Convenient Synthesis of 2,3-Dihydro-1,2,4-thiadiazoles, 4,5-Dihydro-1,3-thiazoles, and 1,3-Thiazoles through a [4+1]-Type Oxidative Ring Closure of Isolable 1,3-Thiaza-1,3-butadienes

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Supporting Information

Contents

I. General Information

The melting points were determined with a Barnstead International MEL-TEMP, and were uncorrected. ^{1}H NMR spectra were recorded on a Bruker DRX 400-P spectrometer (400 MHz) or a Bruker DRX 500-P NMR spectrometer (500 MHz), and the chemical shifts of the ^{1}H NMR spectra are given in δ relative to internal tetramethylsilane (TMS). ^{13}C NMR spectra were recorded using a Bruker DRX-400P (101 MHZ) or a Bruker AVANCE III 500 (126 MHZ). Mass spectra were recorded on a JEOL JMS-700T mass spectrometer with electron-impact ionization or electrospray ionization. High resolution mass spectra (HRMS) were also recorded on a JEOL JMS-700T spectrometer. IR spectra were measured as thin-film (neat) or KBr disks on a JASCO FT/IR-7300 spectrometer. Elemental analyses were performed using a Yanagimoto CHN corder MT-5.

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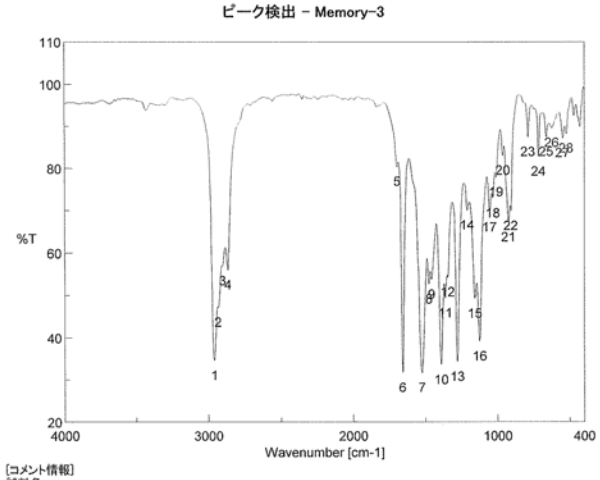
II. Spectral data for the compounds

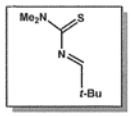
(1) 1,3-Thiaza-1,3-butadienes (5, 6):

5a ($R^1 = NMe_2$, $R^2 = t\text{-}C_4H_9$):

IR Spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部



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		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
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エンド	4600.36 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	4358	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

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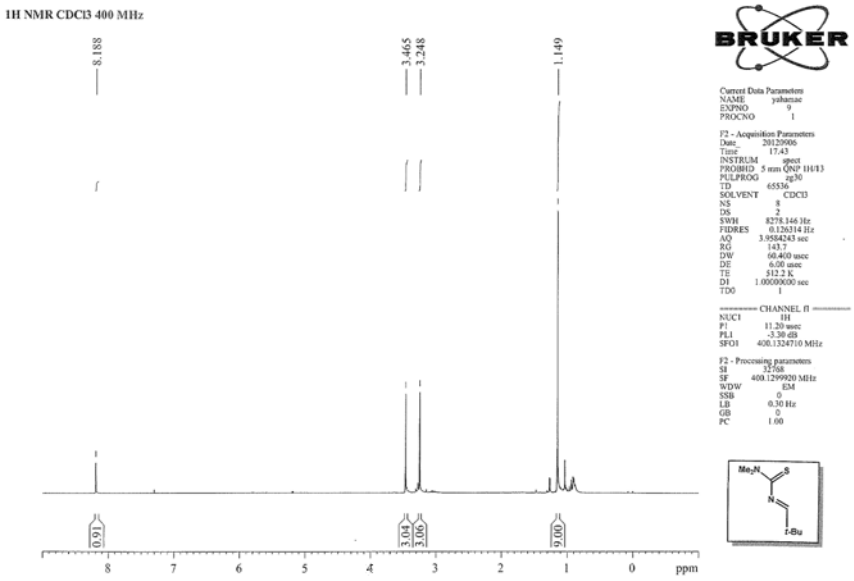
4	2868.6	56	5	1697.1	80	6	1658.5	32
7	1525.4	32	8	1477.2	53	9	1458.9	54
10	1392.4	34	11	1363.4	49	12	1347.0	54
13	1280.5	34	14	1212.0	70	15	1159.0	49
16	1125.3	39	17	1056.8	70	18	1035.6	73
19	1012.5	78	20	965.2	83	21	925.7	67
22	909.3	70	23	790.7	87	24	718.4	83
25	664.4	87	26	625.8	90	27	549.6	87
28	525.5	88						

^{1}H NMR spectrum



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PROCNO 1

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FIDRES 0.126314 Hz
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RG 143.7
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TE 312.2 K
D1 1.00000000 sec
TD0 1

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F2 - Processing parameters
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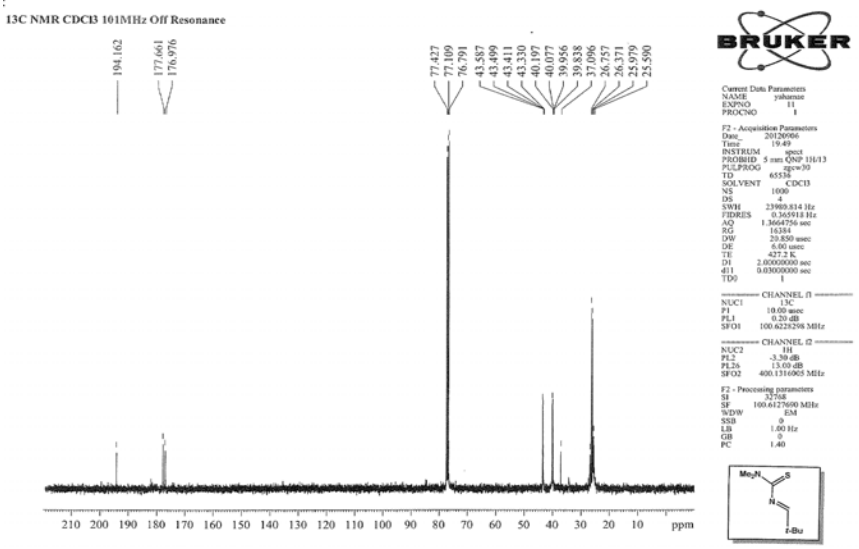
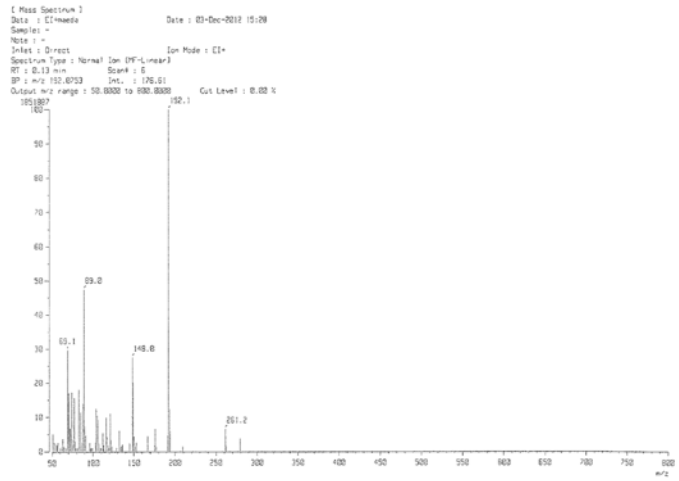
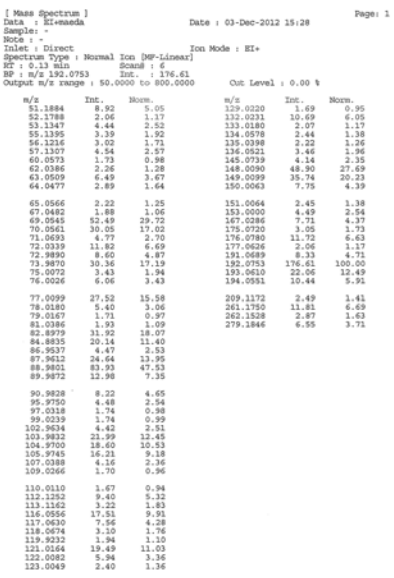
^{13}C NMR spectrum



5b ($R^1 = NMe_2$, $R^2 = C_6H_5$):

Mass Spectrum





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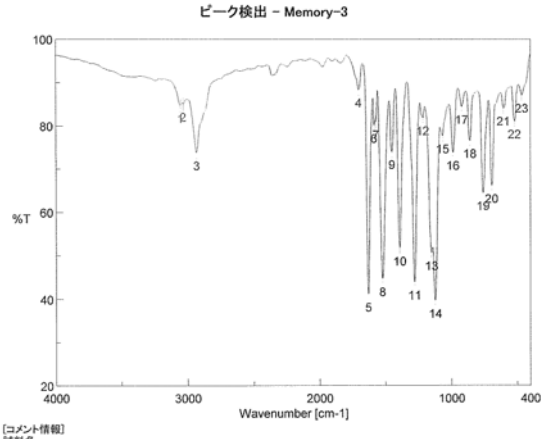
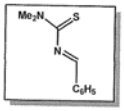
53.1347	4.44	2.52	133.0180	2.07	1.17
55.1395	3.39	1.92	134.0578	2.44	1.38
56.1216	3.02	1.71	135.0398	2.22	1.26
57.1307	4.54	2.57	136.0521	3.46	1.96
60.0573	1.73	0.98	145.0739	4.14	2.35
62.0386	2.26	1.28	148.0090	48.90	27.69
63.0509	6.49	3.67	149.0099	35.74	20.23
64.0477	2.89	1.64	150.0063	7.75	4.39
65.0566	2.22	1.25	151.0064	2.45	1.38
67.0482	1.88	1.06	153.0000	4.49	2.54
69.0545	52.49	29.72	167.0286	7.71	4.37
70.0561	30.05	17.02	175.0720	3.05	1.73
71.0693	4.77	2.70	176.0780	11.72	6.63
72.0339	11.82	6.69	177.0626	2.06	1.17
72.9890	8.60	4.87	191.0689	8.33	4.71
73.9870	30.36	17.19	192.0753	176.61	100.00
75.0072	3.43	1.94	193.0610	22.06	12.49
76.0026	6.06	3.43	194.0551	10.44	5.91
77.0099	27.52	15.58	209.1172	2.49	1.41
78.0180	5.40	3.06	261.1750	11.81	6.69
79.0167	1.71	0.97	262.1528	2.87	1.63
81.0386	1.93	1.09	279.1846	6.55	3.71
82.8979	31.92	18.07			
84.8835	20.14	11.40			
86.9537	4.47	2.53			
87.9612	24.64	13.95			
88.9801	83.93	47.53			
89.9872	12.98	7.35			
90.9828	8.22	4.65			
95.9750	4.48	2.54			
97.0318	1.74	0.98			
99.0239	1.74	0.99			
102.9634	4.42	2.51			
103.9832	21.99	12.45			
104.9700	18.60	10.53			
105.9745	16.21	9.18			
107.0388	4.16	2.36			
109.0266	1.70	0.96			
110.0110	1.67	0.94			
112.1252	9.40	5.32			
113.1162	3.22	1.83			
116.0556	17.51	9.91			
117.0630	7.56	4.28			
118.0674	3.10	1.76			
119.9232	1.94	1.10			
121.0164	19.49	11.03			
122.0082	5.94	3.36			
123.0049	2.40	1.36			

IR Spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部



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データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	349.053 cm-1	積算回数	20
エンド	7800.65 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	7729	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

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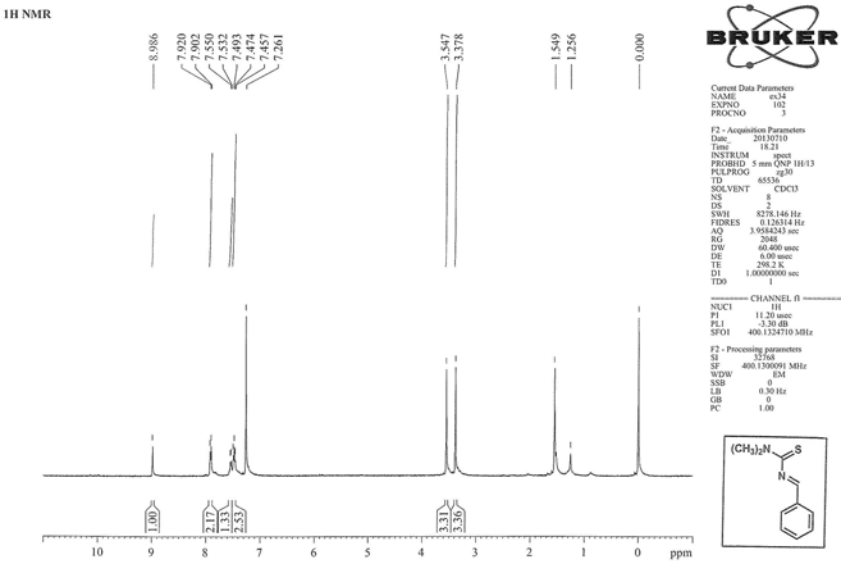
7	1572.7	81	8	1521.6	45	9	1451.2	74
10	1392.4	52	11	1278.6	44	12	1215.9	82
13	1151.3	51	14	1122.4	40	15	1066.4	78
16	987.4	74	17	921.8	84	18	859.1	77
19	758.9	64	20	692.3	66	21	603.6	84
22	518.8	81	23	464.8	87			

^{1}H NMR spectrum



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PROCNO 3

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DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 2048
DW 60.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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F2 - Processing parameters
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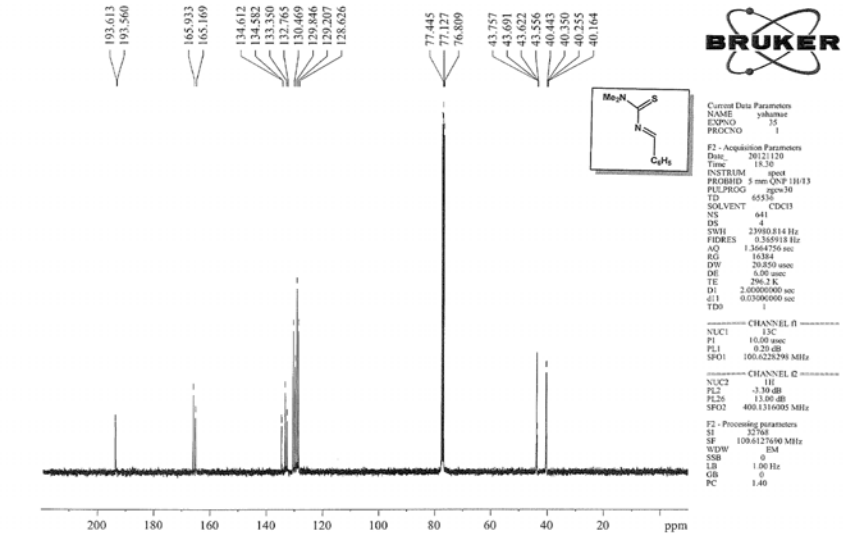
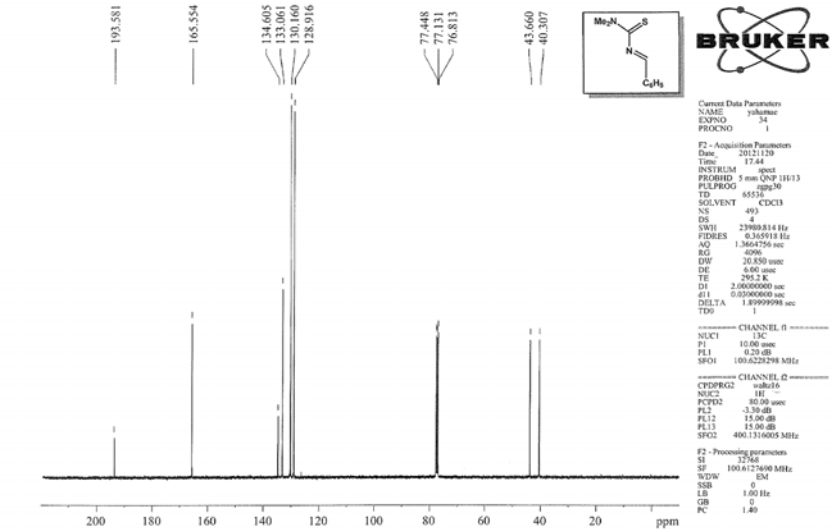
GB 0
PC 1.00

