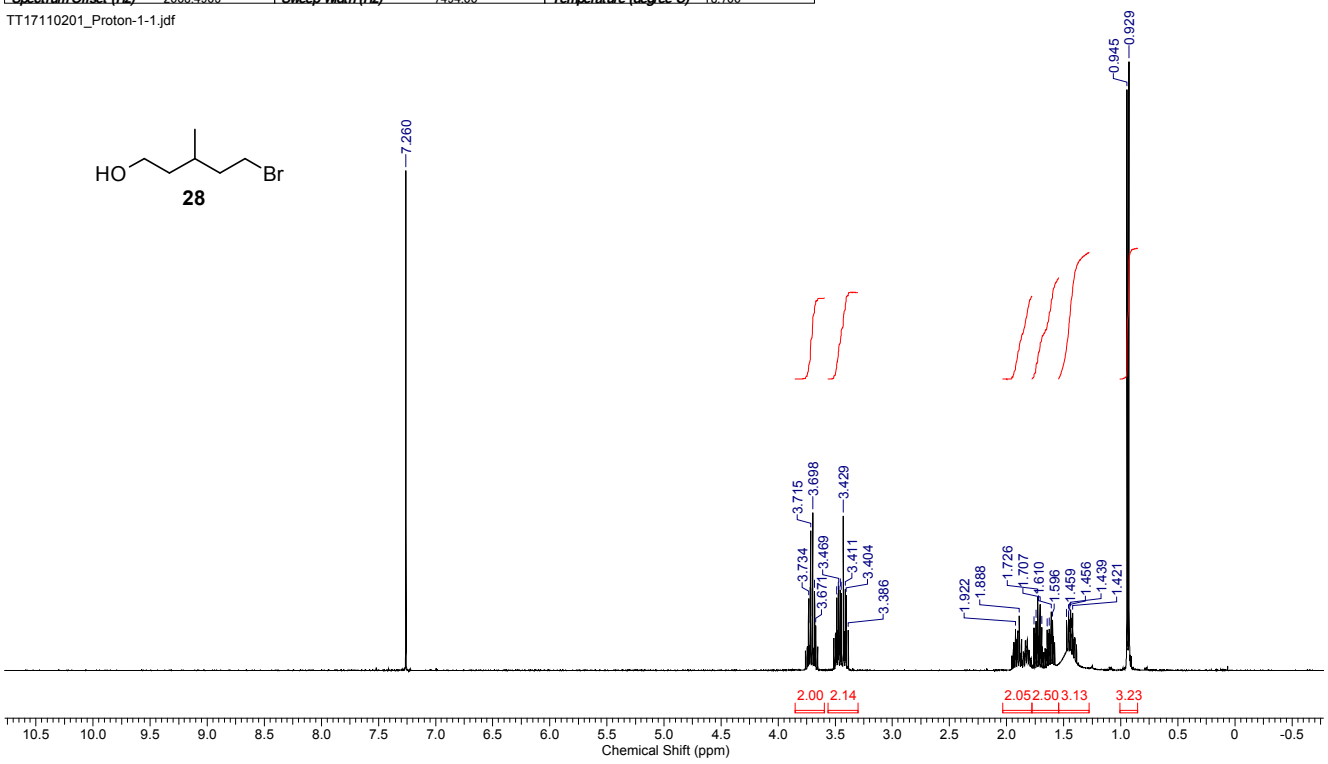


2019/03/05 18:55:51

Acquisition Time (sec)	2.1863	Comment	single_pulse	Date	02 Nov 2017 12:17:42
Date Stamp	02 Nov 2017 12:16:51				
File Name	¥¥Mac¥iCloud¥ [illegible]NMR [illegible]¥2017NMR K¥2017NMR(JEOL)¥ [illegible]TT17110201 Proton-1-1.jdf			Frequency (MHz)	399.78
Nucleus	1H	Number of Transients	8	Origin	ECA
Original Points Count	16384	Owner	delta	Points Count	32768
Pulse Sequence	proton.jxp	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2003.4905
Sweep Width (Hz)	7494.00	Temperature (degree C)	18.700		

TT17110201_Proton-1-1.jdf

28

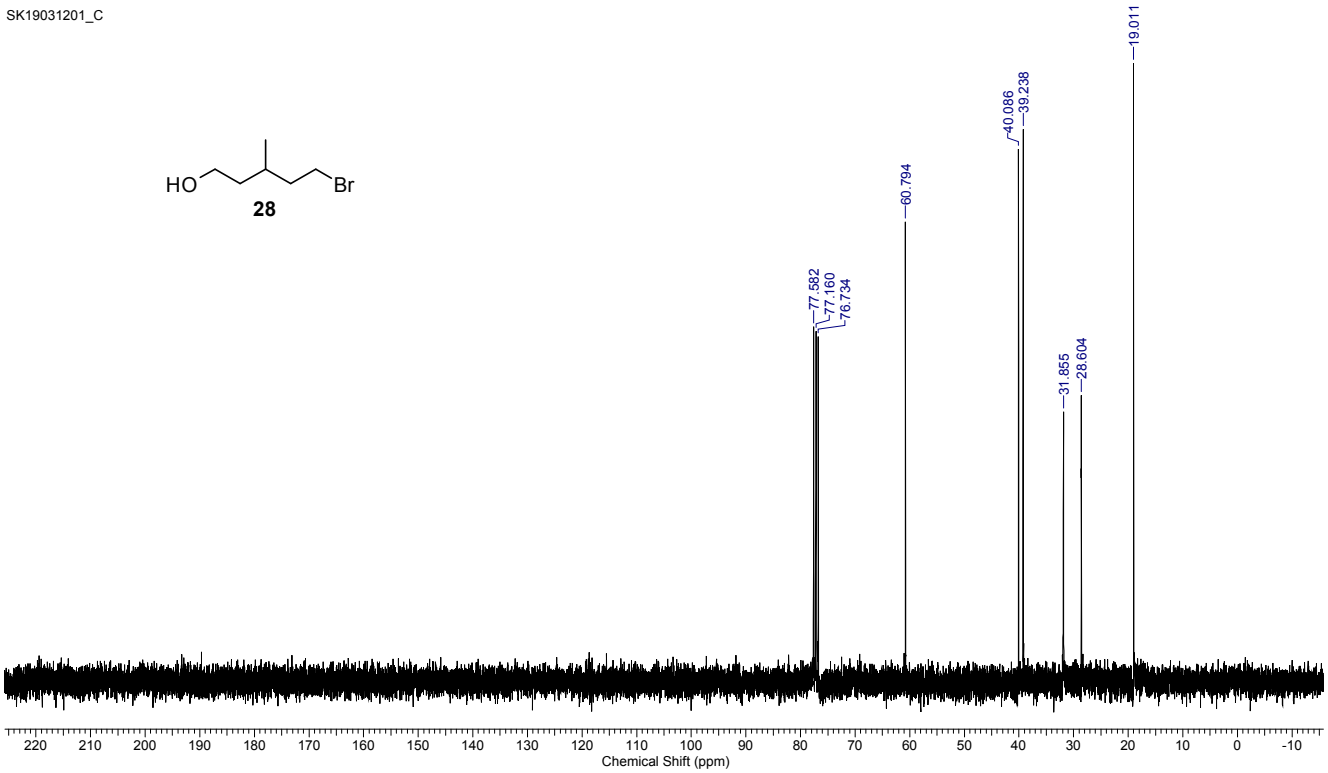


2019/03/12 12:14:16

Acquisition Time (sec)	0.8527	Comment	c13-NMR	Date	Mar 12 2019	Date Stamp	Mar 12 2019
File Name	¥¥Mac¥iCloud¥ [illegible]NMR [illegible]¥2019NMR K¥koba¥SK19031201 C.fid¥fid					Frequency (MHz)	75.46
Nucleus	13C	Number of Transients	192	Original Points Count	19335	Points Count	65536
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	8953.8359
Spectrum Type	STANDARD	Sweep Width (Hz)	22675.74	Temperature (degree C)	AMBIENT TEMPERATURE		

SK19031201_C

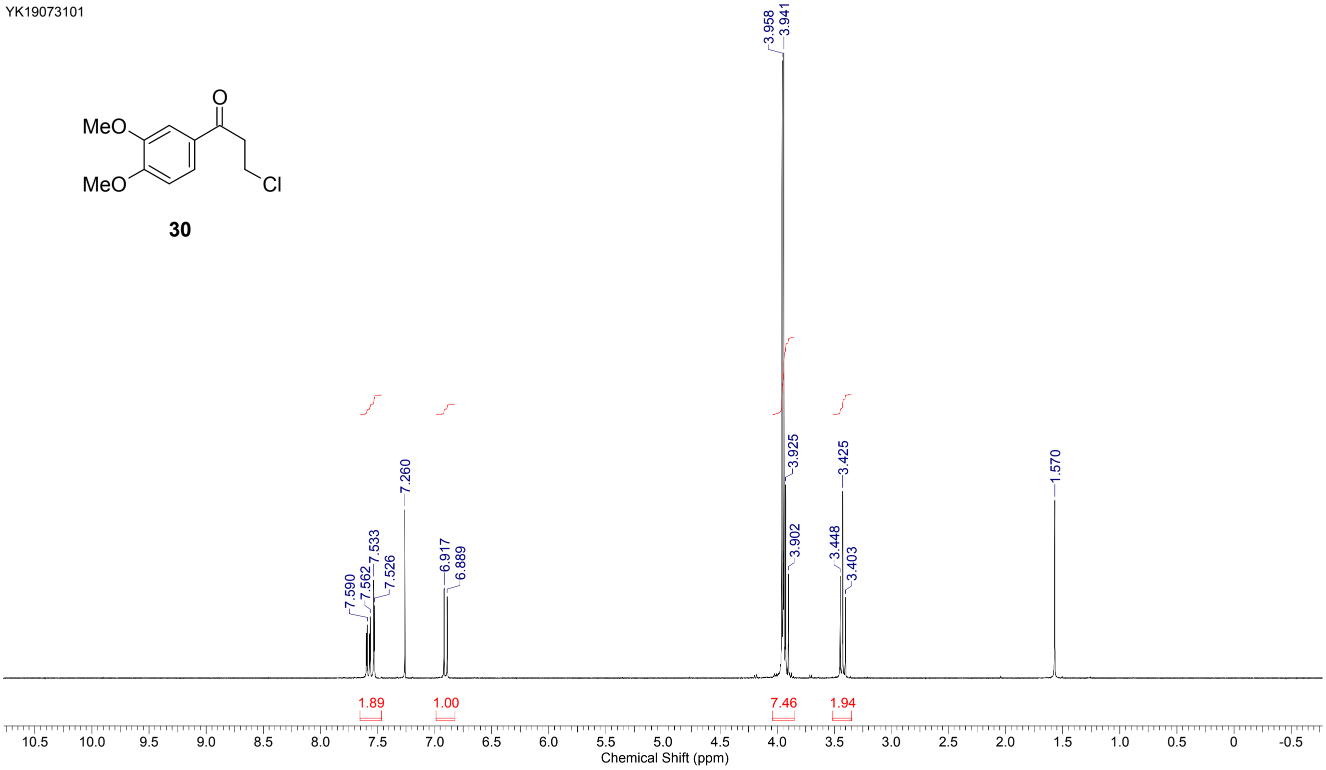
28



2019/08/05 14:50:29

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Jul 31 2019
Date Stamp	Jul 31 2019	*File Name*	¥¥Mac¥iCloud¥_HHHHHH¥NMR_K HHH HHH HH¥2019NMR_K¥2019NMR(agilent)¥kuroda¥YK19073101.fid¥fid				
Frequency (MHz)	300.05	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	34.00	*Solvent*	pyridine
Spectrum Offset (Hz)	1605.9590	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