^{13}C NMR spectrum

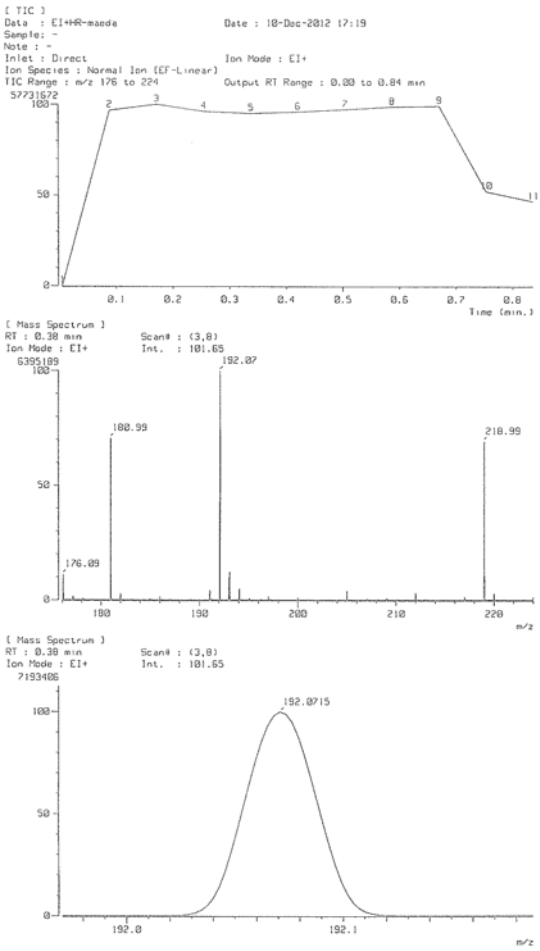
13C NMR CDCl3 298 K Off Resonance



13C NMR CDCl3 298 K



HRMS

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[ Elemental Composition ]
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Sample: -
Note : -
Inlet : Direct                         Ion Mode : EI+
RT : 0.38 min                          Scan#: (3,8)
Elements : C 10/0, H 12/0, N 2/0, S 1/0
Mass Tolerance          : 5mmu
Unsaturation (U.S.) : -0.5 - 10.0

Observed m/z Int%   Err[ppm / mmu]    U.S.  Composition
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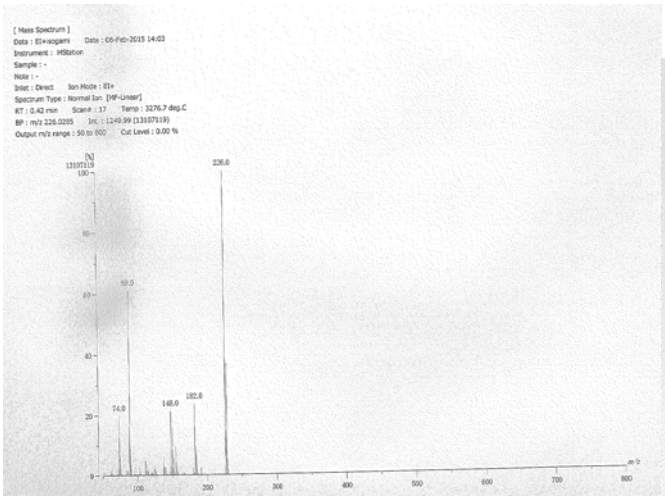
5c (R^1 = NMe_2, R^2 = *p*-ClC_6H_4):

Mass spectrum

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[ Mass Spectrum ]
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Instrument :  MStation
Sample : -
Note  : -
Inlet : Direct                         Ion Mode : EI+
Spectrum Type : Normal Ion    [MF-Linear]
RT : 0.42 min          Scan# : 17      Temp : 3276.7 deg.C
BP : m/z 226.0285      Int. : 1249.99 (13107119)
Output m/z range : 50.0000 to 800.0000     Cut Level : 3.00 %

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 73.9606   250.16    20.01   2623103
 74.9675    51.93     4.15    544495
 88.0141   206.02    16.48   2160255
 89.0234   765.08    61.21   8022399
 90.0207    47.11     3.77    493967
110.9969    59.85     4.79    627599
112.9984    44.46     3.56    466223
124.0033    40.36     3.23    423199
138.0122    78.12     6.25    819119
148.0153   268.38    21.47   2814127
150.0100   198.26    15.86   2078895
152.0091    73.99     5.92    775855
154.9687   121.87     9.75   1277871
156.9704    48.08     3.85    504127
181.9871   295.79    23.66   3101615
182.9801   100.51     8.04   1053871
183.9831   118.96     9.52   1247407
184.9810    40.07     3.21    420127
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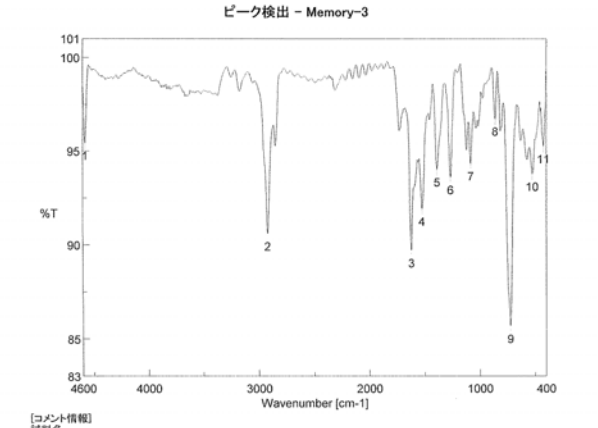
IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2015/02/03 18:27
データタイプ 等間隔データ
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縦軸 %T
スタート 399.193 cm-1
エンド 4800.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

[ピーク検出結果]

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7	1087.7	94.3343	8	864.9	96.7332	9	725.1	85.6905
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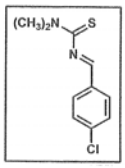
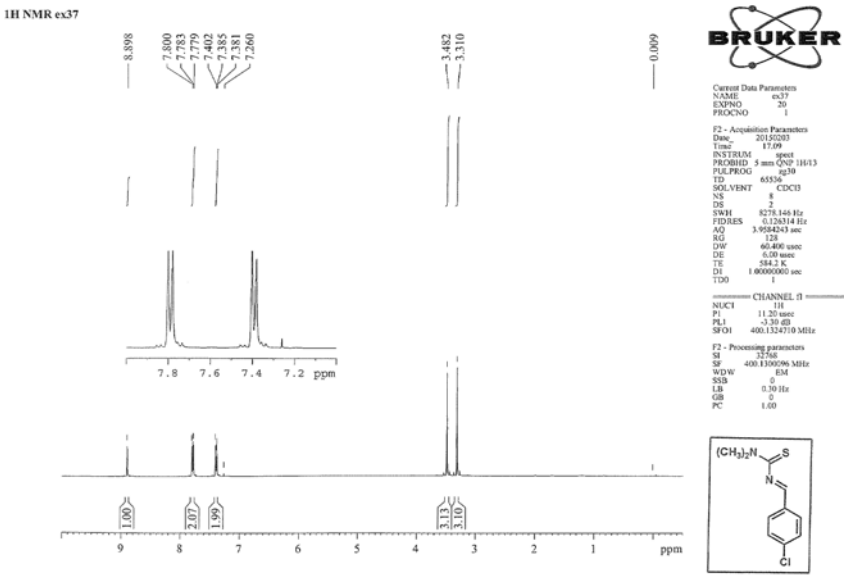
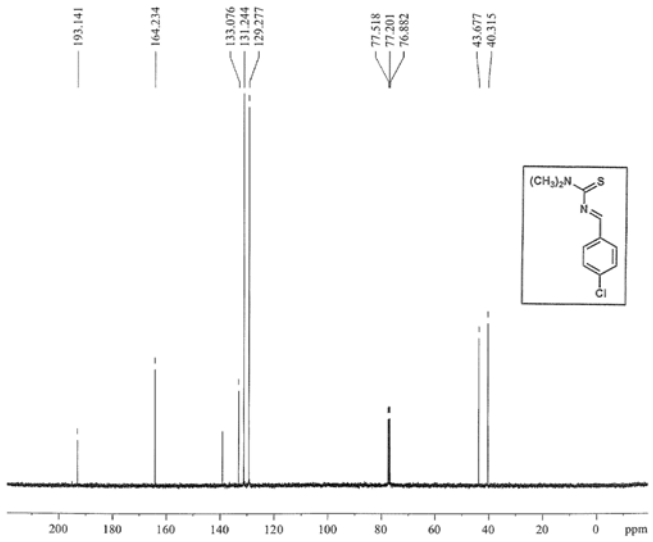


^{1}H NMR



^{13}C NMR

13C NMR ex37 CPD



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SOLVENT CDCl3
NS 63
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FIDRES 0.365918 Hz
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RG 20642.5
DW 20.850 usec
DE 6.00 usec
TE 584.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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SFO1 100.6228298 MHz

========== CHANNEL f2 ==========
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PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
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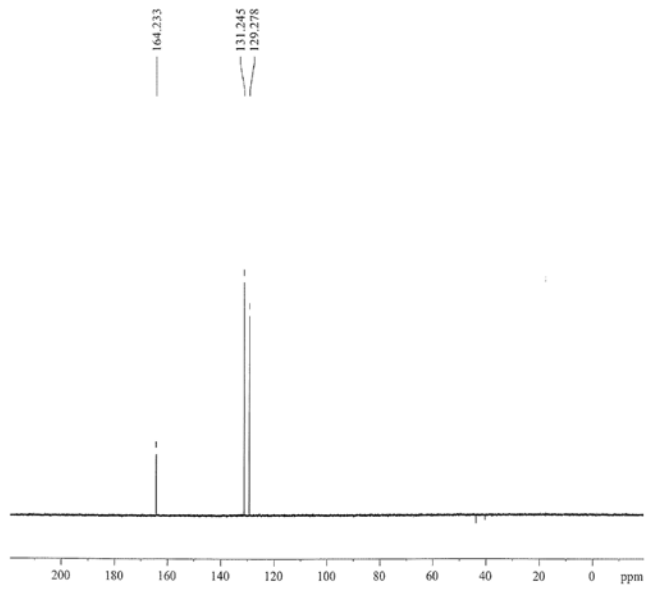
13C NMR ex37 dept90



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PROCNO 1

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FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 41285.1
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DE 6.00 usec
TE 584.3 K
CNST2 145.0000000
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d2 0.00344828 sec
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DELTA 0.00001273 sec
TD0 1

========== CHANNEL f1 ==========
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p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
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p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
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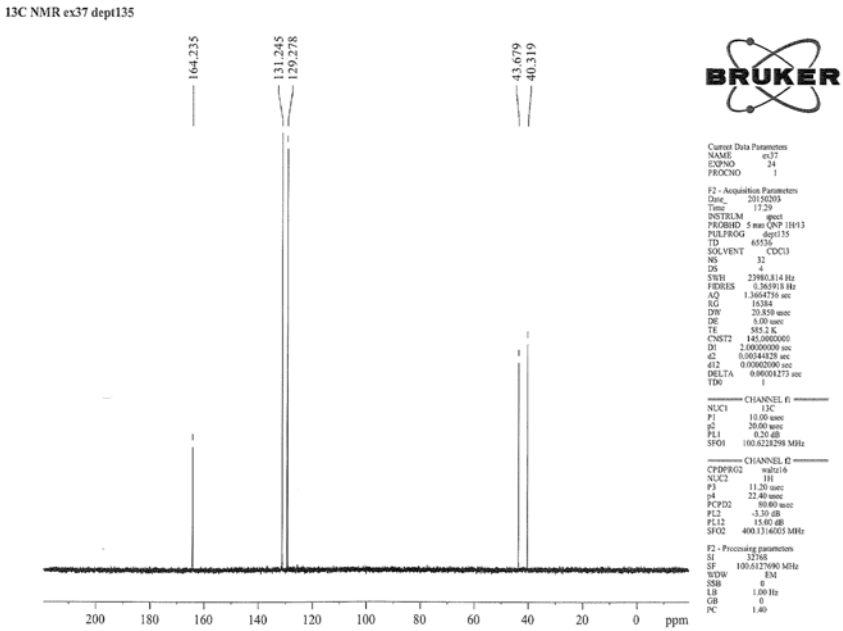
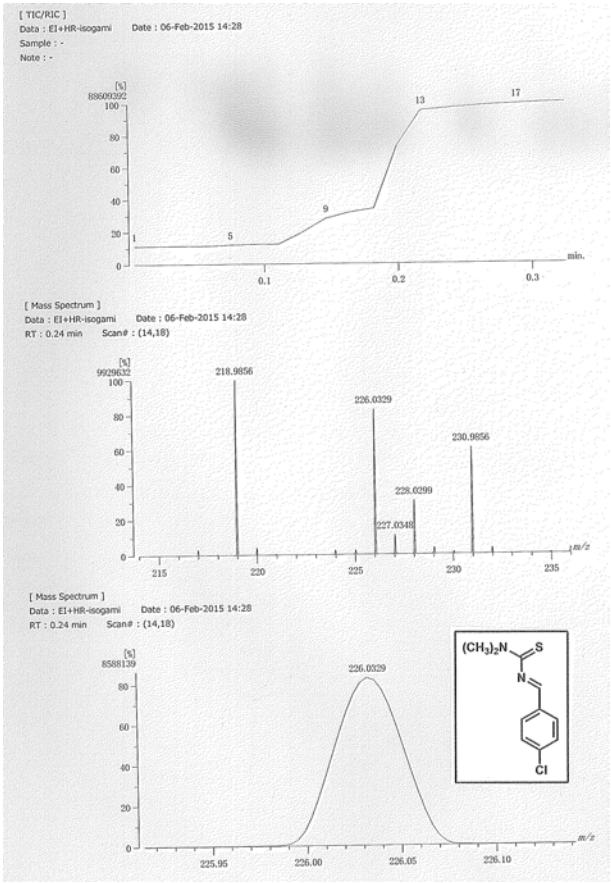


HRMS



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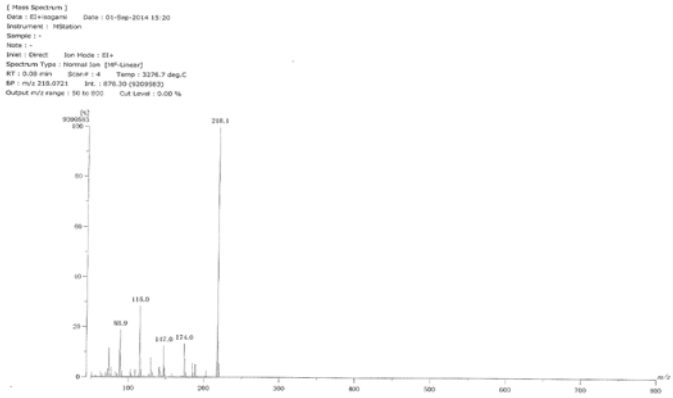
Elements : C 10/0, H 11/0, 35Cl 1/0, 37Cl 1/0, N 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 10.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	226.0329	82.81	-1.1 / -0.2	7.0	C10 H11 35Cl N2 S

5d ($R^1 = NMe_2$, $R^2 = CH{=}CHC_6H_5$):

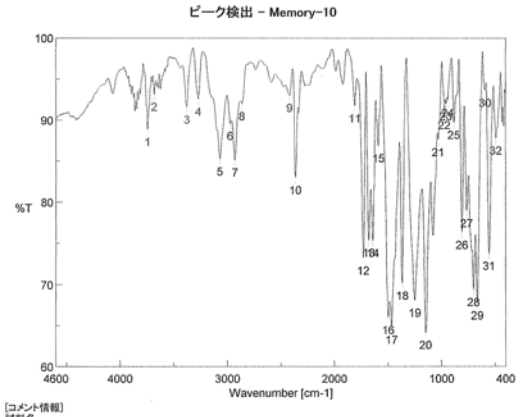
Mass Spectrum



[Mass Spectrum]
Data : EI+isogami Date : 01-Sep-2014 15:20
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.08 min Scan# : 4 Temp : 3276.7 deg.C
BP : m/z 218.0721 Int. : 878.30 (9209583)
Output m/z range : 50.0000 to 800.0000 Cut Level : 1.00 %

m/z	Int.	Norm.	
51.2761	17.56	2.00	184079
63.0763	18.71	2.13	196175
65.0727	11.87	1.35	124431
69.0643	17.10	1.95	179311
70.0522	9.64	1.10	101103
71.0621	13.42	1.53	140767
71.9777	21.55	2.45	226015
72.9756	29.06	3.31	304767
73.9806	102.71	11.69	1076959
74.9824	10.99	1.25	115279
75.9856	11.25	1.28	117951
76.9960	34.19	3.89	358543
77.9967	10.46	1.19	109663
82.8726	18.93	2.16	198495
84.8614	12.44	1.42	130463
87.9422	95.26	10.85	998879
88.9486	165.79	18.88	1738463
89.9451	13.32	1.52	139679
90.9634	22.50	2.56	235903
101.9734	16.40	1.87	172015
102.9862	26.90	3.06	282095
103.9915	12.76	1.45	133759
109.0126	26.49	3.02	277807
114.0256	13.35	1.52	139999
115.0458	249.75	28.44	2618847
116.0564	68.23	7.77	715487
117.0711	26.47	3.01	277599
126.9983	10.58	1.20	110911
129.0000	11.07	1.26	116031
130.0169	66.50	7.57	697311
131.0043	26.29	2.99	275679
132.0119	16.05	1.83	168271
140.0035	9.37	1.07	98255
141.0176	34.47	3.92	361439
142.0283	20.77	2.36	217775
143.0426	20.41	2.32	213999
147.0027	110.18	12.54	1155295
148.0117	33.37	3.80	349871
149.0099	10.03	1.14	105215
158.0593	13.00	1.48	136335
174.0281	116.77	13.30	1224415
175.0302	65.58	7.47	687647
176.0351	17.31	1.97	181519
185.0917	49.16	5.60	515455
186.0900	15.48	1.76	162335
189.0534	44.73	5.09	469007
203.0573	23.20	2.64	243263
217.0655	56.34	6.41	590751
218.0721	878.30	100.00	9209583
219.0723	125.68	14.31	1317871
220.0746	47.54	5.41	498447

IR Spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/07/29 17:25
更新日時 2014/07/29 17:26

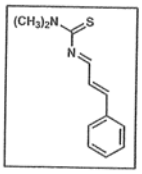
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018