YK19073101

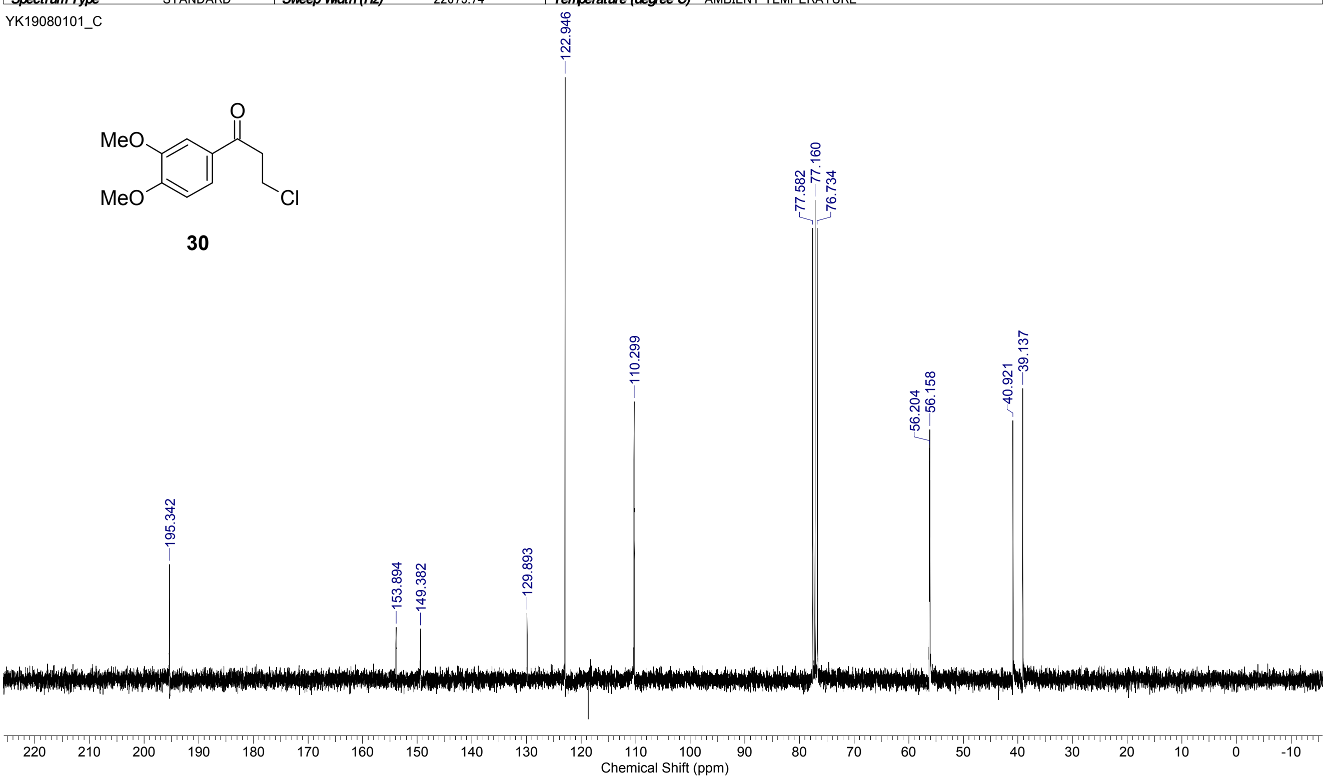


30

2019/08/05 15:40:21

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Aug 1 2019	*Date Stamp*	Aug 1 2019
File Name	¥¥Mac¥iCloud¥_HHHHHH¥NMR_K HHH HHH HH¥2019NMR_K¥2019NMR(agilent)¥kuroda¥YK19080101_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	640	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d	*Spectrum Offset (Hz)*	8955.5654
Spectrum Type	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE		

YK19080101_C

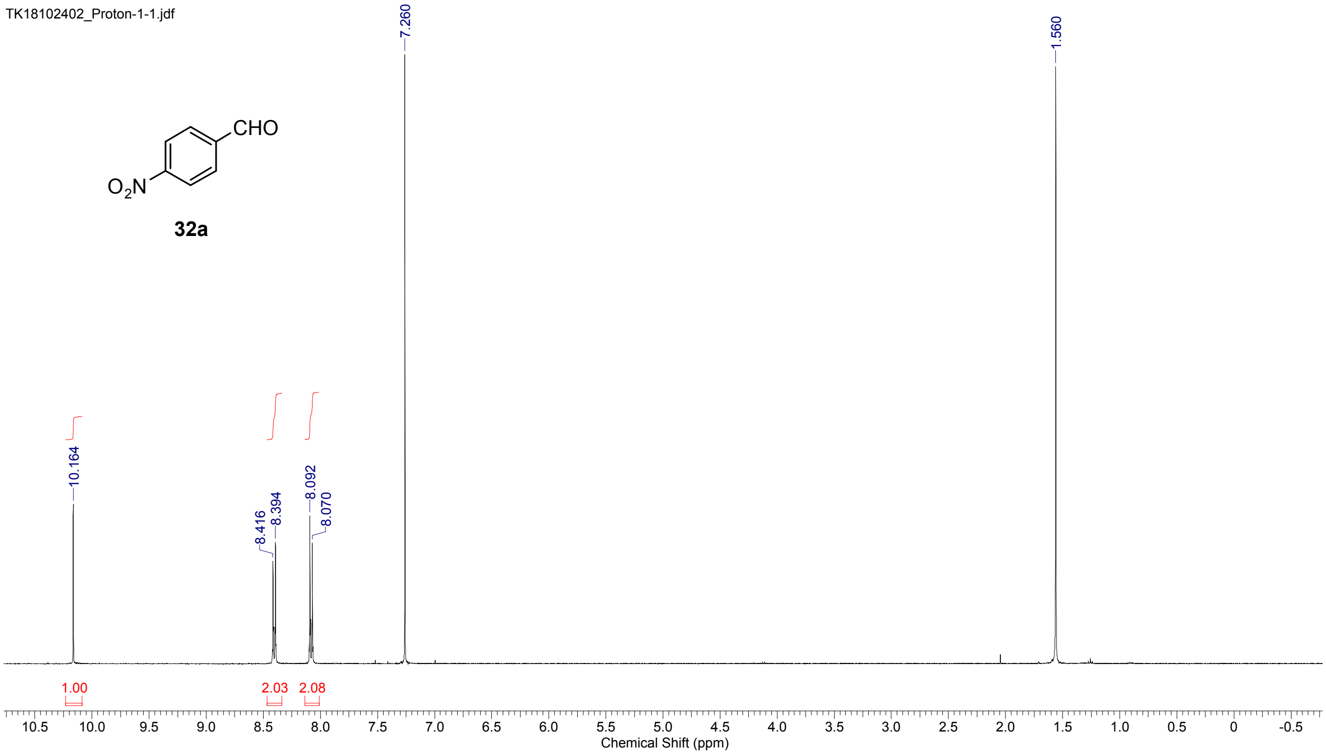


30

2019/03/06 20:23:46

Acquisition Time (sec)	2.1863	Comment	single_pulse	Date	24 Oct 2018 09:43:15		
Date Stamp	24 Oct 2018 09:42:23						
File Name	¥¥Mac¥iCloud¥_[illegible]NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK18102402_Proton-1-1.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8	Origin	ECA
Original Points Count	16384	Owner	delta	Points Count	32768	Pulse Sequence	proton.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2003.4905	Sweep Width (Hz)	7494.00	Temperature (degree C)	18.900

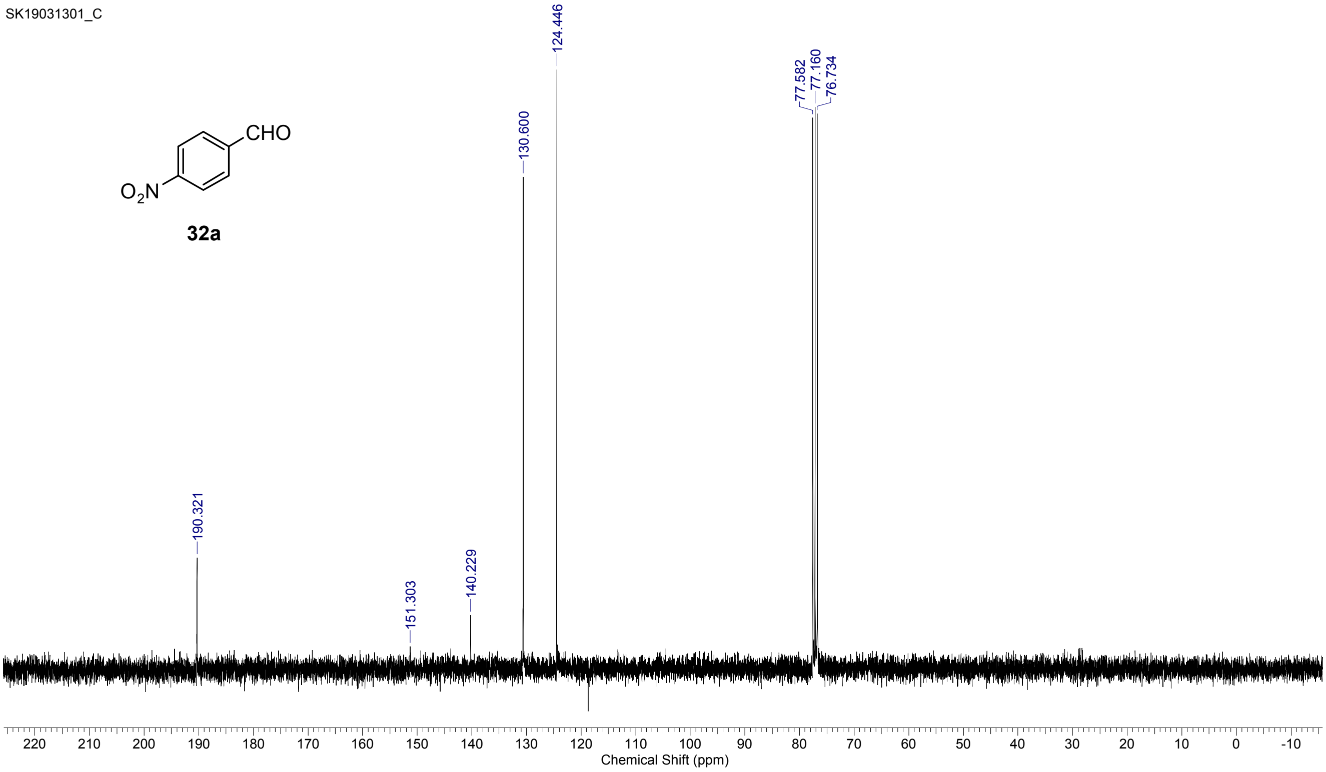
TK18102402_Proton-1-1.jdf



2019/03/13 20:13:54

Acquisition Time (sec)	0.8527	Comment	c13-NMR	Date	Mar 13 2019	Date Stamp	Mar 13 2019		
File Name	¥¥Mac¥iCloud¥_[illegible]NMR_[illegible]¥2019NMR_K¥koba¥SK19031301_C.fid¥fid					Frequency (MHz)	75.46	Nucleus	13C
Number of Transients	672	Original Points Count	19335	Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	30.00
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	8956.6035	Spectrum Type	STANDARD	Sweep Width (Hz)	22675.74
Temperature (degree C)	AMBIENT TEMPERATURE								

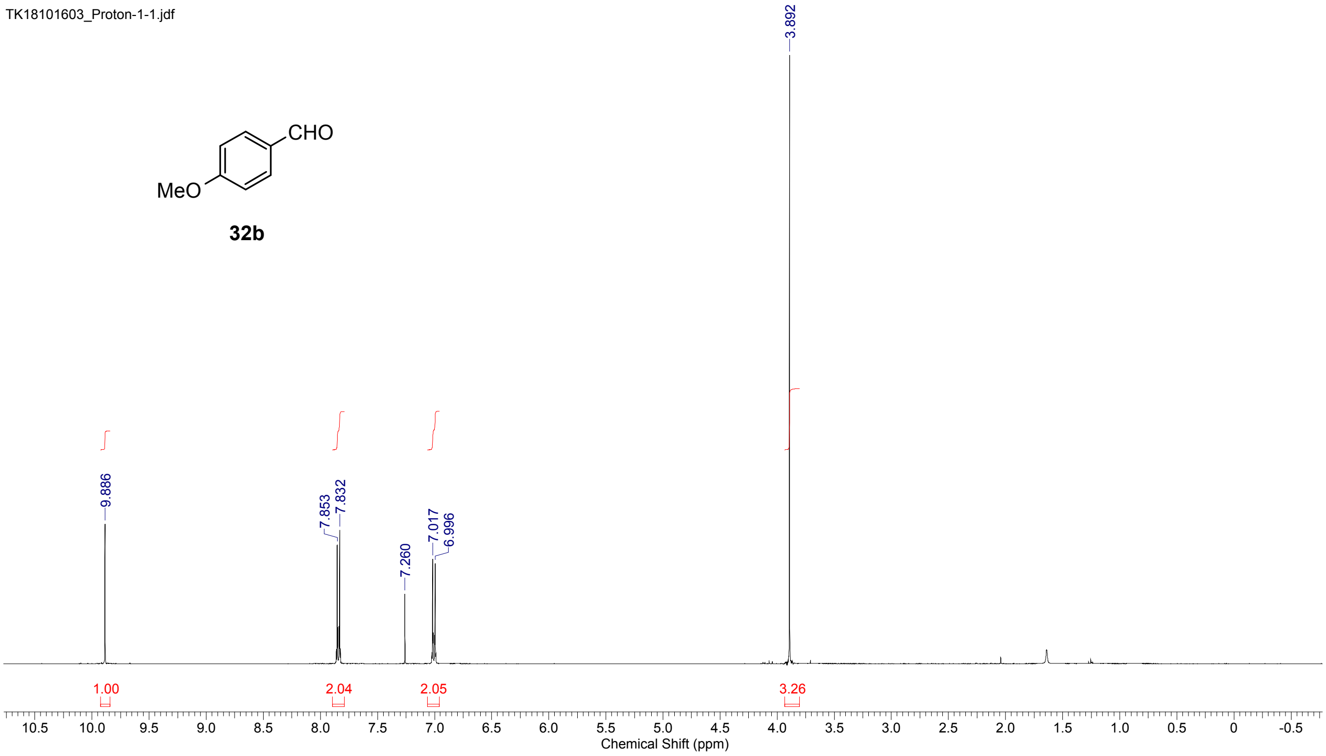
SK19031301_C



2019/03/07 14:48:08

Acquisition Time (sec)	2.1863	Comment	single_pulse	Date	16 Oct 2018 08:24:46		
Date Stamp	16 Oct 2018 08:23:55						
File Name	¥¥Mac¥iCloud¥[illegible]¥NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK18101603_Proton-1-1.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8	Origin	ECA
Original Points Count	16384	Owner	delta	Points Count	32768	Pulse Sequence	proton.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2003.4905	Sweep Width (Hz)	7494.00	Temperature (degree C)	17.700

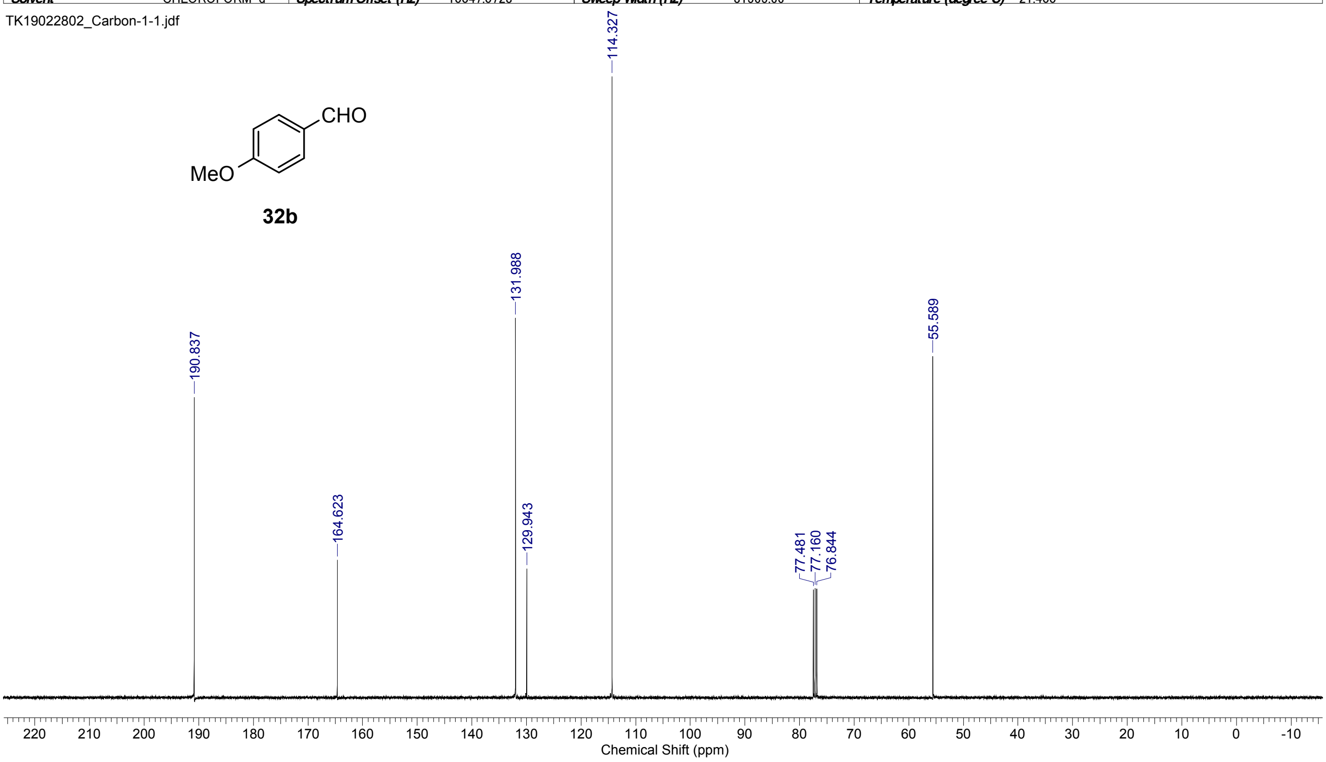
TK18101603_Proton-1-1.jdf



2019/03/07 14:50:46

Acquisition Time (sec)	1.0381	Comment	single pulse decoupled gated NOE			Date	01 Mar 2019 09:33:38
Date Stamp	01 Mar 2019 09:23:36						
File Name	¥¥Mac¥iCloud¥[illegible]¥NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK19022802_Carbon-1-1.jdf						
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	256	Origin	ECA
Original Points Count	32768	Owner	delta	Points Count	65536	Pulse Sequence	carbon.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10047.0723	Sweep Width (Hz)	31565.66	Temperature (degree C)	21.400