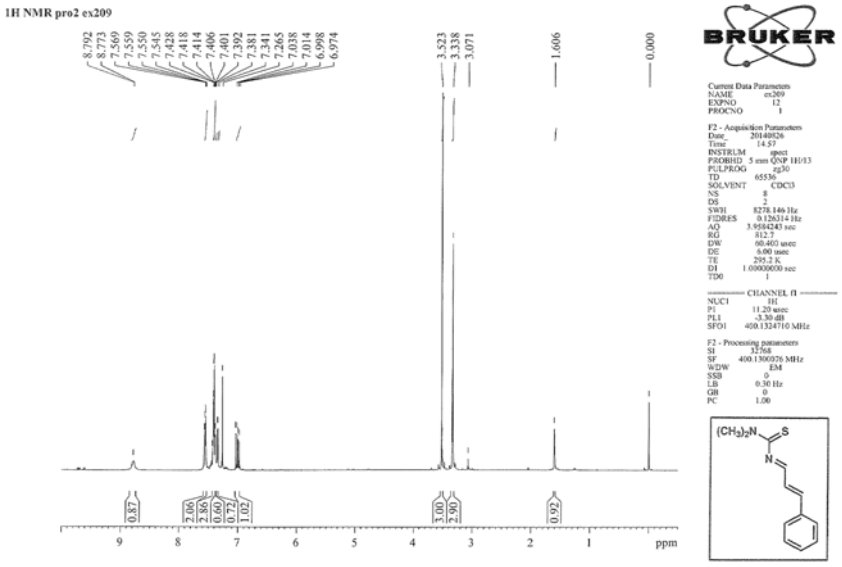
測定日時 2014/07/29 17:21
光源 標準光源
検出器 TGS
積算回数 48
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (64)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

[ピーク検出結果]

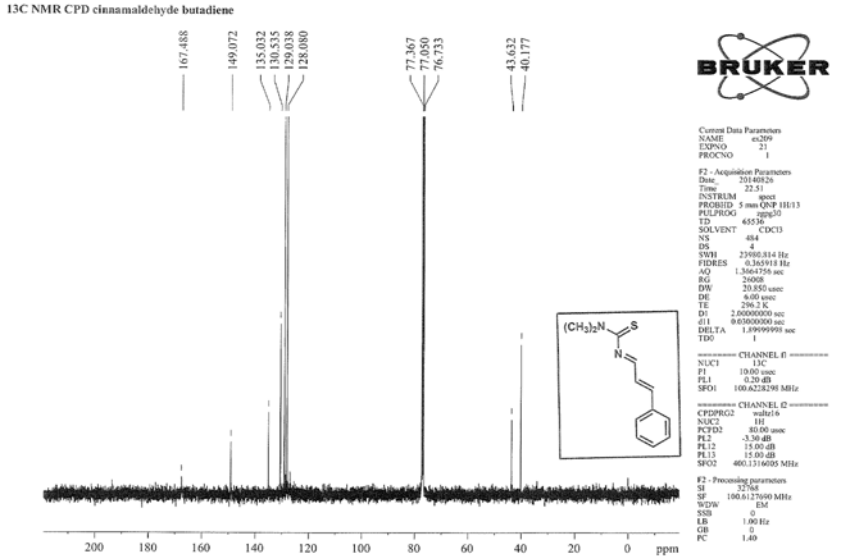
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3743.2	88.8657	2	3681.4	93.1674	3	3375.8	91.6043
4	3269.7	92.6021	5	3067.2	85.2612	6	2969.8	89.6075
7	2927.4	85.1419	8	2861.8	92.0115	9	2419.3	93.0485
10	2363.3	82.9993	11	1808.9	91.7596	12	1729.8	73.2246
13	1678.7	75.4084	14	1641.1	75.3604	15	1589.1	86.8669
16	1497.5	66.0101	17	1466.6	64.8111	18	1366.3	70.1922
19	1250.6	68.1112	20	1147.4	64.1758	21	1030.8	87.6275
22	971.0	90.9382	23	957.5	92.0336	24	941.1	92.4522
25	882.3	89.7331	26	808.0	76.3426	27	763.7	78.9885
28	700.0	69.4076	29	665.3	67.7922	30	593.0	93.6767
31	555.4	73.8147	32	490.8	87.8344			



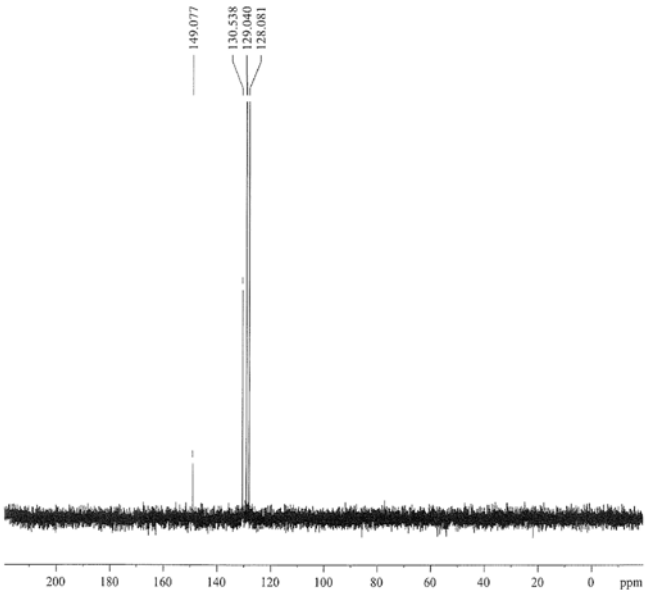
^{1}H NMR


1H NMR pro2 ex209
8.792
8.773
7.569
7.559
7.550
7.545
7.428
7.418
7.414
7.406
7.401
7.392
7.381
7.341
7.265
7.038
7.014
6.998
6.974
3.523
3.338
3.071
1.606
0.000
0.87
2.06
2.86
0.60
0.72
1.02
3.00
2.90
0.92
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME ex209
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140826
Time 14.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 812.7
DW 60.402 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
(CH3)2N
S
N

^{13}C NMR


13C NMR CPD cinnamaldehyde butadiene
167.488
149.072
135.032
130.535
129.038
128.080
77.367
77.050
76.733
43.632
40.177
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME ex209
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140826
Time 22.51
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 484
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 26008
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
(CH3)2N
S
N

13C NMR dept 90 cinnamaldehyde butadiene



Current Data Parameters
NAME ex209
EXPNO 23
PROCNO 1

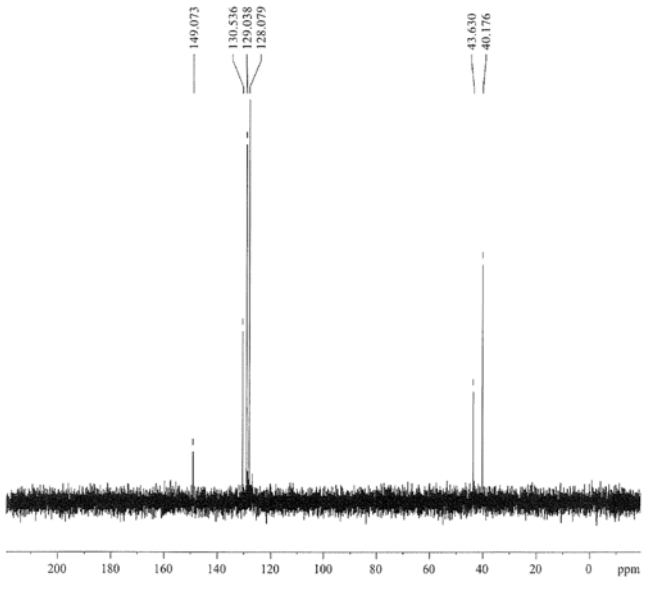
F2 - Acquisition Parameters
Date_ 20140826
Time 23.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 101
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.60 usec
TE 296.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.90 dB
SFO2 400.1316005 MHz

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

13C NMR DEPT135 cinnamaldehyde butadiene



Current Data Parameters
NAME ex209
EXPNO 25
PROCNO 1

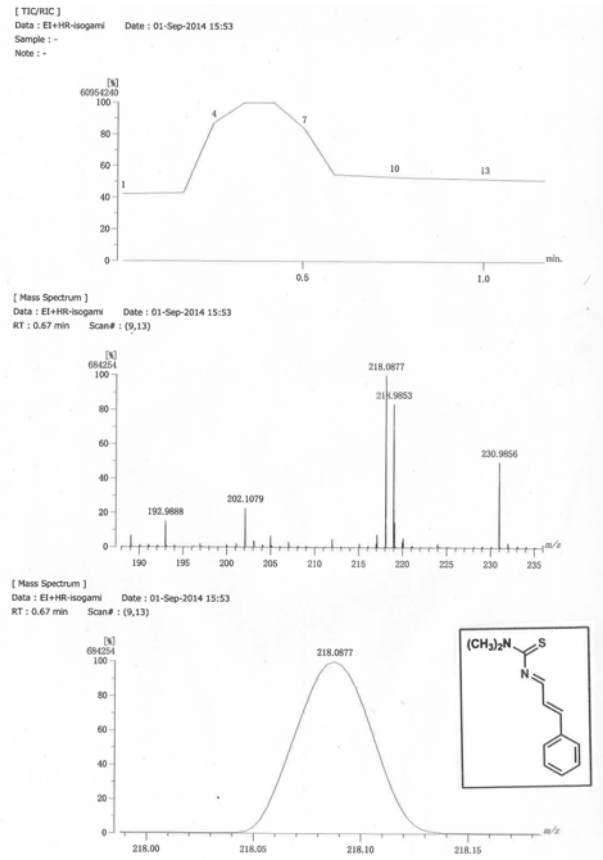
F2 - Acquisition Parameters
Date_ 20140826
Time 23.19
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 106
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 29193
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

HRMS



Data : EI+HR-isogami Date : 01-Sep-2014 15:53
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.67 min Scan# : (9,13)
Elements : C 12/0, H 14/0, N 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 10.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	218.0877	100.00	-0.3 / -0.1	8.0	C12 H14 N2 S

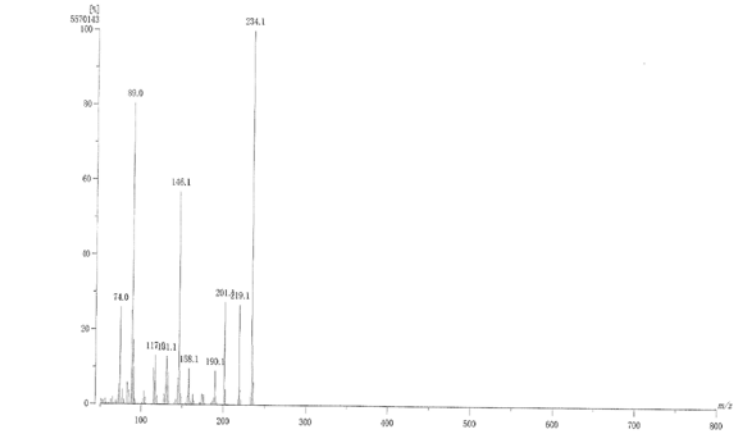
[Theoretical Ion Distribution]
Molecular Formula : C12 H14 N2 S
(m/z 218.0878, MW 218.3226, U.S. 8.0)
Base Peak : 218.0878, Averaged MW : 218.3198(a), 218.3212(w)

m/z	INT.
218.0878	100.0000
219.0906	14.8708
220.0854	5.4577
221.0872	0.6676
222.0875	0.0629
223.0883	0.0046
224.0900	0.0002

5e (R^1 = NMe_2, R^2 = Mes):

Mass Spectrum

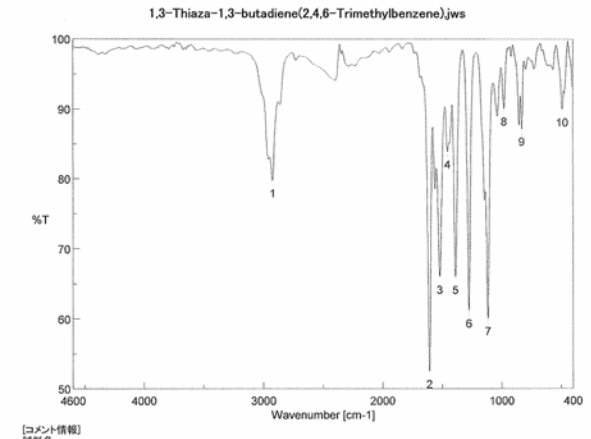
[Mass Spectrum]
Data : EI+isogami Date : 09-May-2014 13:23
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.13 min Scan# : 6 Temp : 3276.7 deg.C
BP : m/z 234.1124 Int. : 531.21 (5570143)
Output m/z range : 50 to 800 Cut Level : 0.09 %



[Mass Spectrum]
Data : EI+isogami Date : 09-May-2014 13:23
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.13 min Scan# : 6 Temp : 3276.7 deg.C
BP : m/z 234.1124 Int. : 531.21 (5570143)
Output m/z range : 100.0000 to 800.0000 Cut Level : 1.00 %

m/z	Int.	Norm.	
102.0946	8.33	1.57	87359
103.1088	19.30	3.63	202335
104.1040	10.49	1.98	110047
105.1221	10.25	1.93	107439
115.1042	52.24	9.83	547759
116.1134	31.08	5.85	325903
117.0485	70.21	13.22	736239
118.1241	9.69	1.82	101647
119.1447	12.84	2.42	134623
127.0989	6.70	1.26	70239
128.1001	15.01	2.83	157423
129.1114	12.71	2.39	133263
130.1059	46.45	8.74	487071
131.1105	68.31	12.86	716271
132.1184	46.22	8.70	484703
133.0744	26.76	5.04	280639
134.0618	5.38	1.01	56415
142.0813	7.54	1.42	79039
143.0871	6.99	1.32	73295
144.0909	26.72	5.03	280127
145.1127	38.42	7.23	402847
146.0664	301.81	56.81	3164655
147.0594	47.94	9.02	502703
148.0768	15.90	2.99	166751
149.0689	10.91	2.05	114351
156.1069	11.87	2.24	124495
157.1184	12.77	2.40	133903
158.1260	51.34	9.66	538351
159.1208	9.94	1.87	104207
163.0592	15.28	2.88	160207
174.0562	15.07	2.84	158031
176.0468	14.63	2.75	153439
187.1186	5.83	1.10	61167
189.0595	10.36	1.95	108607
190.0617	48.03	9.04	503679
191.0740	12.77	2.40	133935
201.0971	145.39	27.37	1524575
202.0983	22.33	4.20	234095
218.1319	8.87	1.67	92991
219.0929	141.59	26.65	1484639
220.0963	21.14	3.98	221647
221.0933	8.18	1.54	85727
233.0988	11.98	2.25	125567
234.1124	531.21	100.00	5570143
235.1014	84.53	15.91	886367
236.1006	32.97	6.21	345759

IR Spectrum



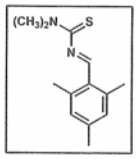
[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/05/12 17:49
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

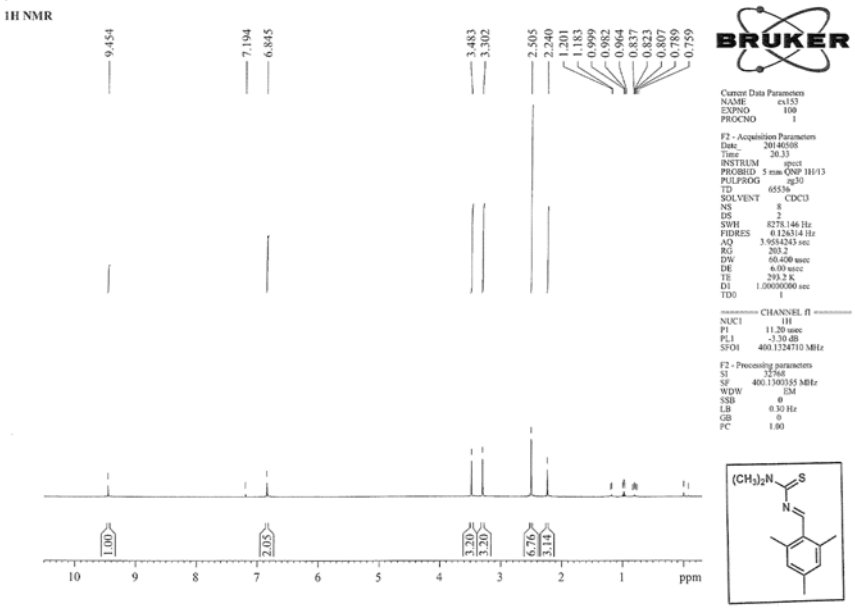
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2923.6	79.7688	2	1606.4	52.4972	3	1518.7	66.0015
4	1454.1	83.8932	5	1387.5	65.9955	6	1274.7	61.193
7	1115.6	60.0758	8	980.6	90.0797	9	831.2	87.1653
10	491.8	89.9661						