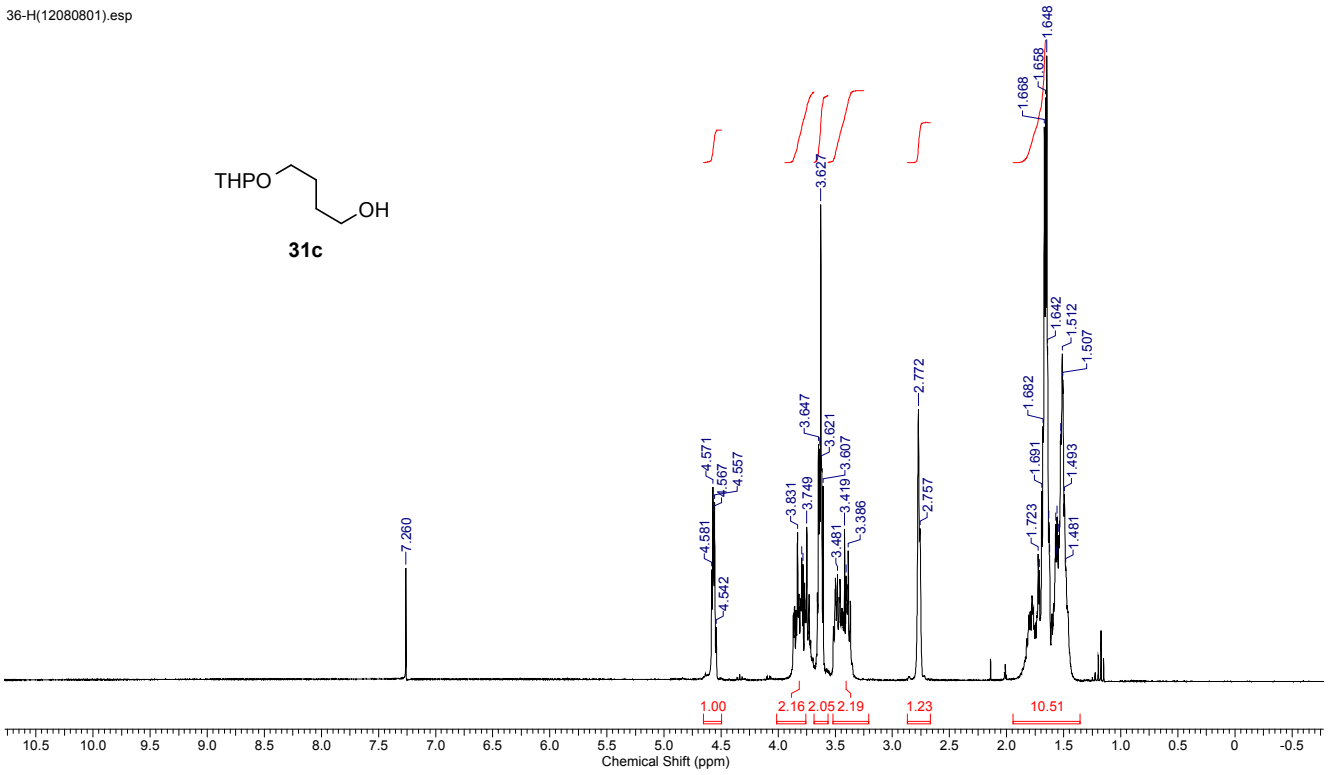
TK19022802_Carbon-1-1.jdf



2019/03/07 16:29:29

Acquisition Time (sec)	3.5561	*Comment*	STANDARD 1H OBSERVE			*Date*	Aug 8 2012
Date Stamp	Aug 8 2012	*File Name*	¥¥Mac¥iCloud¥ [illegible]¥NMR [illegible]¥2012NMR K¥saka¥12080801.fid¥fid				
Frequency (MHz)	300.06	*Nucleus*	1H	*Number of Transients*	16	*Original Points Count*	17080
Points Count	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	16.00	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	1752.1255	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	4803.07	*Temperature (degree C)*	AMBIENT TEMPERATURE

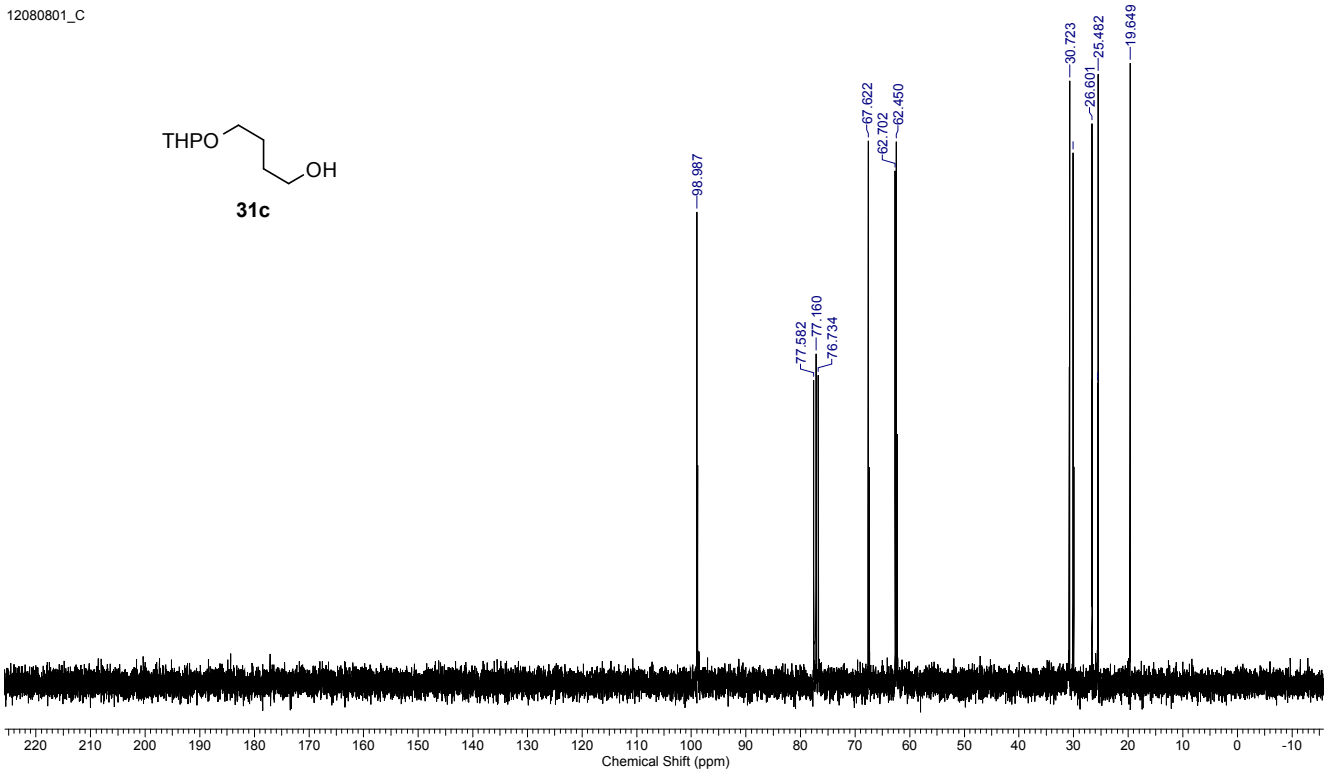
36-H(12080801).esp



2019/03/07 16:38:11

Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Aug 8 2012	*Date Stamp*	Aug 8 2012		
File Name	¥¥Mac¥iCloud¥ [illegible]¥NMR [illegible]¥2012NMR K¥saka¥12080801_C.fid¥fid					*Frequency (MHz)*	75.46	*Nucleus*	13C
Number of Transients	96	*Original Points Count*	19335	*Points Count*	65536	*Pulse Sequence*	s2pul	*Receiver Gain*	30.00
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	8966.3594	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74
Temperature (degree C)	AMBIENT TEMPERATURE								

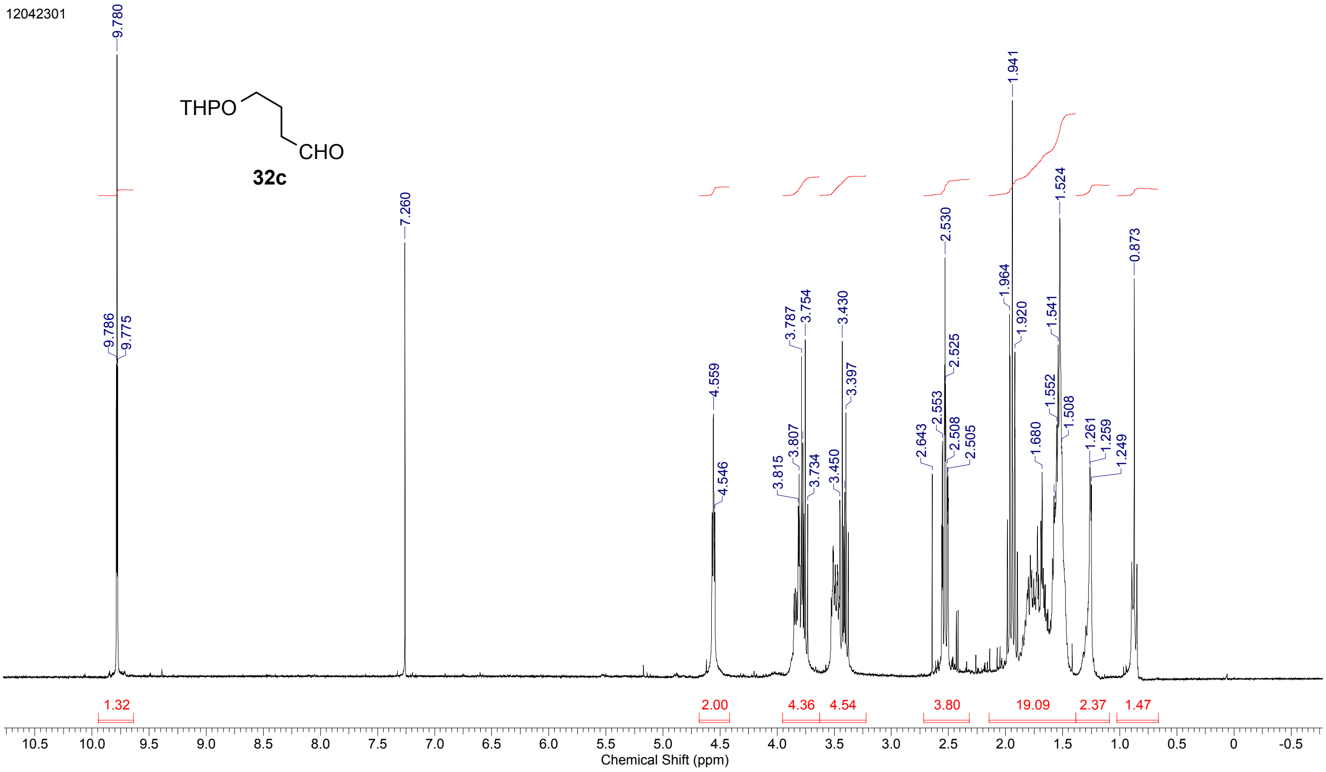
12080801_C



2019/03/07 15:02:26

Acquisition Time (sec)	3.5561	Comment	STANDARD 1H OBSERVE			Date	Apr 23 2012
Date Stamp	Apr 23 2012	File Name	¥¥Mac¥iCloud¥ ... ¥NMR ... ¥2012NMR_K¥saka¥12042301.fid¥fid				
Frequency (MHz)	300.06	Nucleus	1H	Number of Transients	16	Original Points Count	17080
Points Count	65536	Pulse Sequence	s2pul	Receiver Gain	24.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1767.8837	Spectrum Type	STANDARD	Sweep Width (Hz)	4803.07	Temperature (degree C)	AMBIENT TEMPERATURE