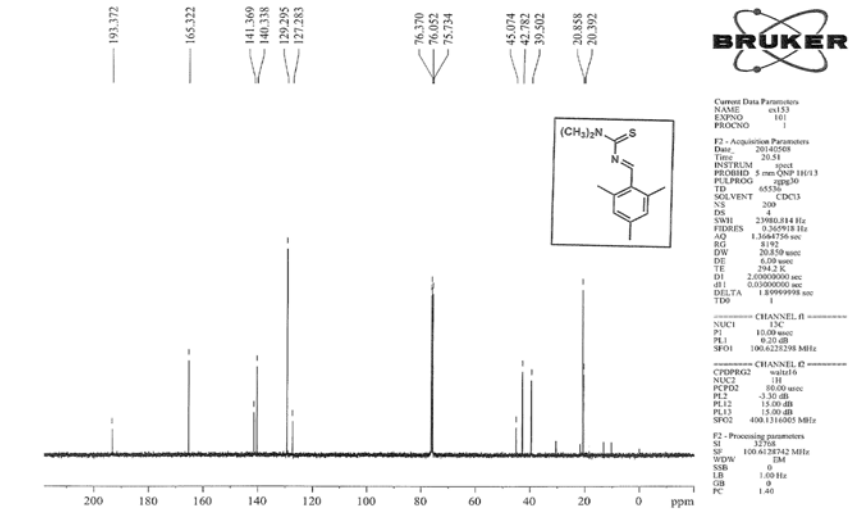
^{1}H NMR

1H NMR

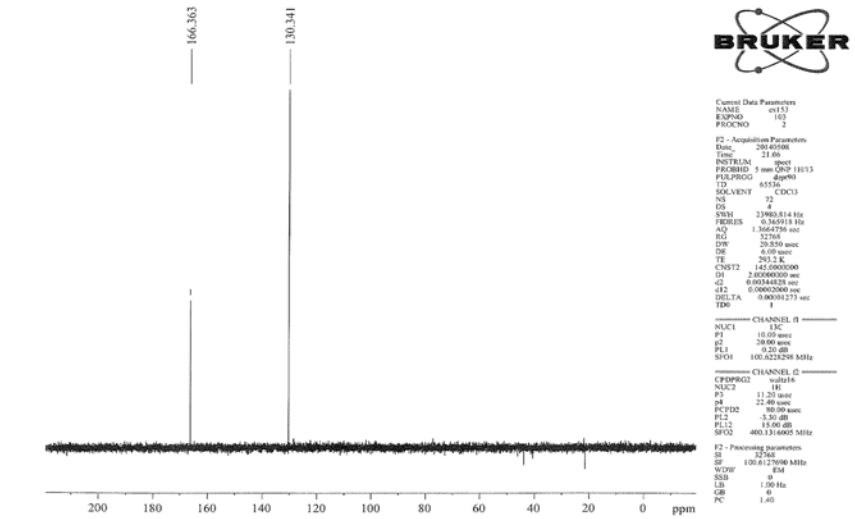


^{13}C NMR

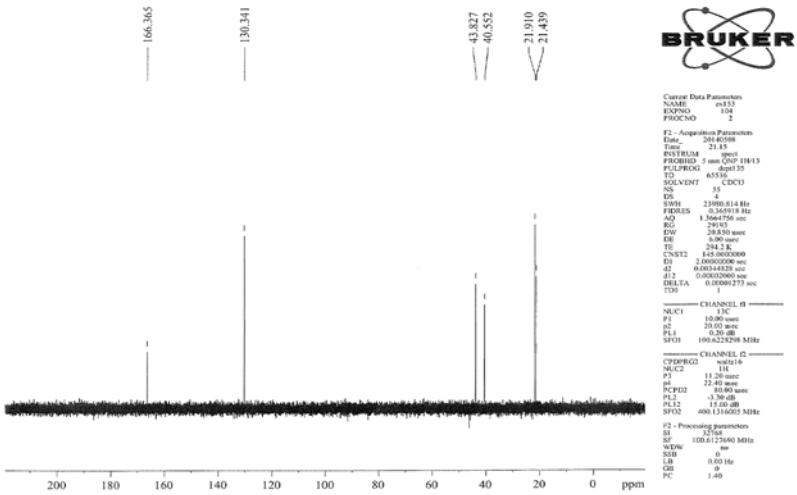
13C NMR



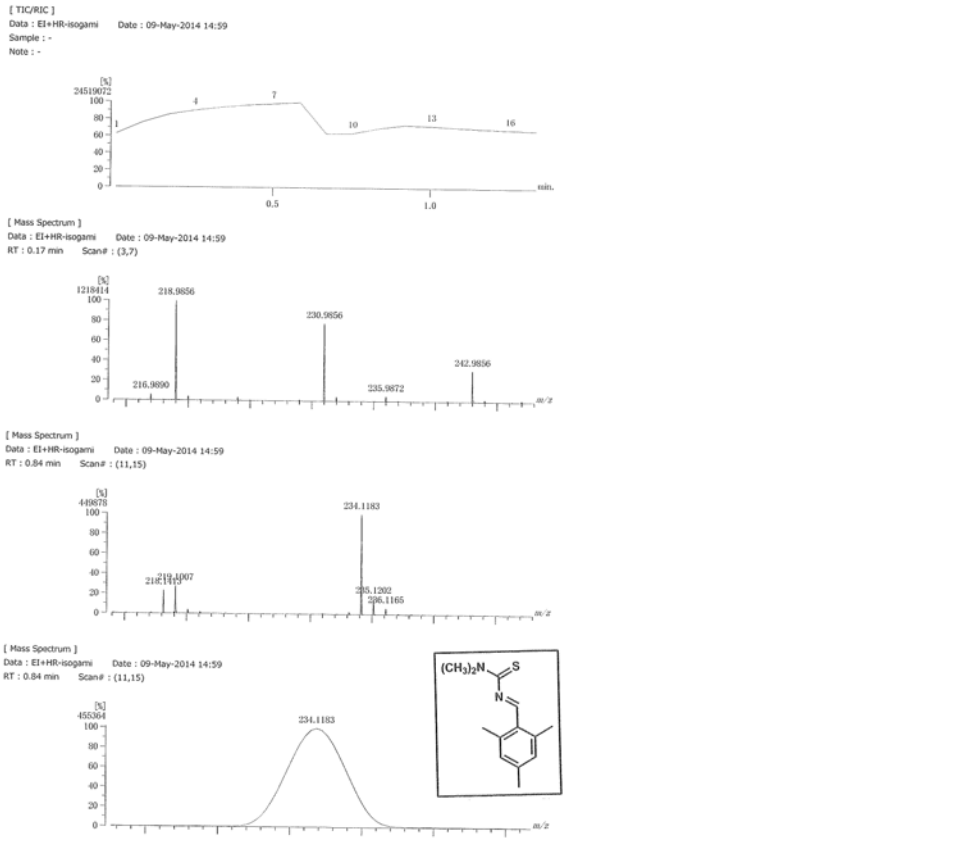
13C dept90



13C dept135



HRMS



Data : EI+HR-isogami Date : 09-May-2014 14:59
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.84 min Scan# : (11,15)
Elements : C 13/0, H 18/0, N 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 10.0

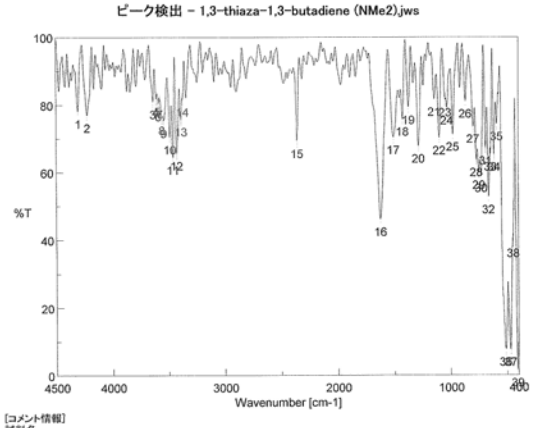
	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	234.1183	100.00	-3.3 / -0.8	7.0	C13 H18 N2 S

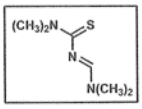
[Theoretical Ion Distribution]
Molecular Formula : C13 H18 N2 S
(m/z 234.1191, MW 234.3653, U.S. 7.0)
Base Peak : 234.1191, Averaged MW : 234.3622(a), 234.3635(w)

m/z	INT.
234.1191	100.0000
235.1219	15.9830
236.1170	5.6231
237.1186	0.7283
238.1191	0.0703
239.1199	0.0053
240.1216	0.0003

5f ($R^1 = R^2 = NMe_2$)[7]:

IR spectrum





[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/09/29 12:37

データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 349.053 cm-1
エンド 7800.65 cm-1
データ間隔 0.964233 cm-1
データ数 7729

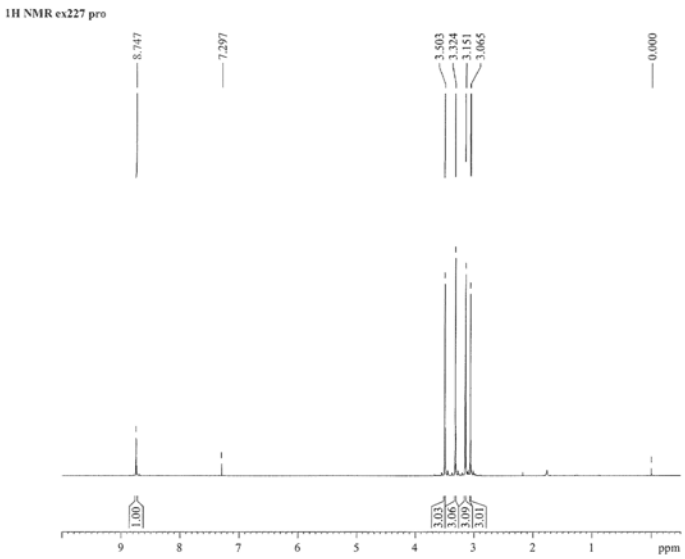
[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018

光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (128)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	4306.3	78.1972	2	4224.3	76.9976	3	3641.9	81.0074
4	3613.0	81.7197	5	3600.5	81.8451	6	3591.8	80.3617
7	3581.2	81.0942	8	3561.9	76.2637	9	3546.5	75.3913
10	3492.5	70.4943	11	3465.5	64.4894	12	3431.7	65.7291
13	3393.1	75.8383	14	3380.6	81.7096	15	2365.3	69.2873
16	1623.8	46.1617	17	1509.0	70.3968	18	1428.0	75.8428
19	1376.0	79.2796	20	1286.3	67.8317	21	1146.5	81.708
22	1101.2	70.2502	23	1049.1	81.5466	24	1034.6	79.16
25	981.6	71.3406	26	869.7	81.1411	27	801.3	73.6506
28	773.3	63.7442	29	751.1	59.9797	30	730.9	59.048
31	690.4	67.1895	32	665.3	52.71	33	648.0	65.397
34	617.1	65.3117	35	593.0	74.3903	36	514.9	7.70481
37	471.5	7.655	38	449.3	39.7943	39	409.8	1.54022

^{1}H NMR

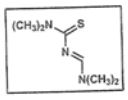


Current Data Parameters
NAME ex227
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140925
Time 21.39
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

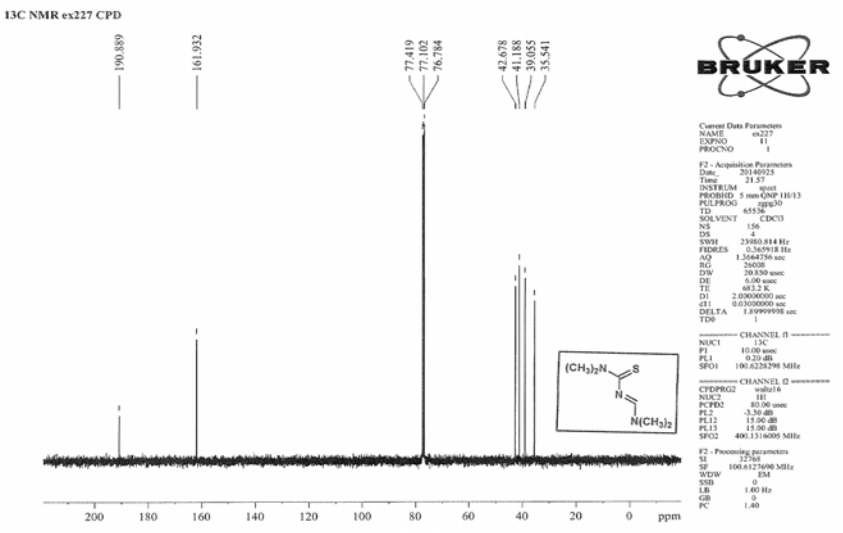
========== CHANNEL f1 ==========
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299648 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

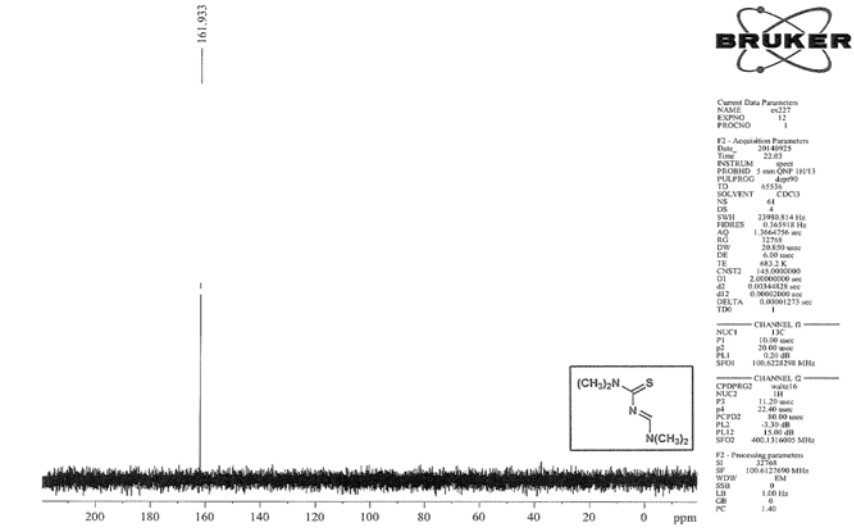


^{13}C NMR

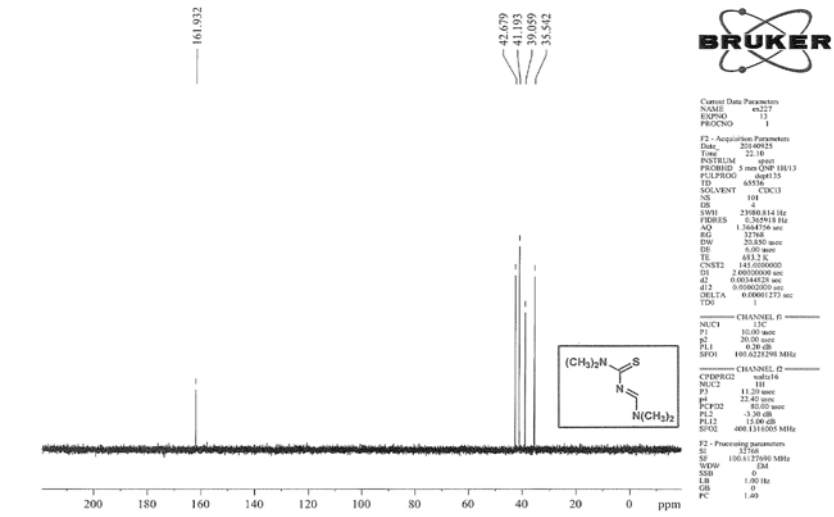
13C NMR ex227 CPD



13C NMR ex227 dept90

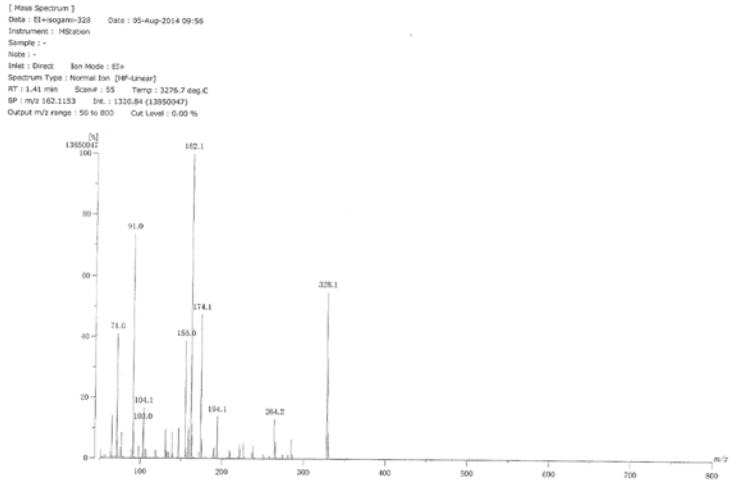


13C NMR ex227 dept135



6 ($R^1 = C_6H_5$, $R^2 = NMe_2$):[8]

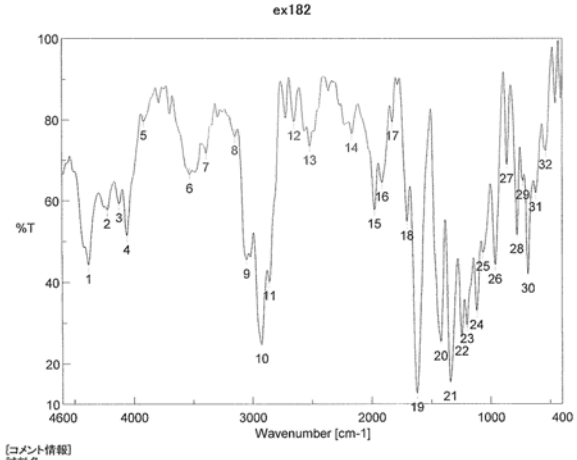
Mass spectrum



[Mass Spectrum]
Data : EI+isogami-328 Date : 05-Aug-2014 09:56
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.41 min Scan# : 55 Temp : 3276.7 deg.C
BP : m/z 162.1153 Int. : 1320.84 (13850047)
Output m/z range : 100.0000 to 800.0000 Cut Level : 2.00 %

m/z	Int.	Norm.	
102.9749	150.48	11.39	1577871
104.0558	220.89	16.72	2316175
104.9816	43.17	3.27	452719
107.0682	41.25	3.12	432527
118.0632	36.94	2.80	387343
119.0318	34.03	2.58	356815
131.0383	129.90	9.83	1362111
132.5402	32.25	2.44	338159
135.0285	26.97	2.04	282799
138.9913	116.11	8.79	1217471
147.0935	131.15	9.93	1375167
155.0129	512.15	38.77	5370303
156.0221	46.55	3.52	488095
157.0120	27.98	2.12	293439
159.0967	137.91	10.44	1446079
161.1038	81.00	6.13	849343
162.1153	1320.84	100.00	13850047
163.1147	152.75	11.56	1601727
174.0922	627.48	47.51	6579647
175.1031	87.27	6.61	915135
190.0829	47.35	3.58	496511
194.0960	183.22	13.87	1921215
195.1023	30.48	2.31	319615
209.1171	37.12	2.81	389263
210.1143	27.46	2.08	287919
221.1116	61.86	4.68	648623
222.0750	42.15	3.19	441935
226.0537	68.13	5.16	714431
237.1053	29.17	2.21	305903
238.0741	55.99	4.24	587055
264.1867	173.07	13.10	1814719
265.1836	75.70	5.73	793791
285.0621	84.40	6.39	884991
328.1106	727.22	55.06	7625471
329.1212	439.26	33.26	4605951
330.1228	116.43	8.81	1220863
331.1269	28.76	2.18	301551

IR spectrum



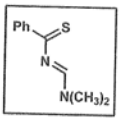
[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/06/23 15:41
更新日時 2014/06/23 15:42

データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018

光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (128)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

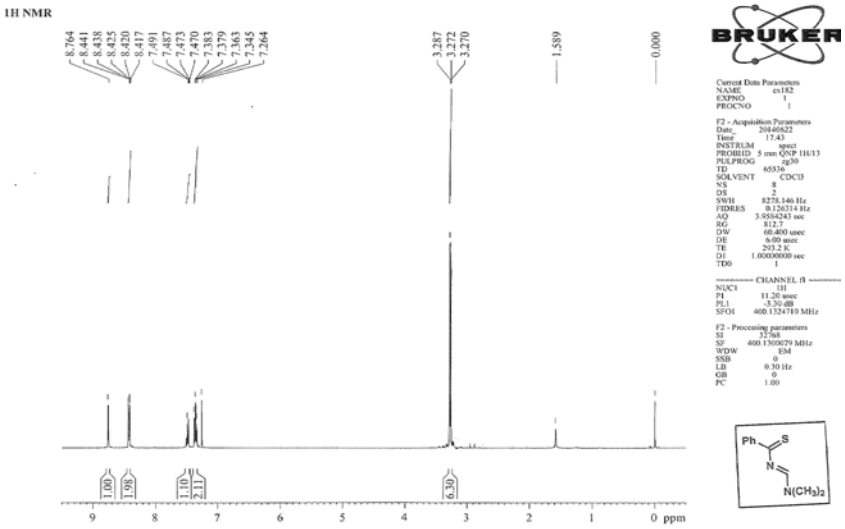


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	4381.5	44.2649	2	4222.4	57.7574	3	4124.0	59.2775
4	4059.4	51.4447	5	3914.8	79.6427	6	3532.0	66.5108
7	3393.1	71.7374	8	3151.1	75.8895	9	3052.8	45.5259
10	2926.5	24.7172	11	2859.9	40.1574	12	2654.5	79.5047
13	2522.4	73.4669	14	2169.5	76.508	15	1978.6	57.7747
16	1915.0	64.4299	17	1829.2	79.4747	18	1704.8	54.9021
19	1621.8	12.7287	20	1421.3	25.3485	21	1340.3	15.4468
22	1243.9	26.5656	23	1201.4	29.5798	24	1118.5	33.0377
25	1066.4	47.3362	26	963.3	44.2224	27	864.9	68.9105
28	780.1	51.6354	29	730.9	64.9329	30	687.5	41.9796
31	622.9	61.9204	32	539.0	72.365			

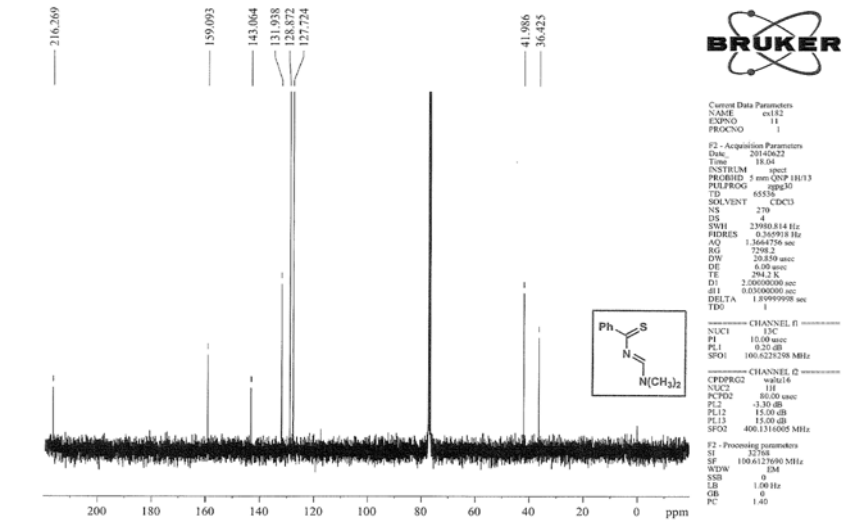
^{1}H NMR

1H NMR

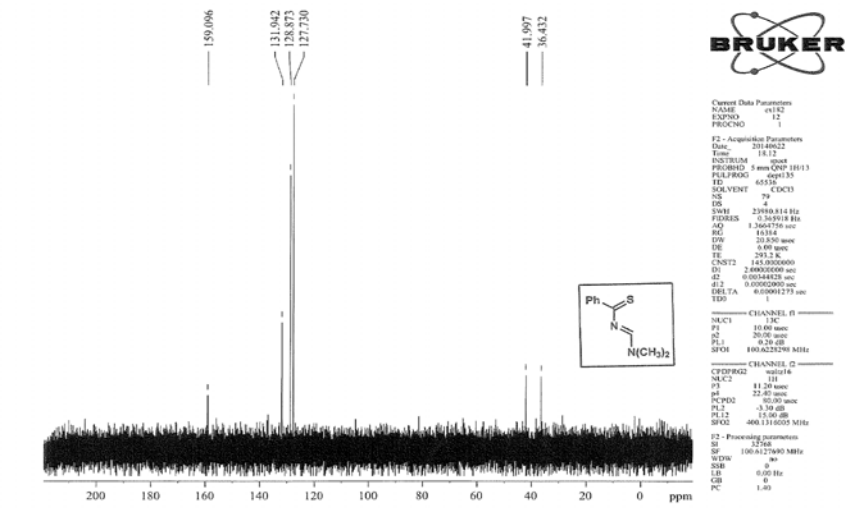


^{13}C NMR

13C NMR



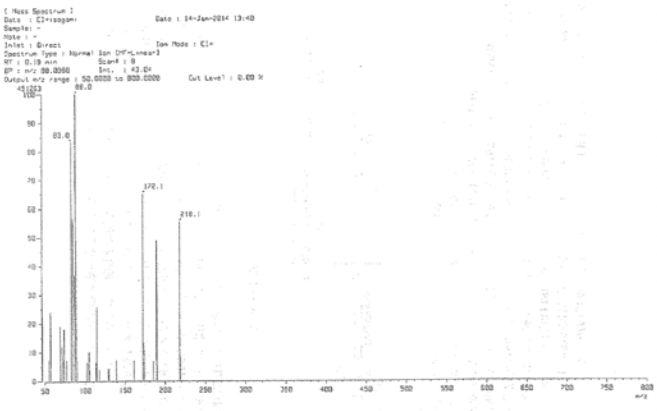
13C NMR dept 135



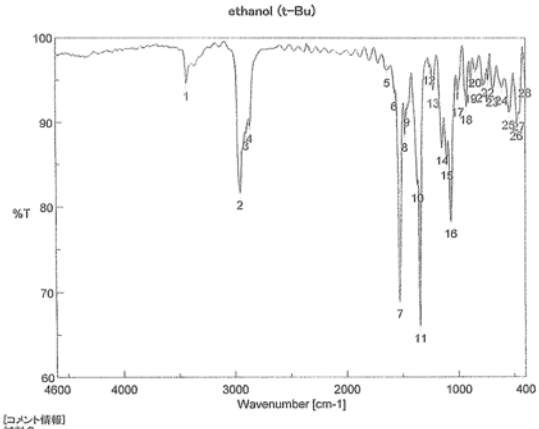
(2) 1,3-Thiaza-1,3-butadiene-Ethanol Adduct (7):

7a (R^1 = NMe_2, R^2 = *t*- C_4H_9):

Mass spectrum



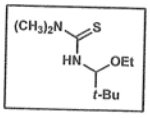
IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社　岩手大学　工学部

[データ情報]
作成日時　2013/12/20 21:16
データタイプ　等間隔データ
横軸　Wavenumber [cm-1]
縦軸　%T
スタート　399.193 cm-1
エンド　4600.36 cm-1
データ間隔　0.964233 cm-1
データ数　4358

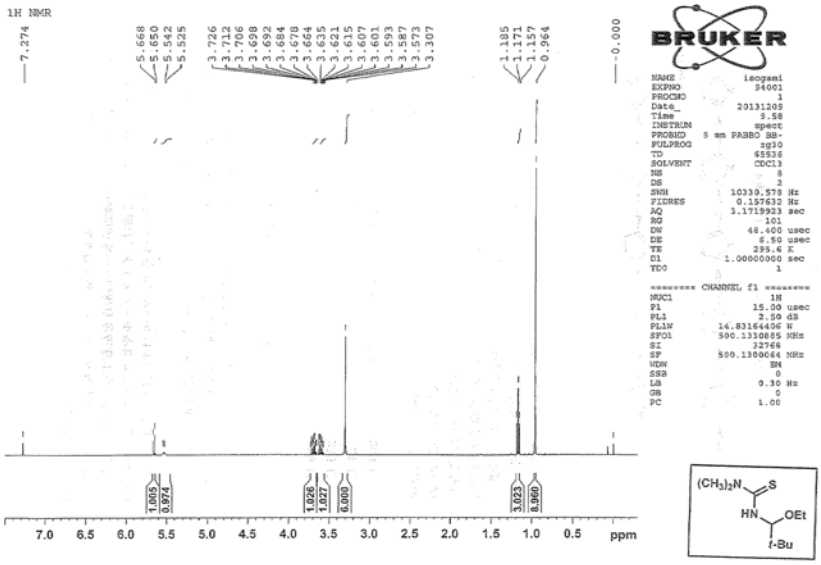
[測定情報]
機種名　FT/IR-4200typeA
シリアル番号　B061661018
光源　標準光源
検出器　TGS
積算回数　16
分解　4 cm-1
ゼロフィリング　On
アポダイゼーション　Cosine
ゲイン　Auto (8)
アパーチャー　Auto (7.1 mm)
スキャンスピード　Auto (2 mm/sec)
フィルタ　Auto (30000 Hz)



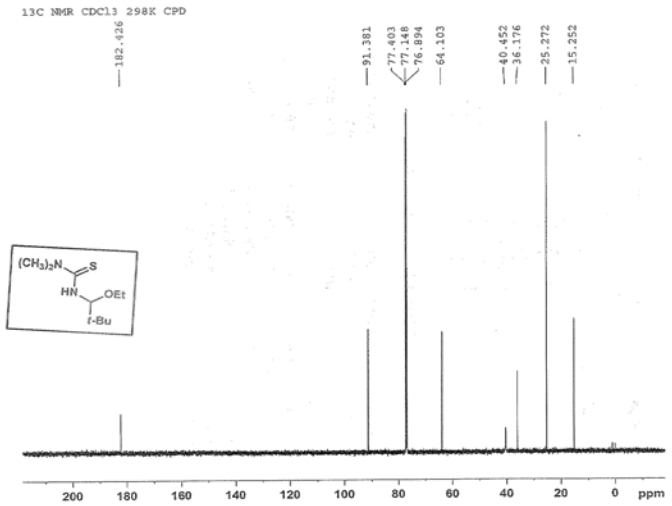
[ピーク検出結果]

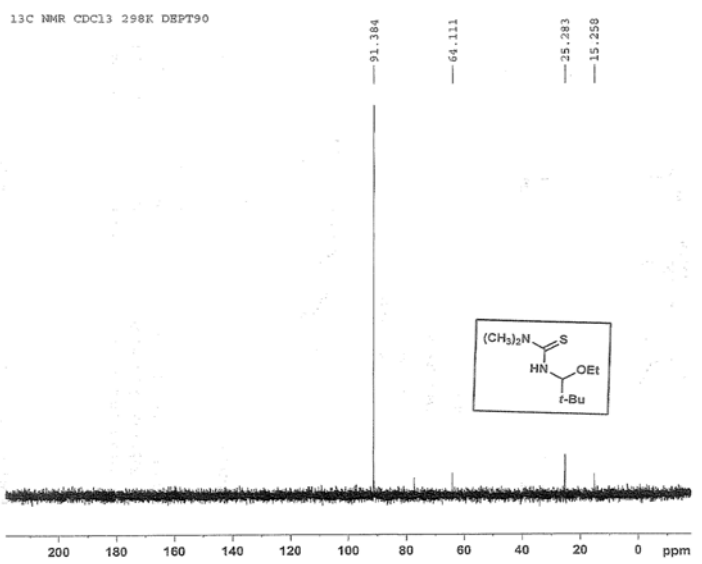
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3437.5	94.6486	2	2960.2	81.7482	3	2906.2	88.7821
4	2871.5	89.813	5	1641.1	96.2432	6	1573.6	93.4601
7	1526.4	69.0096	8	1480.1	88.5979	9	1461.8	91.5636
10	1369.2	82.584	11	1344.1	66.1059	12	1261.2	96.5499
13	1226.5	93.8181	14	1147.4	86.9915	15	1105.0	85.238
16	1069.3	78.3864	17	1006.7	92.7397	18	929.5	91.856
19	889.0	94.3607	20	847.6	96.216	21	779.1	94.4243
22	735.7	95.0377	23	692.3	93.9435	24	611.3	94.1275
25	547.7	91.2457	26	477.3	89.9643	27	454.2	91.0418
28	402.1	95.0229						

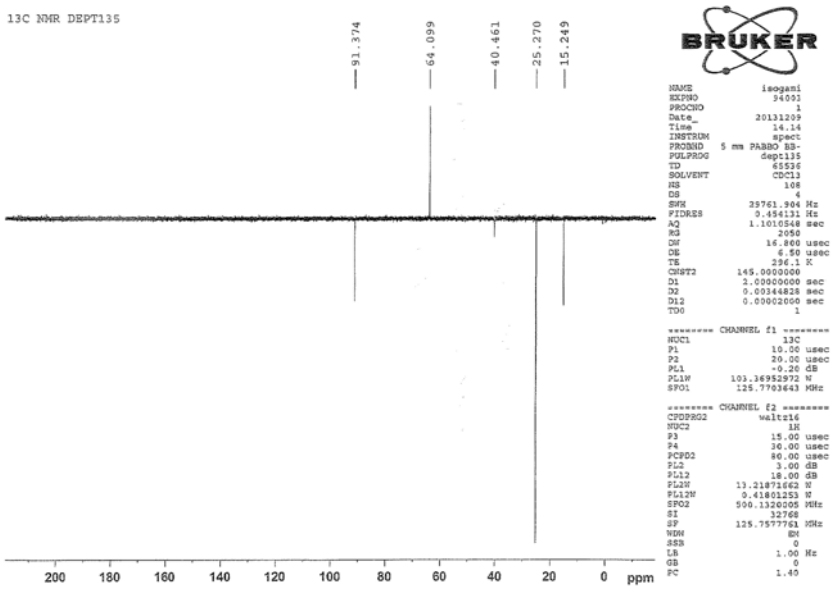
^{1}H NMR


1H NMR
7.274
5.668
5.650
5.542
5.525
3.726
3.712
3.706
3.698
3.692
3.684
3.678
3.664
3.635
3.621
3.615
3.607
3.601
3.593
3.587
3.573
3.307
1.185
1.171
1.157
0.964
0.000
1.005
0.974
1.826
1.027
6.000
3.023
8.860
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
BRUKER
NAME isogami
EXPNO 94001
PROCNO 1
Date_ 20131209
Time_ 9.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 101
DW 48.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 2.50 dB
PL1W 14.83164496 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
(CH3)2N
S
HN
OEt
t-Bu

^{13}C NMR


13C NMR CDCl3 298K CPD
182.426
91.381
77.403
77.148
76.894
64.103
40.452
36.176
25.272
15.252
200 180 160 140 120 100 80 60 40 20 0 ppm
(CH3)2N
S
HN
OEt
t-Bu
BRUKER
NAME isogami
EXPNO 94101
PROCNO 1
Date_ 20131209
Time_ 13.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 257
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.20 dB
PL1W 103.36952972 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 18.00 dB
PL13 18.00 dB
PL2W 13.21871662 W
PL12W 0.41801253 W
PL13W 0.41801253 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577756 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