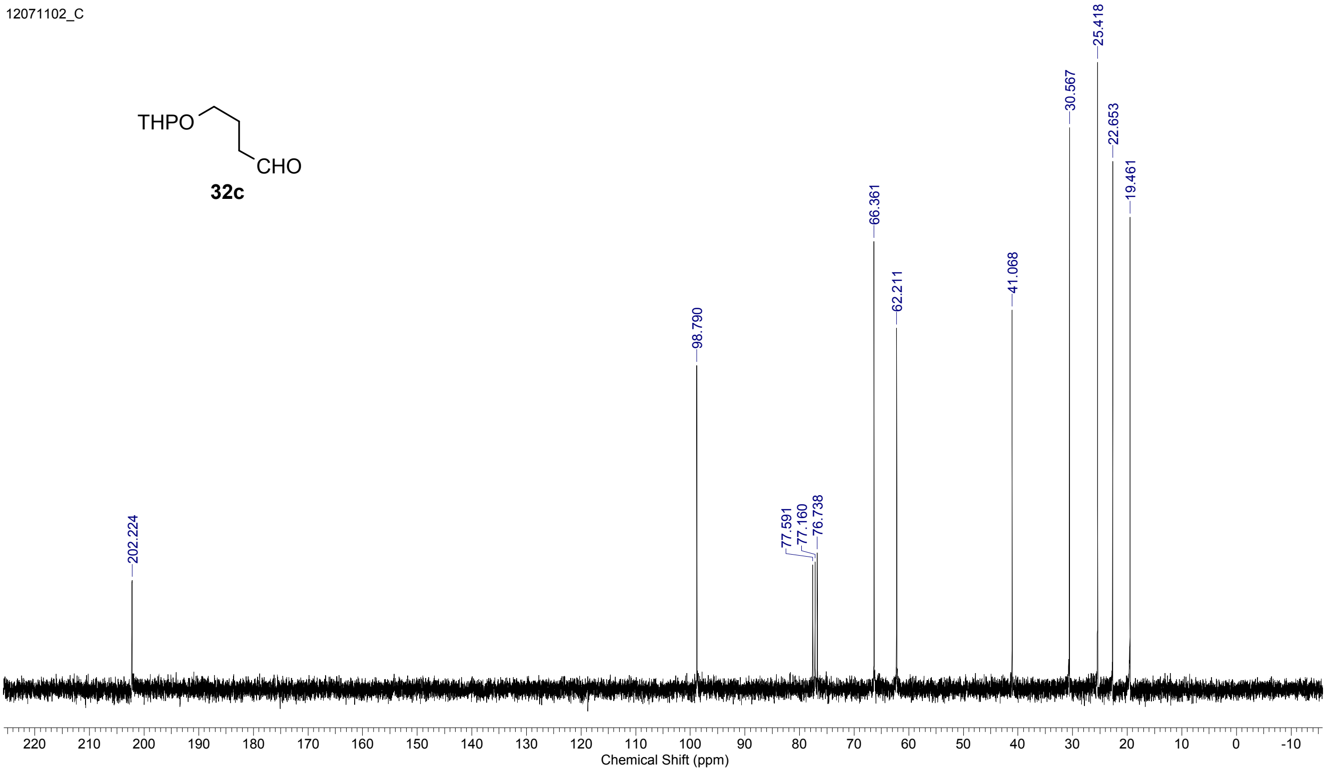
12042301



2019/03/07 17:19:56

Acquisition Time (sec)	0.8527	Comment	c13-NMR	Date	Jul 11 2012	Date Stamp	Jul 11 2012
File Name	¥¥Mac¥iCloud¥ ... ¥NMR ... ¥2012NMR_K¥saka¥12071102_C.fid¥fid			Frequency (MHz)	75.46	Nucleus	13C
Number of Transients	64	Original Points Count	19335	Points Count	65536	Pulse Sequence	s2pul
Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	8962.2070	Spectrum Type	STANDARD
Sweep Width (Hz)	22675.74	Temperature (degree C)	AMBIENT TEMPERATURE				

12071102_C

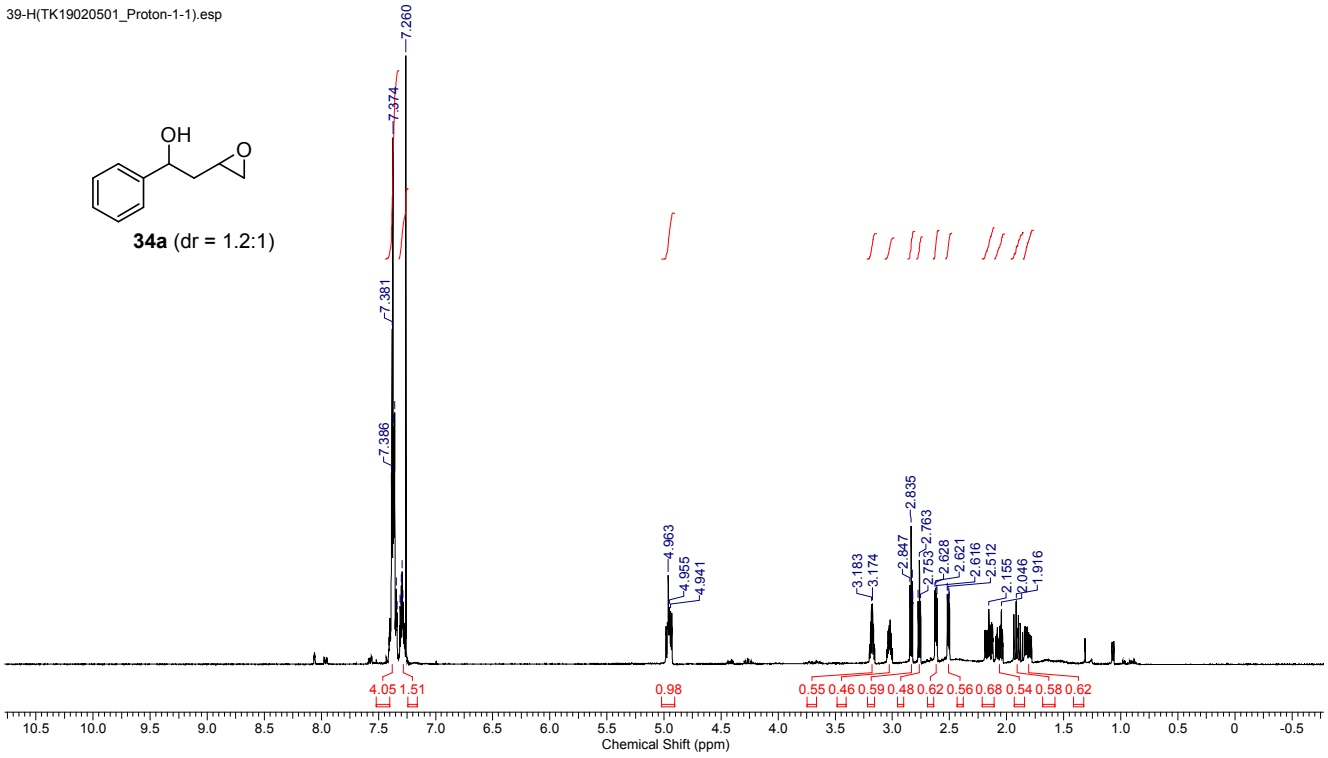


2019/03/07 18:13:26

Acquisition Time (sec)	2.1863	***Comment***	single_pulse	***Date***	05 Feb 2019 13:33:59		
Date Stamp	05 Feb 2019 13:33:08						
File Name	¥¥Mac¥iCloud¥ [illegible]NMR [illegible]¥2018NMR K¥2018NMR(JEOL)¥ [illegible]NMR2018¥TK19020501_Proton-1-1.jdf						
Frequency (MHz)	399.78	***Nucleus***	1H	***Number of Transients***	8	***Origin***	ECA
Original Points Count	16384	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp
Solvent	CHLOROFORM-d	***Spectrum Offset (Hz)***	2003.4905	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	22.100

39-H(TK19020501_Proton-1-1).esp

34a (dr = 1.2:1)