13C NMR CDCl3 298K DEPT90
91.384
64.111
25.283
15.258
200 180 160 140 120 100 80 60 40 20 0 ppm
(CH3)2N
S
HN
OEt
t-Bu
BRUKER
NAME isogami
EXPNO 94102
PROCNO 1
Date_ 20131209
Time_ 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 141
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PL1 -0.20 dB
PL1W 103.36952972 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PL2 3.00 dB
PL12 18.00 dB
PL2W 13.21871662 W
PL12W 0.41801253 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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NAME                isogami
EXPNO                  34051
PROCNO                     1
Date_               20131209
Time                   14.14
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG              dept135
TD                     65536
SOLVENT                CDCl3
NS                       108
DS                         4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                      2050
DW                   16.800 usec
DE                    6.50 usec
TE                   296.1 K
CNST2              145.0000000
D1                   3.00000000 sec
D2                   0.00344828 sec
D12                  0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.06 usec
P2                     20.00 usec
PL1                    -0.20 dB
PL1W            103.16952972 W
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
P3                     15.00 usec
P4                     30.00 usec
PCPD2                  80.00 usec
PL2                     3.00 dB
PL12                   18.00 dB
PL2W            13.21871662 W
PL12W            0.41801253 W
SFO2             500.1320005 MHz
SI                       32768
SF               125.7577761 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40
```

7b ($R^1 = NMe_2$, $R^2 = C_6H_5$):

MS spectrum

```
[ Mass Spectrum ]
Data   : EI+isogami                    Date : 14-Jan-2014 13:40
Sample: -
Note : -
Inlet : Direct                         Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.19 min          Scan# : 8
BP : m/z 88.0360       Int.  : 43.04
Output m/z range : 50.0000 to 800.0000       Cut Level : 0.00 %

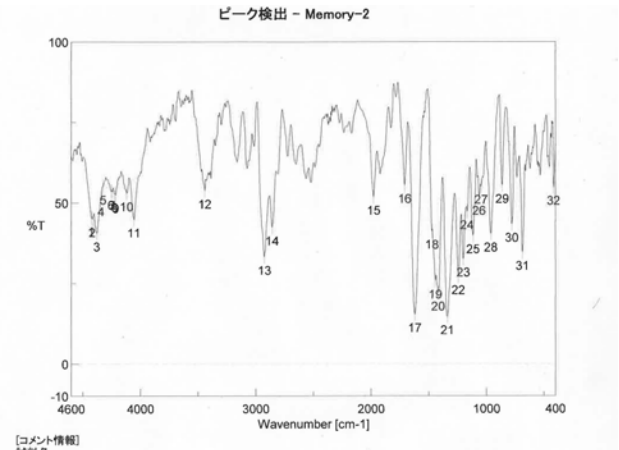
    m/z         Int.     Norm.
  55.0119      3.23      7.50
  56.0263      2.01      4.67
  57.0341     10.31     23.95
  69.0647      8.25     19.16
  70.0531      4.33     10.07
  71.0585      5.17     12.01
  72.0346      4.09      9.51
  72.9910      3.19      7.41
  73.9896      7.79     18.09
  77.0125      3.06      7.12

  82.9767     35.85     83.29
  84.9667     24.47     56.86
  86.0230      2.16      5.02
  87.0967     15.88     36.91
  88.0360     43.04    100.00
  89.0376     21.08     48.97
  90.0214      3.14      7.31
 102.0887      2.73      6.34
 104.0444      2.80      6.52
 105.0384      4.31     10.02

 106.0363      1.65      3.84
 114.0383      2.83      6.57
 115.0497     11.09     25.76
 117.9067      1.64      3.82
 129.0431      1.78      4.13
 130.0933      1.80      4.19
 139.1172      3.10      7.21
 161.0580      3.07      7.14
 172.1024     28.08     65.26
 173.1084      5.79     13.46

 174.1163      4.55     10.58
 185.1497      2.96      6.89
 189.0978     21.18     49.21
 190.1314      2.33      5.42
 218.1466     24.00     55.76
 219.1480      3.46      8.04
```

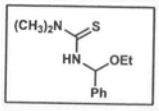
IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2015/03/16 10:05
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

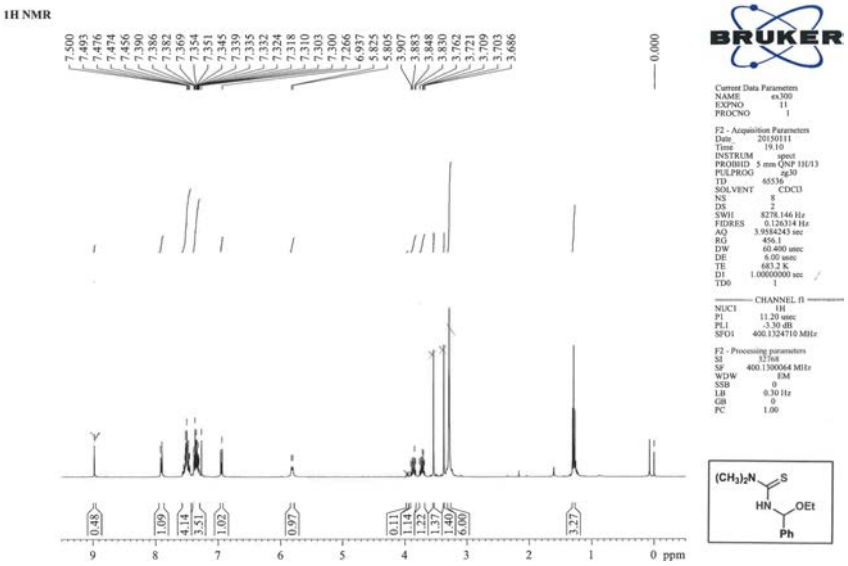
[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (128)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)



[ピーク検出結果]

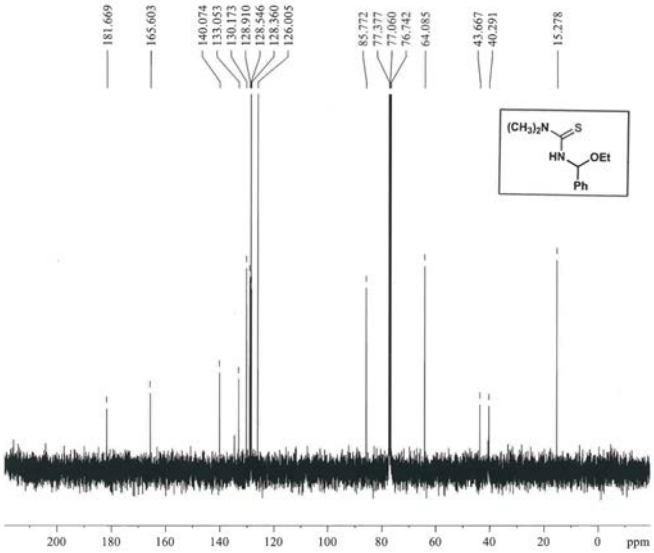
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	4424.9	45.2712	2	4416.2	44.9951	3	4378.6	40.5401
4	4342.9	51.4874	5	4325.6	55.0517	6	4255.2	53.4879
7	4246.5	53.4175	8	4225.3	52.7778	9	4216.6	52.479
10	4122.1	53.0061	11	4056.5	44.8153	12	3442.3	53.7951
13	2925.5	33.145	14	2859.0	42.3376	15	1977.6	51.8236
16	1707.7	55.4578	17	1621.8	15.3816	18	1471.4	41.2601
19	1444.4	25.7493	20	1418.4	22.0263	21	1338.4	14.843
22	1244.8	27.0958	23	1201.4	32.6146	24	1168.7	47.2662
25	1115.6	39.7985	26	1063.6	51.7252	27	1046.2	55.1572
28	961.3	40.3477	29	863.0	55.3703	30	779.1	43.2992
31	688.5	34.5645	32	416.6	54.8255			

^{1}H NMR



^{13}C NMR

13C NMR



Current Data Parameters
NAME ex300
EXPNO 12
PROCNO 1

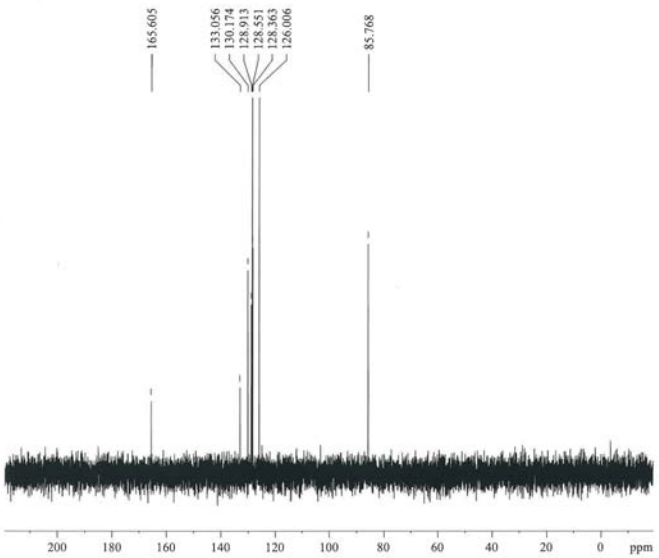
F2 - Acquisition Parameters
Date_ 20150111
Time 19:20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 85
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept90



Current Data Parameters
NAME ex300
EXPNO 13
PROCNO 1

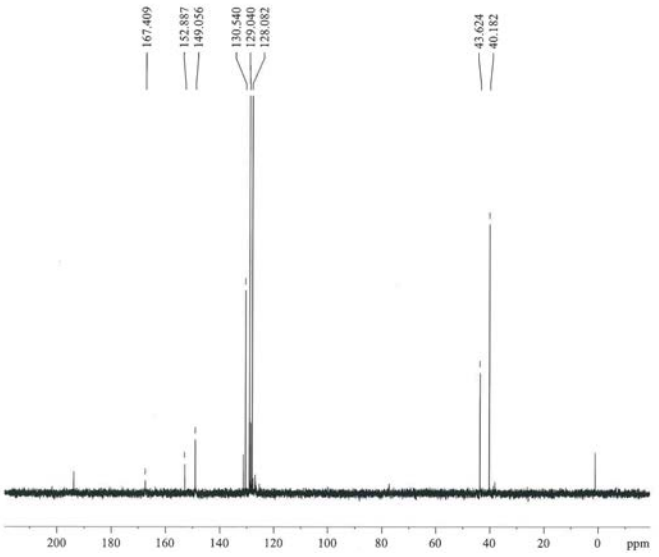
F2 - Acquisition Parameters
Date_ 20150111
Time 19:24
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 24
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept135



Current Data Parameters
NAME ex295
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141219
Time 0.59
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 178
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 26008
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

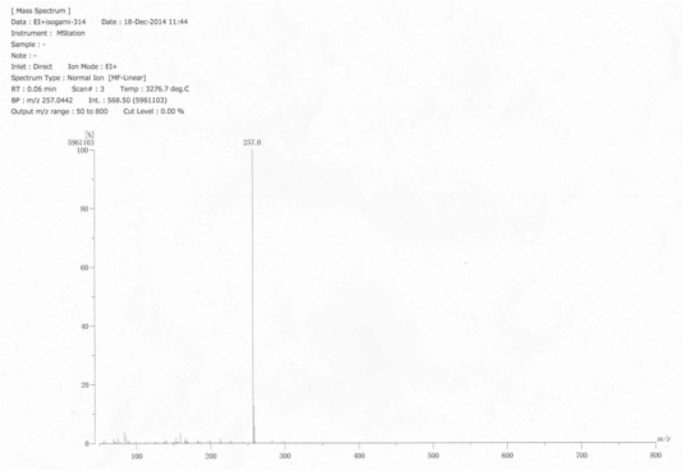
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

(3) 1,3-Thiaza-1,3-butadiene-[4+2]-Cycloadducts (9~12):

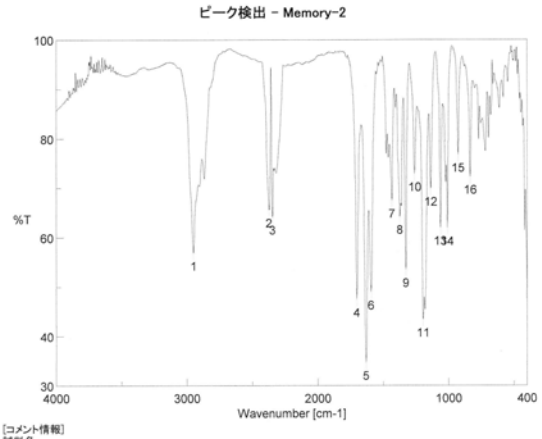
9a (R^1 = NMe_2, R^2 = *t*-C_4H_9, R^3 =H, R^4 = CO_2Me):

Mass spectrum



m/z	Int.	Norm.	
150.9909	1.90	0.33	19887
151.9800	2.54	0.45	26655
153.0027	10.87	1.91	114015
153.9771	2.89	0.51	30319
154.9908	2.90	0.51	30431
155.9797	1.90	0.33	19871
158.9944	18.53	3.26	194335
164.9991	5.90	1.04	61823
166.0019	8.87	1.56	93039
167.0229	3.54	0.62	37119
168.0163	4.02	0.71	42127
169.0048	2.17	0.38	22719
181.0208	1.69	0.30	17759
181.9713	6.94	1.22	72815
183.0020	3.50	0.62	36671
185.0339	2.44	0.43	25535
187.0191	2.44	0.43	25631
197.0494	3.80	0.67	39839
199.0703	6.01	1.06	63023
212.0478	1.81	0.32	18943
213.0510	8.63	1.52	90495
214.0213	1.84	0.32	19263
226.0252	6.26	1.10	65631
227.0253	1.75	0.31	18383
229.0595	2.42	0.43	25375
243.0136	2.46	0.43	25823
257.0442	568.50	100.00	5961103
258.0501	72.55	12.76	760719
259.0479	34.31	6.03	359743
260.0666	3.73	0.66	39119
283.0874	6.98	1.23	73151
295.0894	1.99	0.35	20911
299.0811	4.47	0.79	46863
326.0494	1.93	0.34	20239

IR spectrum

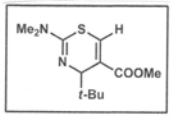


[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]		[測定情報]	
作成日時	2014/12/03 11:12	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	399.193 cm-1	積算回数	16
エンド	4000.6 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	3736	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

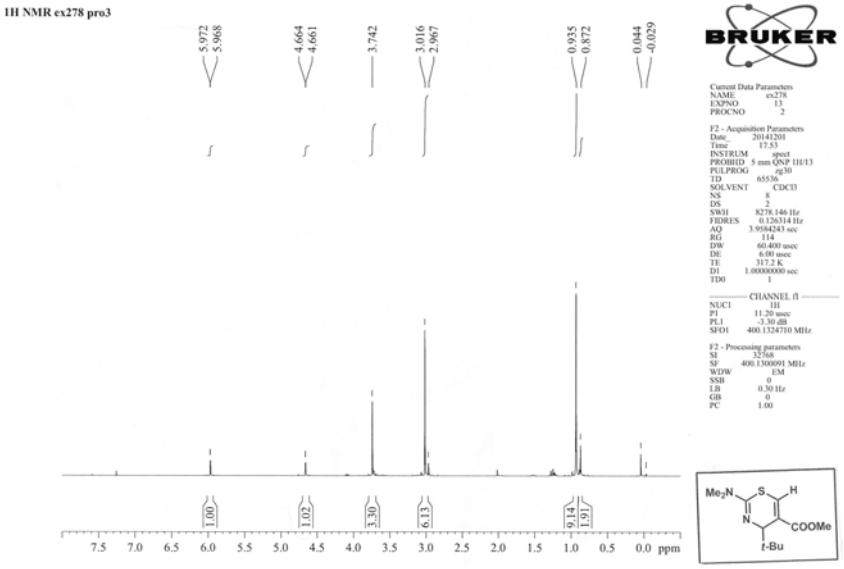
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2951.5	56.9126	2	2373.9	65.6126	3	2348.9	64.188
4	1702.8	47.4608	5	1632.5	34.716	6	1593.9	48.9584
7	1435.7	67.5465	8	1374.0	64.248	9	1327.8	53.4902
10	1260.3	72.8798	11	1195.7	43.4251	12	1137.8	69.9087
13	1063.6	61.9977	14	1010.5	61.9551	15	928.6	76.7571
16	835.0	72.305						



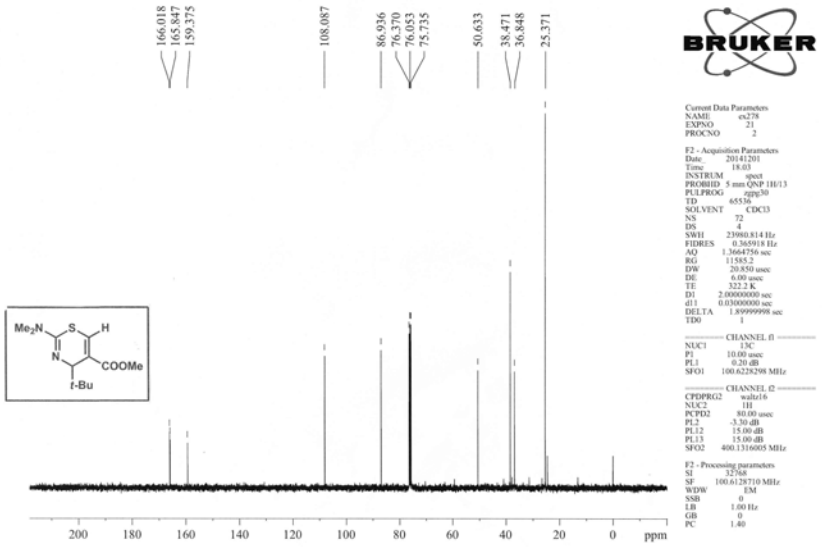
^{1}H NMR

1H NMR ex278 pro3

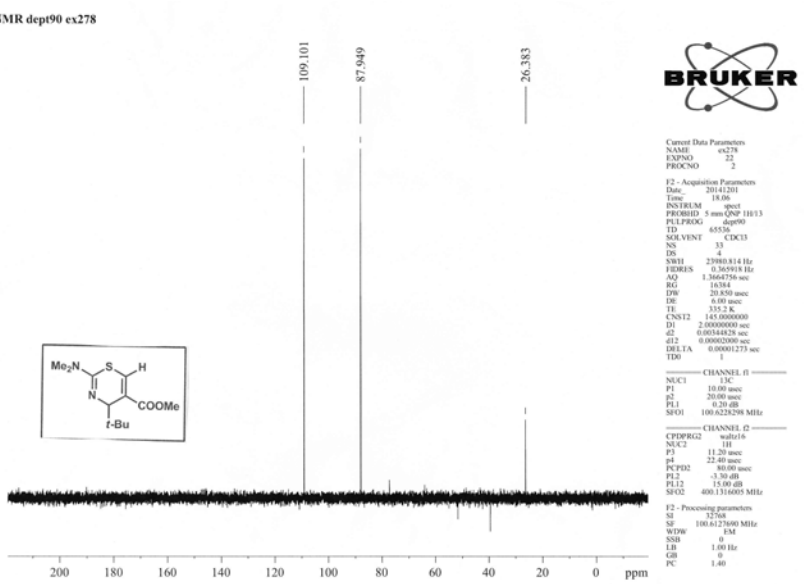


^{13}C NMR

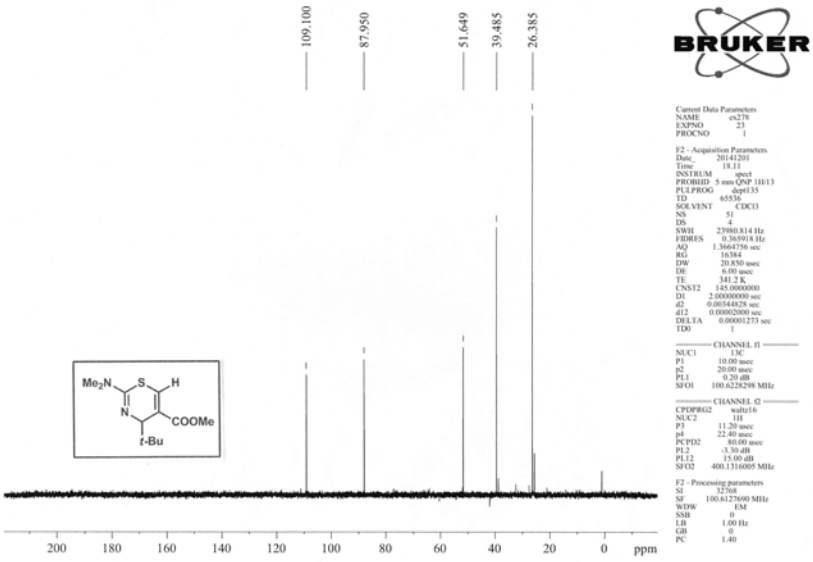
13C NMR CPD ex278



13C NMR dept90 ex278

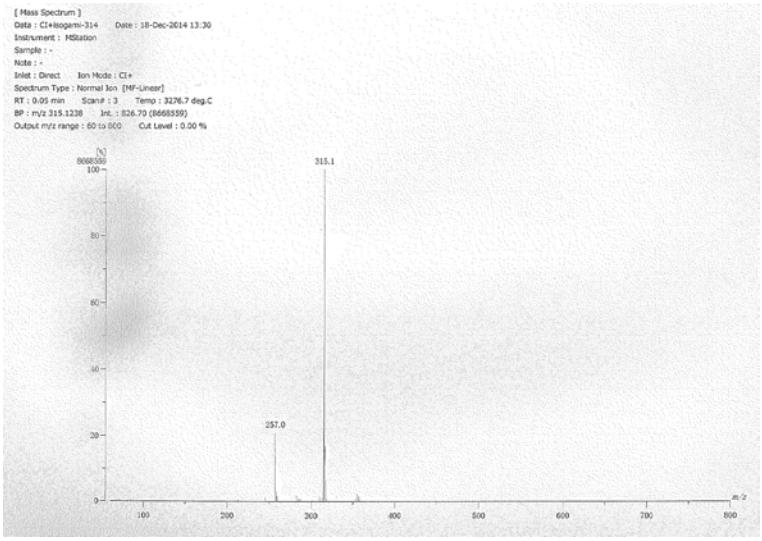


13C NMR dept135 ex278



10a ($R^1 = NMe_2$, $R^2 = t\text{-}C_4H_9$, $R^3 = R^4 = CO_2Me$):

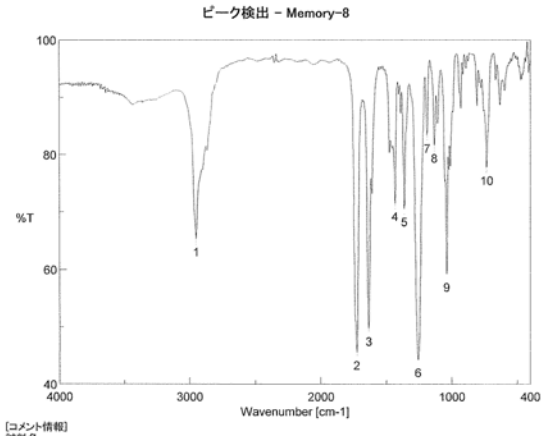
Mass spectrum



[Mass Spectrum]
Data : CI+isogami-314 Date : 18-Dec-2014 13:30
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.05 min Scan# : 3 Temp : 3276.7 deg.C
BP : m/z 315.1238 Int. : 826.70 (8668559)
Output m/z range : 60.0000 to 800.0000 Cut Level : 0.00 %

m/z	Int.	Norm.	
67.0593	2.52	0.30	26399
69.0658	4.33	0.52	45375
71.0712	5.41	0.65	56687
79.0422	1.85	0.22	19375
81.0543	1.96	0.24	20543
85.0903	2.47	0.30	25871
158.9888	2.08	0.25	21791
213.0479	4.77	0.58	50015
245.0625	10.18	1.23	106783
255.0950	1.85	0.22	19439
257.0267	170.50	20.62	1787791
258.0326	25.61	3.10	268495
259.0409	13.47	1.63	141215
283.0668	15.10	1.83	158351
284.0791	2.63	0.32	27599
285.0732	5.87	0.71	61599
287.1064	7.80	0.94	81743
299.0687	1.92	0.23	20143
301.1115	4.09	0.49	42863
310.1116	11.18	1.35	117263
311.0966	1.85	0.22	19391
313.1122	9.55	1.15	100111
314.1225	1.93	0.23	20239
315.1238	826.70	100.00	8668559
316.1254	137.88	16.68	1445775
317.1191	54.34	6.57	569791
318.1244	7.57	0.92	79423
353.1308	7.63	0.92	79983
355.1420	18.71	2.26	196207
356.1596	3.88	0.47	40735
357.1557	13.19	1.60	138303
358.1749	2.83	0.34	29647

IR spectrum



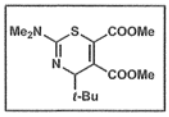
[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/12/03 11:20
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4000.6 cm-1
データ間隔 0.964233 cm-1
データ数 3736

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

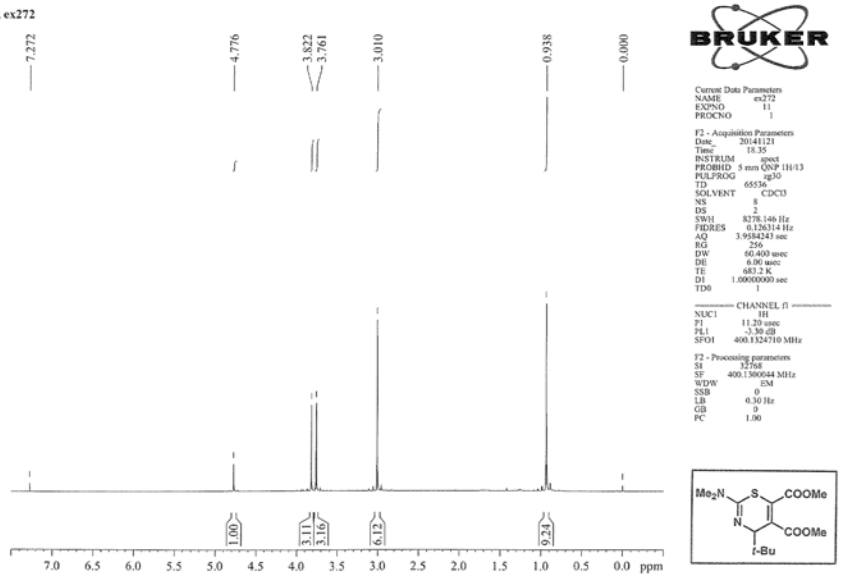
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2952.5	65.3026	2	1726.0	45.5624	3	1635.3	49.751
4	1434.8	71.4657	5	1363.4	70.5298	6	1257.4	44.2838
7	1189.9	83.3644	8	1133.9	81.6217	9	1039.4	59.2024
10	734.8	77.7289						



^{1}H NMR

1H NMR ex272



BRUKER

Current Data Parameters
NAME ex272
EXPNO 11
PROCNO 1

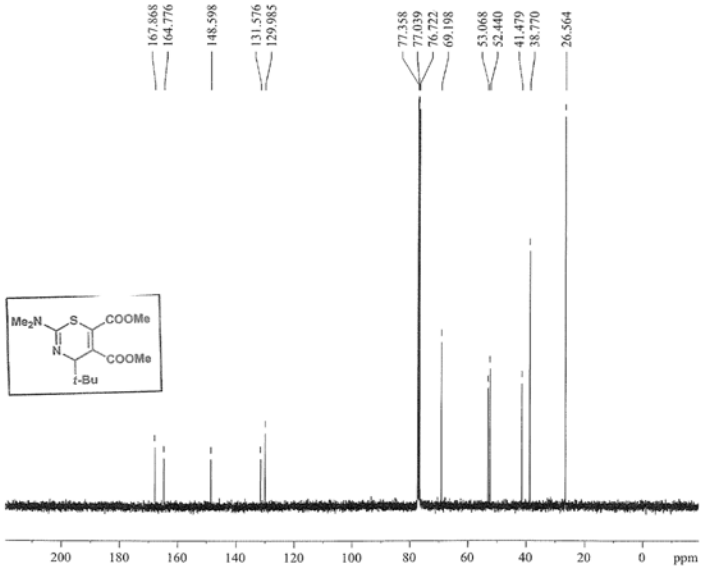
F2 - Acquisition Parameters