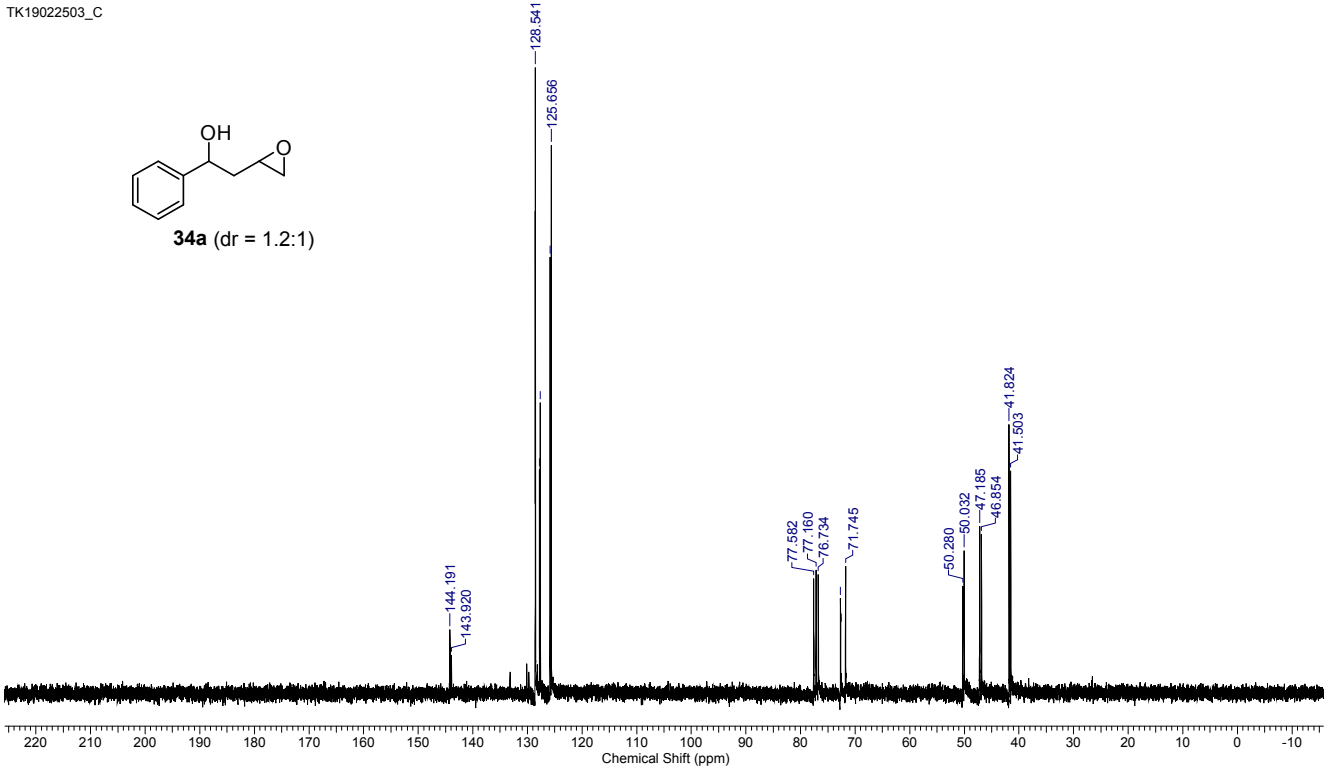


2019/03/07 18:28:29

Acquisition Time (sec)	0.8527	***Comment***	c13-NMR	***Date***	Feb 25 2019	***Date Stamp***	Feb 25 2019
File Name	¥¥Mac¥iCloud¥ [illegible]NMR [illegible]¥2018NMR K¥2018NMR(agilent)¥kawakami¥TK19022503_C.fid¥fid					***Frequency (MHz)***	75.46
Nucleus	13C	***Number of Transients***	128	***Original Points Count***	19335	***Points Count***	65536
Pulse Sequence	s2pul	***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	8949.3369
Spectrum Type	STANDARD	***Sweep Width (Hz)***	22675.74	***Temperature (degree C)***	AMBIENT TEMPERATURE		

TK19022503_C

34a (dr = 1.2:1)

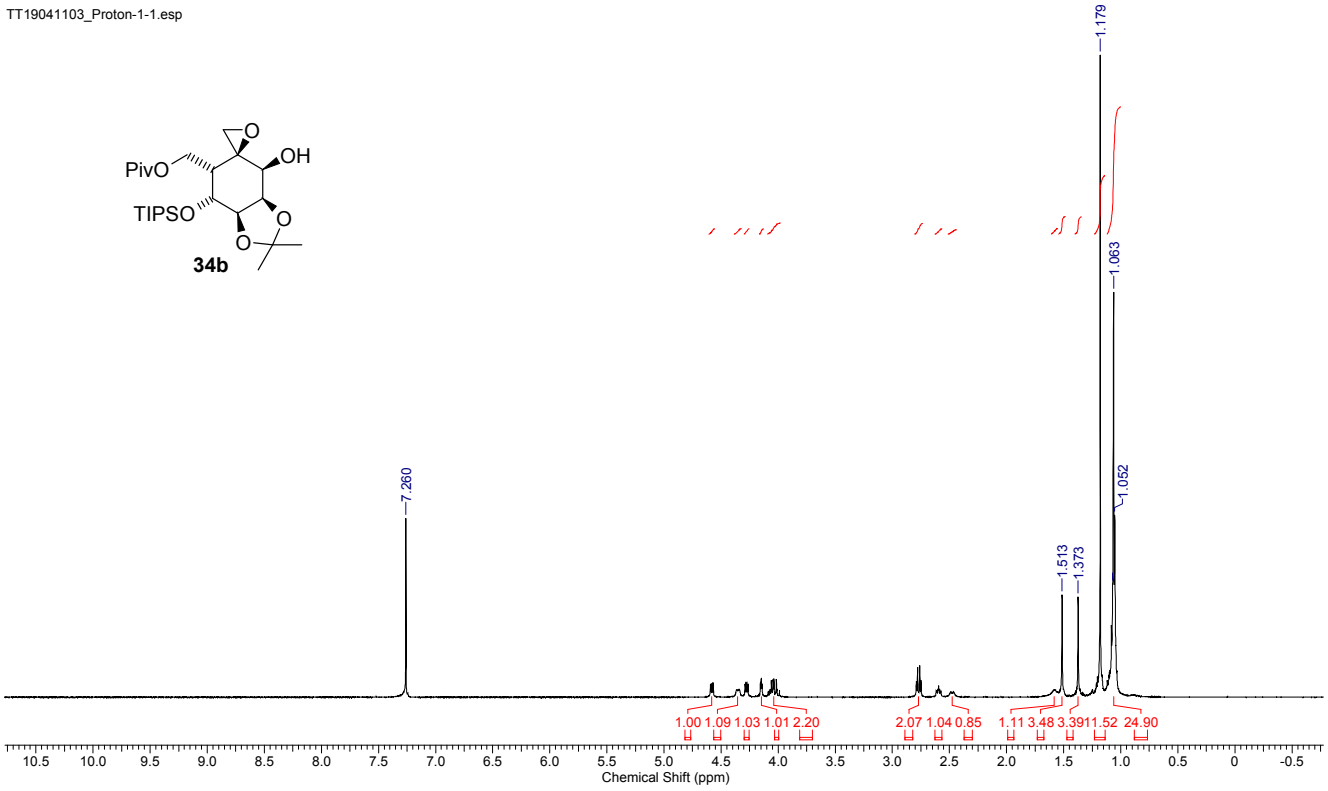


2019/05/20 17:34:35

Acquisition Time (sec)	2.1863	***Comment***	single pulse	***Date***	11 Apr 2019 14:45:44			***Date Stamp***	11 Apr 2019 14:44:53
File Name	¥¥WS¥data¥ ﾋﾋﾋ ﾋ¥TT19041103 Proton-1-1.jdf			***Frequency (MHz)***	399.78	***Nucleus***	1H	***Number of Transients***	8
Origin	ECA	***Original Points Count***	16384	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	proton.jxp
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2003.4905	***Sweep Width (Hz)***	7494.00	***Temperature (degree C)***	16.200

TT19041103_Proton-1-1.esp

34b

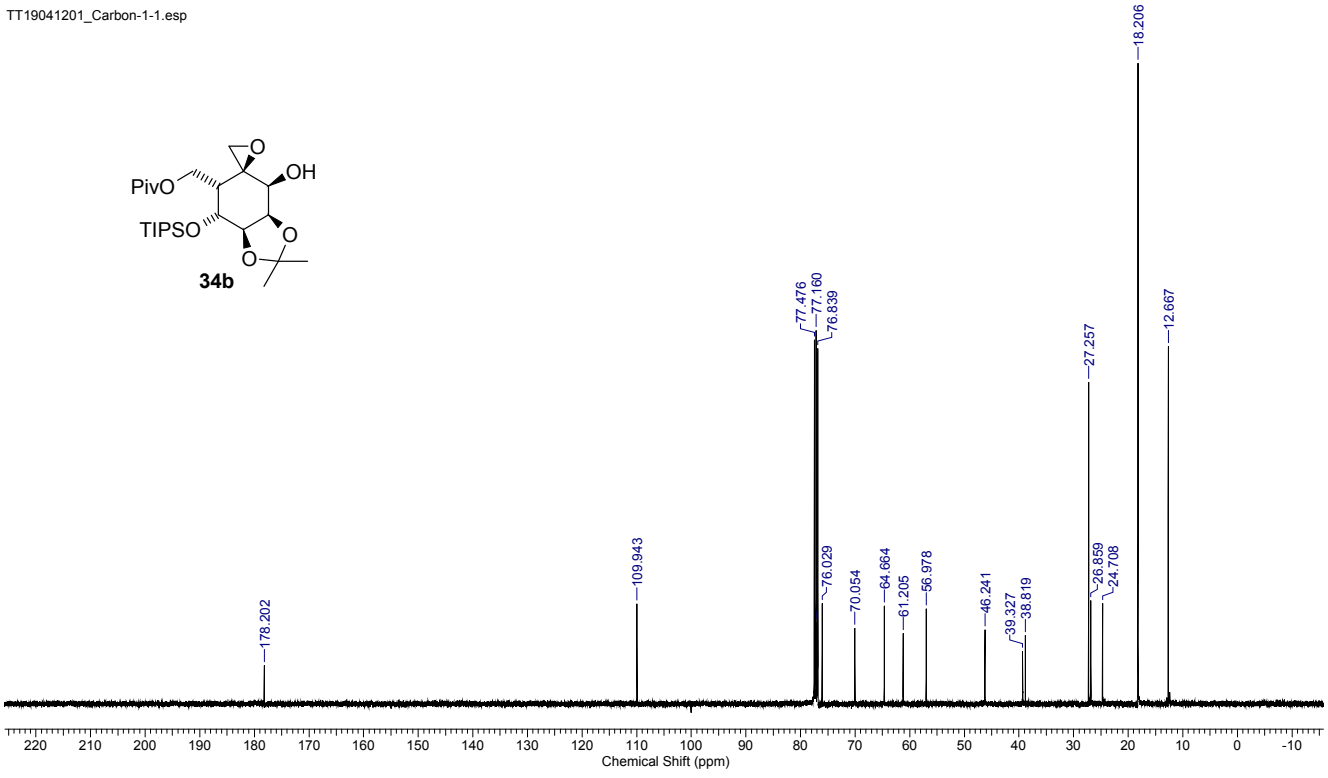


2019/05/20 19:38:10

Acquisition Time (sec)	1.0381	***Comment***	single pulse decoupled gated NOE			***Date***	12 Apr 2019 12:57:55		
Date Stamp	12 Apr 2019 12:18:23			***File Name***	¥¥WS¥data¥ ﾋﾋﾋ ﾋ¥TT19041201 Carbon-1-1.jdf			***Frequency (MHz)***	100.53
Nucleus	13C	***Number of Transients***	1024	***Origin***	ECA	***Original Points Count***	32768	***Owner***	delta
Points Count	65536	***Pulse Sequence***	carbon.jxp	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10056.2236
Sweep Width (Hz)	31565.66	***Temperature (degree C)***	16.600						

TT19041201_Carbon-1-1.esp

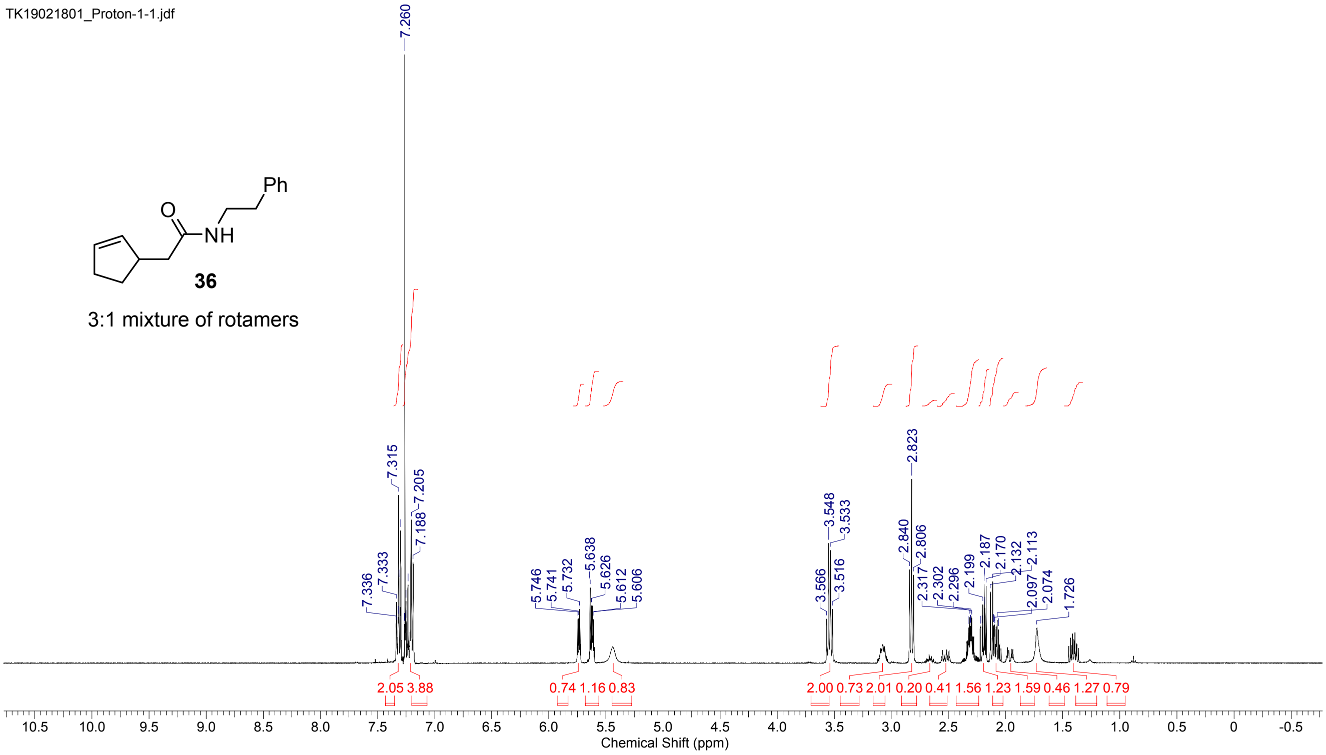
34b



2019/03/11 18:10:06

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	18 Feb 2019 12:01:30		
Date Stamp	18 Feb 2019 12:00:38						
File Name	¥¥Mac¥iCloud¥_[illegible]¥NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK19021801_Proton-1-1.jdf						
Frequency (MHz)	399.78	*Nucleus*	1H	*Number of Transients*	8	*Origin*	ECA
Original Points Count	16384	*Owner*	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Solvent	CHLOROFORM-d	*Spectrum Offset (Hz)*	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	21.300

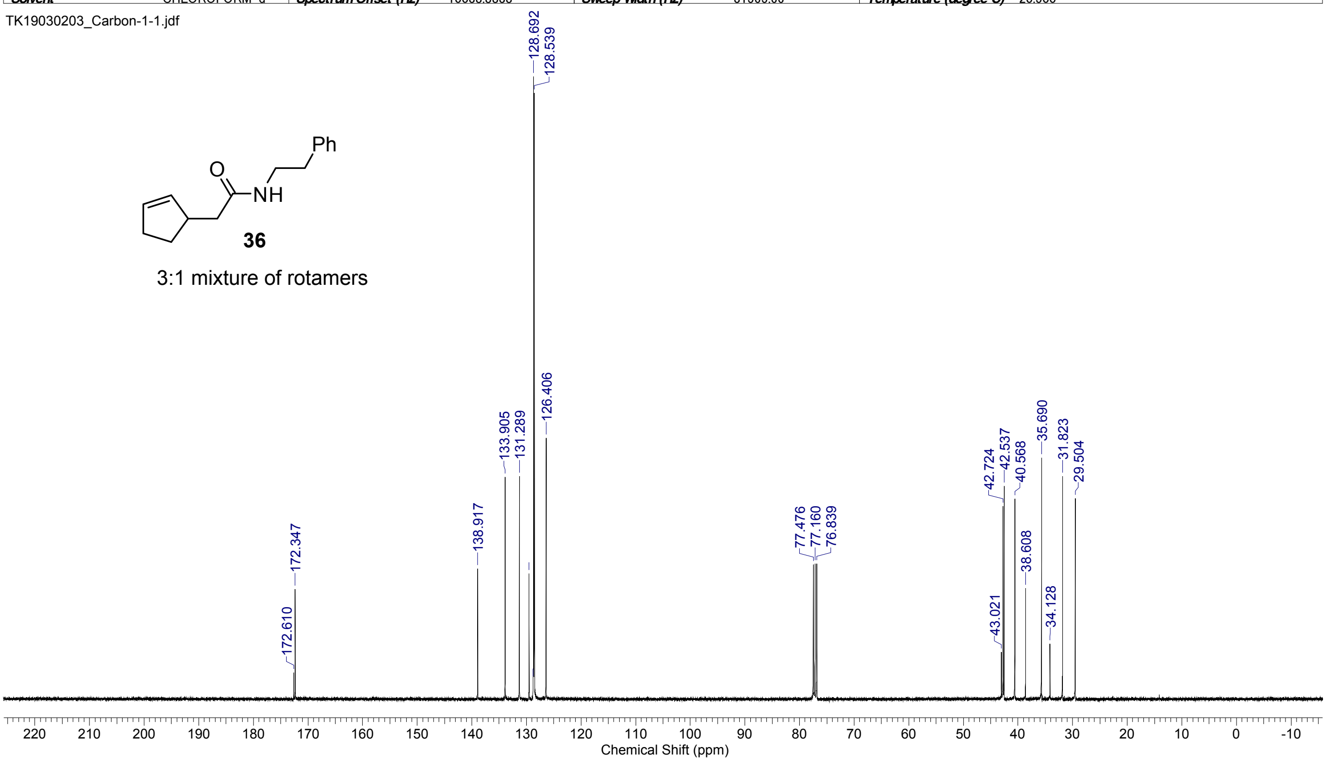
TK19021801_Proton-1-1.jdf



2019/03/11 18:39:28

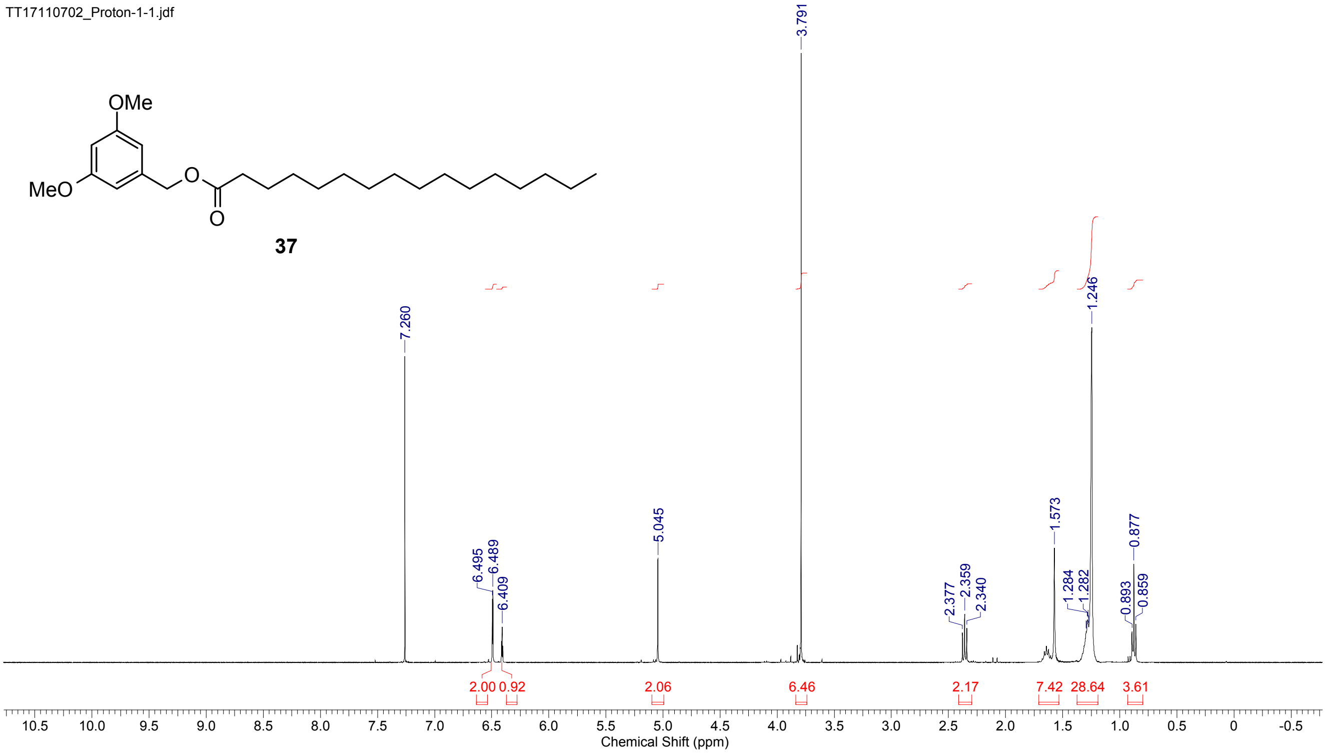
Acquisition Time (sec)	1.0381	*Comment*	single pulse decoupled gated NOE	*Date*	02 Mar 2019 09:12:02		
Date Stamp	02 Mar 2019 08:52:10						
File Name	¥¥Mac¥iCloud¥_[illegible]¥NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK19030203_Carbon-1-1.jdf						
Frequency (MHz)	100.53	*Nucleus*	13C	*Number of Transients*	512	*Origin*	ECA
Original Points Count	32768	*Owner*	delta	*Points Count*	65536	*Pulse Sequence*	carbon.jxp
Solvent	CHLOROFORM-d	*Spectrum Offset (Hz)*	10038.8838	*Sweep Width (Hz)*	31565.66	*Temperature (degree C)*	20.500

TK19030203_Carbon-1-1.jdf



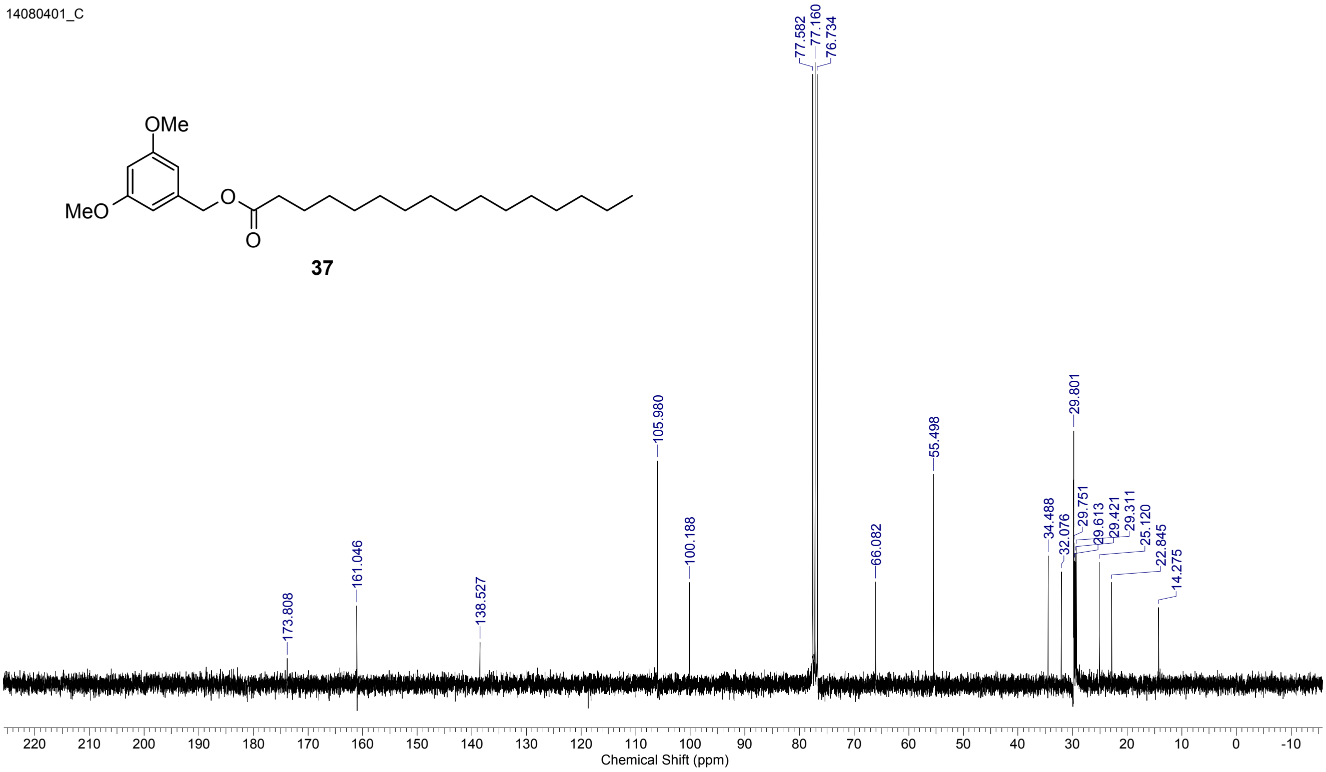
2019/03/07 18:47:57

Acquisition Time (sec)	2.1863	*Comment*	single_pulse	*Date*	07 Nov 2017 09:45:29		
Date Stamp	07 Nov 2017 09:44:38						
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2017NMR_K¥2017NMR(JEOL)¥[illegible]NMR2017¥TT17110702_Proton-1-1.jdf						
Frequency (MHz)	399.78	*Nucleus*	1H	*Number of Transients*	8	*Origin*	ECA
Original Points Count	16384	*Owner*	delta	*Points Count*	32768	*Pulse Sequence*	proton.jxp
Solvent	CHLOROFORM-d	*Spectrum Offset (Hz)*	2003.4905	*Sweep Width (Hz)*	7494.00	*Temperature (degree C)*	18.900



2019/03/07 18:53:59

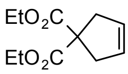
Acquisition Time (sec)	0.8527	*Comment*	c13-NMR	*Date*	Aug 4 2014	*Date Stamp*	Aug 4 2014
File Name	¥¥Mac¥iCloud¥[illegible]NMR[illegible]¥2014NMR_K¥yasumoto¥14080401_C.fid¥fid					*Frequency (MHz)*	75.46
Nucleus	13C	*Number of Transients*	1024	*Original Points Count*	19335	*Points Count*	65536
Pulse Sequence	s2pul	*Receiver Gain*	30.00	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	8955.6230	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	22675.74	*Temperature (degree C)*	AMBIENT TEMPERATURE



2019/03/07 19:01:23

Acquisition Time (sec)	2.1863	Comment	single_pulse	Date	21 Jan 2019 11:16:36		
Date Stamp	21 Jan 2019 11:15:45						
File Name	¥¥Mac¥iCloud¥_[illegible]¥NMR_[illegible]¥2018NMR_K¥2018NMR(JEOL)¥_[illegible]NMR2018¥TK19012101_Proton-1-1.jdf						
Frequency (MHz)	399.78	Nucleus	1H	Number of Transients	8	Origin	ECA
Original Points Count	16384	Owner	delta	Points Count	32768	Pulse Sequence	proton.jxp
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2003.4905	Sweep Width (Hz)	7494.00	Temperature (degree C)	19.300

TK19012101_Proton-1-1.jdf



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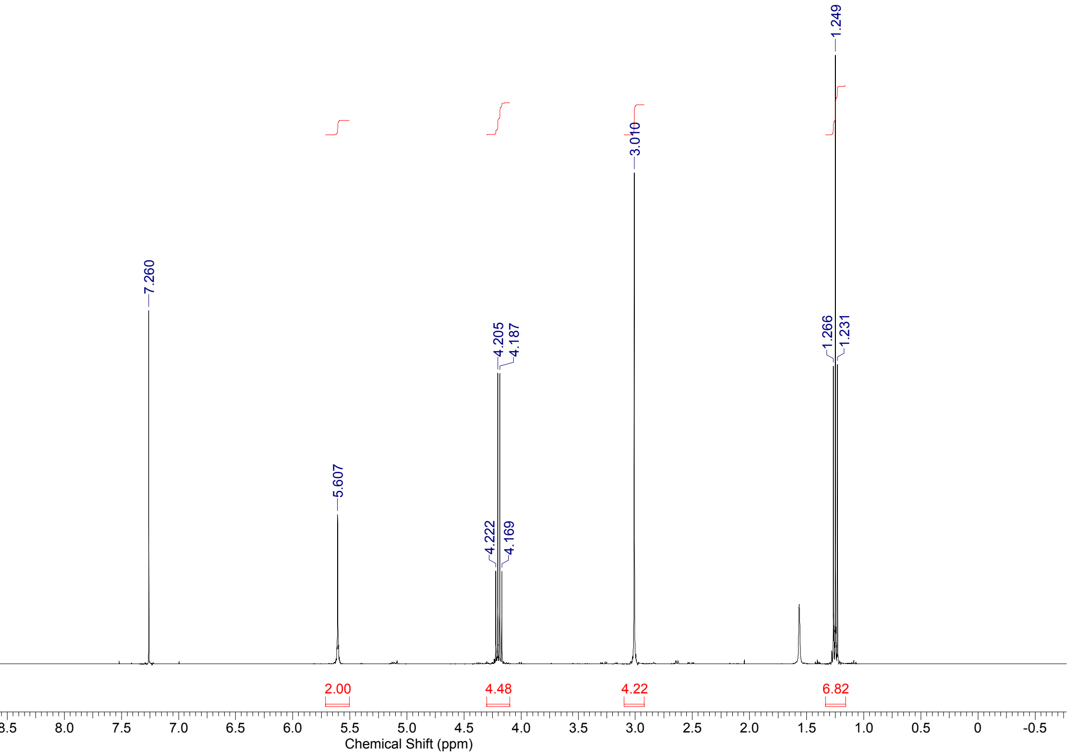
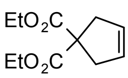


2019/05/27 10:57:10

Acquisition Time (sec)	0.8527	Comment	c13-NMR	Date	Feb 25 2019	Date Stamp	Feb 25 2019
File Name	¥¥Mac¥iCloud¥_[illegible]¥NMR_[illegible]¥2018NMR_K¥2018NMR(agilent)¥kawakami¥TK19022502_C.fid¥fid					Frequency (MHz)	75.46
Nucleus	13C	Number of Transients	64	Original Points Count	19335	Points Count	65536
Pulse Sequence	s2pul	Receiver Gain	30.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	8952.4512
Spectrum Type	STANDARD	Sweep Width (Hz)	22675.74	Temperature (degree C)	AMBIENT TEMPERATURE		

44-C(TK19022502_C).esp



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