Date_ 20141121
Time 18.35
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300644 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR

13C NMR ex272



BRUKER

Current Data Parameters
NAME ex272
EXPNO 12
PROCNO 1

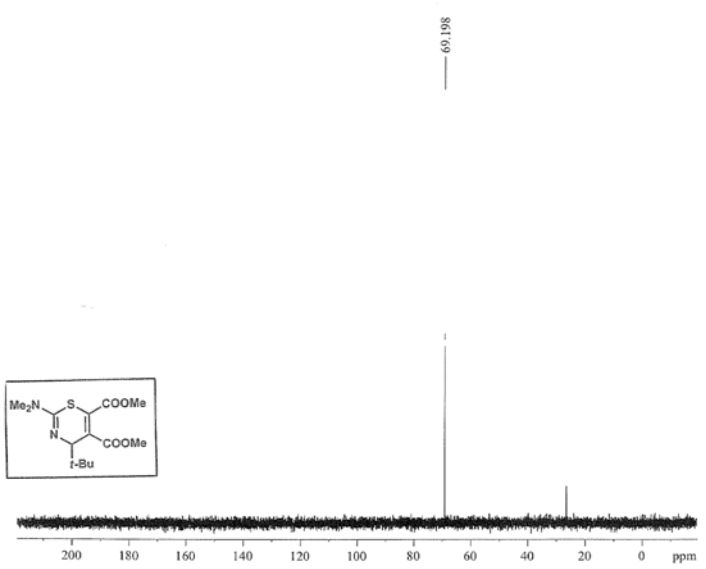
F2 - Acquisition Parameters
Date_ 20141121
Time 18.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 226
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.99999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept90 ex272



BRUKER

Current Data Parameters
NAME ex272
EXPNO 13
PROCNO 1

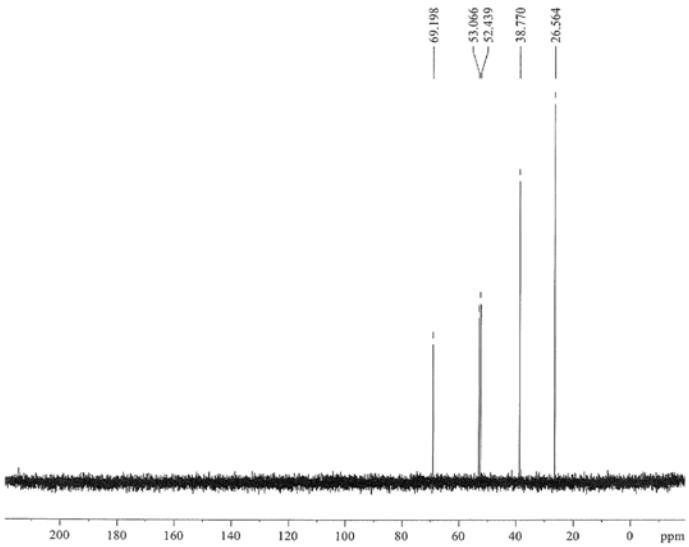
F2 - Acquisition Parameters
Date_ 20141121
Time 15.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 46
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 23170.5
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.09 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept135 ex272



BRUKER

Current Data Parameters
NAME ex272
EXPNO 14
PROCNO 1

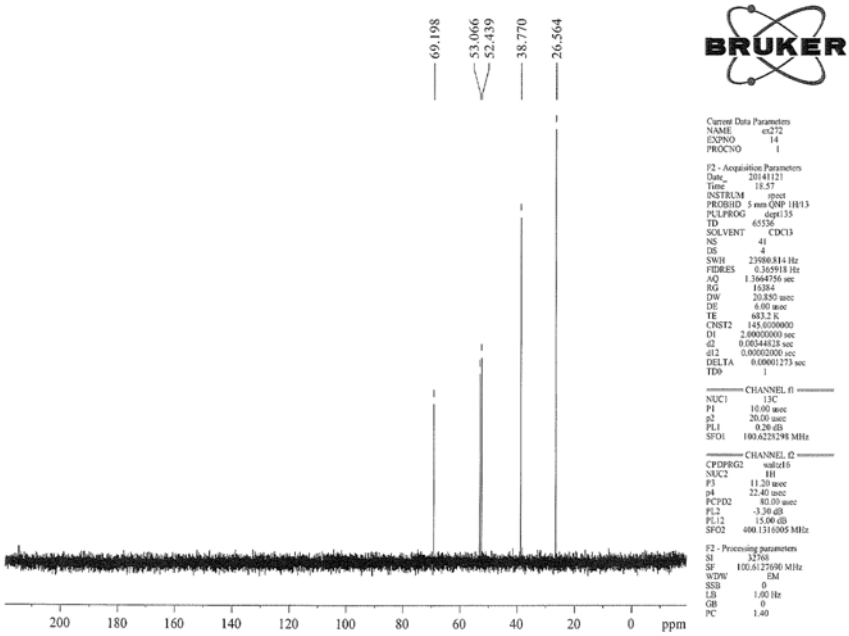
F2 - Acquisition Parameters
Date_ 20141121
Time 18.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 41
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.60 dB
SFO2 400.1316005 MHz

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

13C NMR dept135 ex272



Current Data Parameters
NAME ex272
EXPNO 14
PROCNO 1

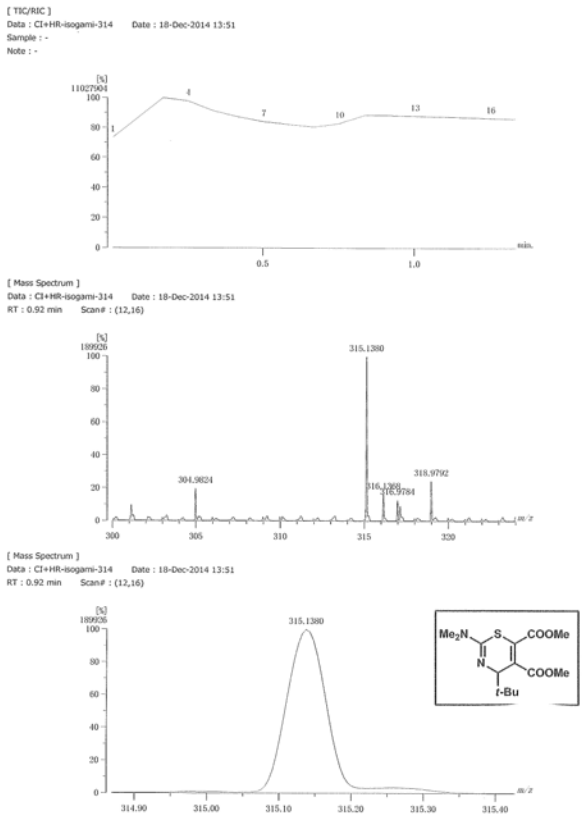
F2 - Acquisition Parameters
Date_ 20141121
Time 18.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 41
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.36 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

HRMS



Data : CI+HR-isogami-314 Date : 18-Dec-2014 13:51
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
RT : 0.92 min Scan# : (12,16)
Elements : C 14/0, H 23/0, N 2/0, O 4/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 5.5

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	315.1380	100.00	+0.5 / +0.1	5.5	C14 H23 N2 O4 S

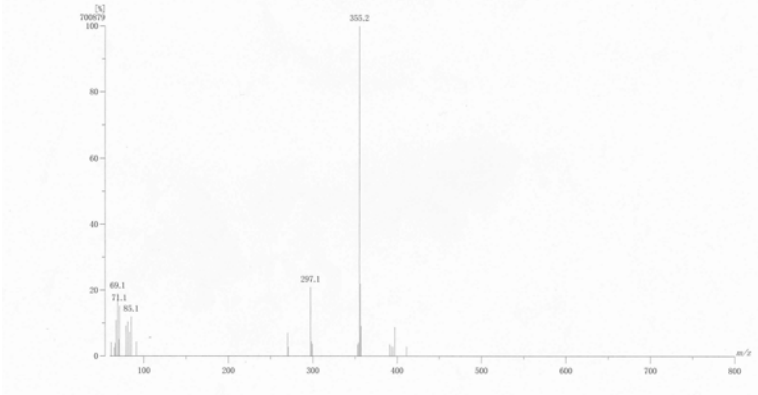
[Theoretical Ion Distribution]
Molecular Formula : C14 H23 N2 O4 S
(m/z 315.1379, MW 315.4136, U.S. 5.5)
Base Peak : 315.1379, Averaged MW : 315.4095(a), 315.4107(w)

m/z	INT.
315.1379	100.0000**********
316.1408	17.2476**********
317.1368	6.6289****
318.1387	0.9377*
319.1391	0.1287
320.1408	0.0130
321.1422	0.0011

11a ($R^1 = NMe_2$, $R^2 = R^3 = t\text{-}C_4H_9$, $R^4 = COCO_2Me$):

Mass spectrum

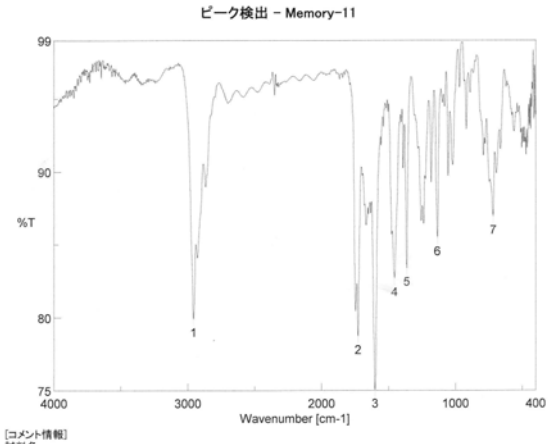
[Mass Spectrum]
Data : CI+isogami-354 Date : 18-Dec-2014 14:26
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.10 min Scan# : 5 Temp : 3276.7 deg.C
BP : m/z 355.1745 Int. : 66.84 (700879)
Output m/z range : 60 to 800 Cut Level : 0.00 %



[Mass Spectrum]
Data : CI+isogami-354 Date : 18-Dec-2014 14:26
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.10 min Scan# : 5 Temp : 3276.7 deg.C
BP : m/z 355.1745 Int. : 66.84 (700879)
Output m/z range : 60.0000 to 800.0000 Cut Level : 0.00 %

m/z	Int.	Norm.	
61.1662	2.77	4.14	29007
65.0487	1.75	2.61	18303
66.0552	2.63	3.93	27551
67.0593	7.29	10.90	76415
69.0658	12.70	19.00	133199
70.0625	3.40	5.09	35647
71.0712	10.16	15.20	106543
79.0422	6.15	9.20	64463
81.0488	6.97	10.42	73055
83.0686	4.85	7.26	50895
85.0847	7.98	11.94	83695
91.0380	2.91	4.35	30463
270.0856	4.70	7.03	49263
271.0477	1.86	2.78	19471
297.0922	13.99	20.93	146671
298.1198	3.02	4.52	31711
299.1187	2.47	3.70	25919
353.1632	2.38	3.56	24943
354.1569	2.78	4.17	29199
355.1745	66.84	100.00	700879
356.1812	14.68	21.96	153919
357.1882	6.10	9.13	63967
391.2308	2.36	3.53	24767
393.1702	1.95	2.92	20463
395.2050	1.88	2.81	19711
397.2338	5.85	8.75	61359
411.1632	1.89	2.83	19855

IR spectrum

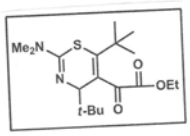


[コメント情報]
試料名
コメント
測定者
所属
会社　岩手大学 工学部

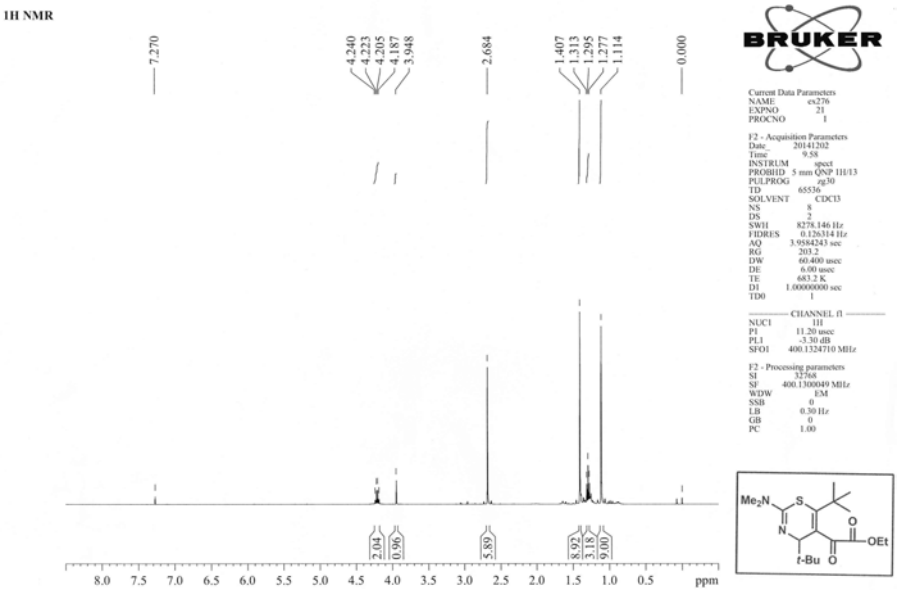
[データ情報]		[測定情報]	
作成日時	2014/12/03 11:27	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	399.193 cm-1	積算回数	16
エンド	4000.6 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	3736	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2957.3	79.9237	2	1727.9	78.7229	3	1600.6	75.0457
4	1457.0	82.6857	5	1365.4	83.3956	6	1134.9	85.4857
7	719.3	86.943						

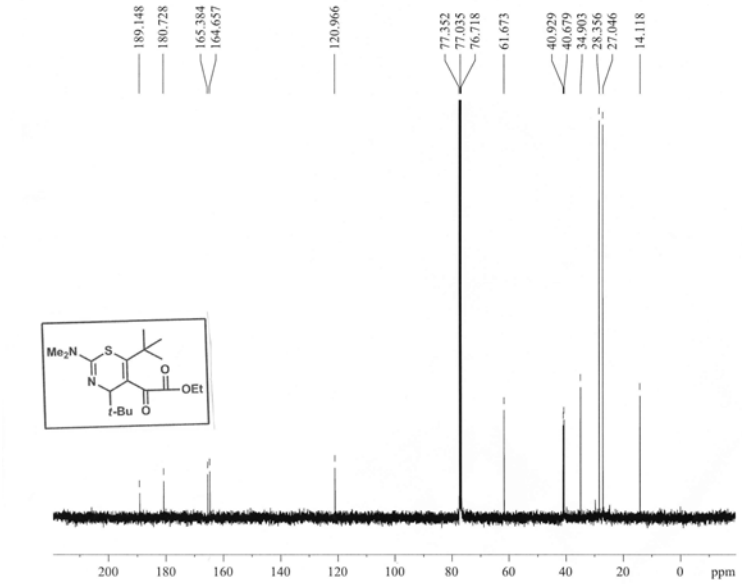


^{1}H NMR



13C NMR

13C NMR CPD



BRUKER

Current Data Parameters
NAME ex276
EXPNO 22
PROCNO 1

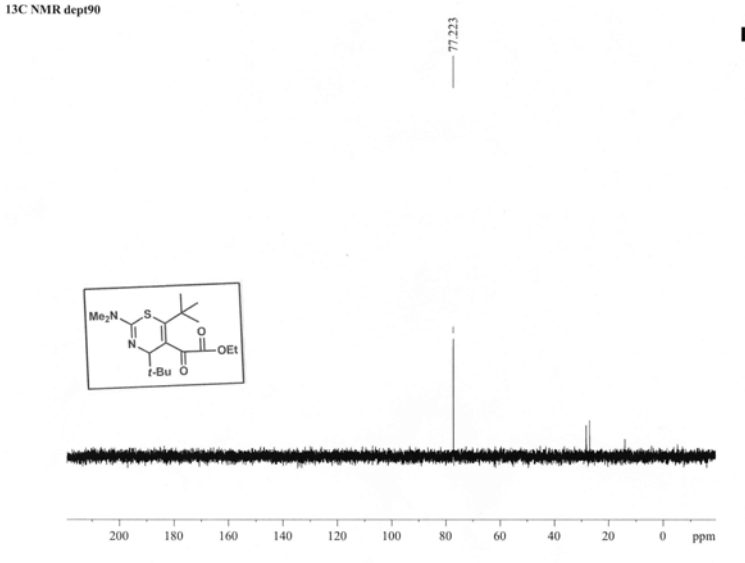
F2 - Acquisition Parameters
Date 20141202
Time 10.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 201
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept90



BRUKER

Current Data Parameters
NAME ex276
EXPNO 25
PROCNO 1

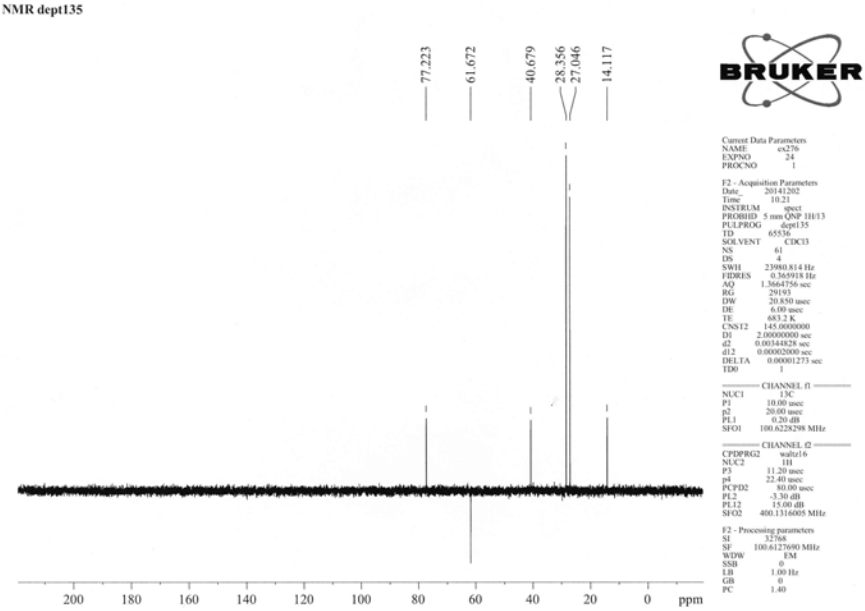
F2 - Acquisition Parameters
Date 20141202
Time 10.26
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 34
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

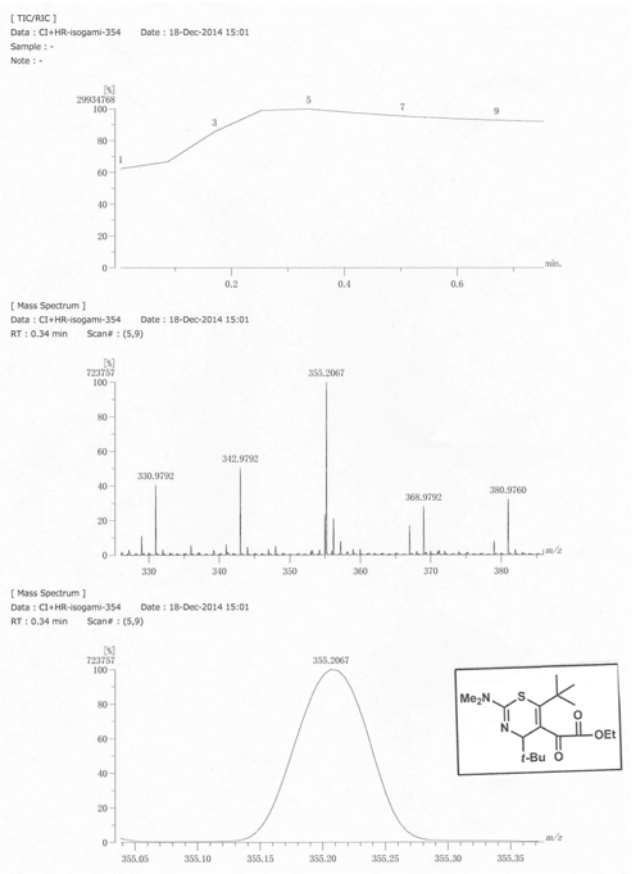
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept135



HRMS



Data : CI+HR-isogami-354 Date : 18-Dec-2014 15:01
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
RT : 0.34 min Scan# : (5,9)
Elements : C 18/0, H 31/0, N 2/0, O 3/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 5.5

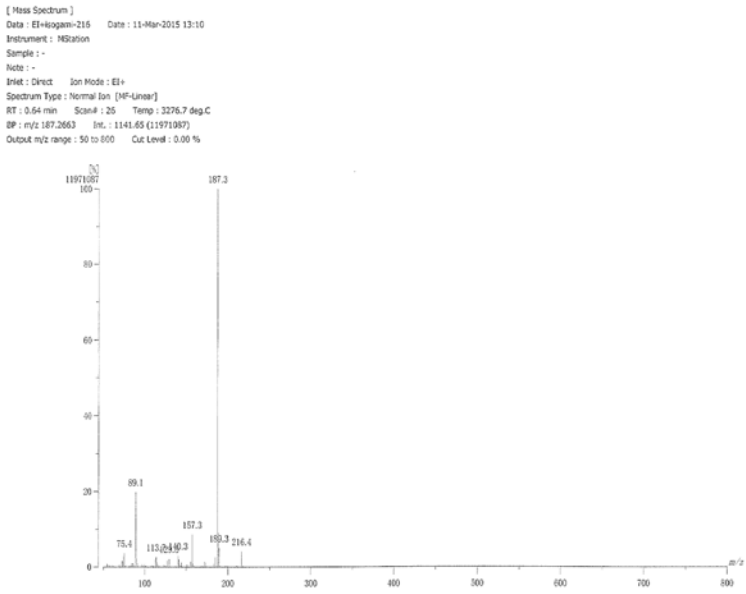
	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	355.2067	100.00	+3.3 / +1.2	5.5	C18 H31 N2 O3 S

[Theoretical Ion Distribution]
Molecular Formula : C18 H31 N2 O3 S
(m/z 355.2055, MW 355.5217, U.S. 5.5)
Base Peak : 355.2055, Averaged MW : 355.5170(a), 355.5181(w)

m/z	INT.
355.2055	100.0000**********
356.2085	21.6585**********
357.2052	7.2617****
358.2066	1.1998*
359.2075	0.1604
360.2089	0.0170
361.2105	0.0015
362.2122	0.0001

12:

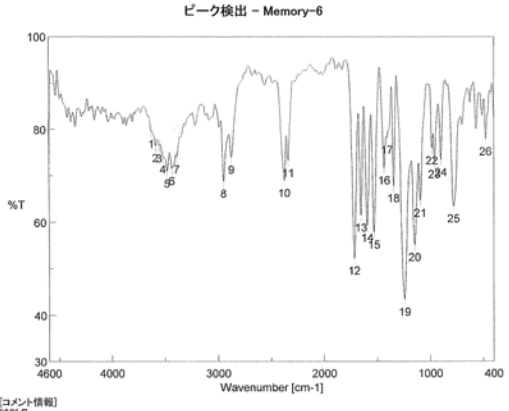
Mass spectrum



[Mass Spectrum]
Data : EI+isogami-216 Date : 11-Mar-2015 13:10
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.64 min Scan# : 26 Temp : 3276.7 deg.C
BP : m/z 187.2663 Int. : 1141.65 (11971087)
Output m/z range : 110.0000 to 800.0000 Cut Level : 0.00 %

m/z	Int.	Norm.	
110.6713	2.91	0.25	30495
112.6589	23.31	2.04	244383
113.6597	30.35	2.66	318207
114.6583	14.47	1.27	151711
115.6609	9.14	0.80	95791
116.6363	2.01	0.18	21087
117.6099	1.73	0.15	18111
123.5415	6.41	0.56	67231
124.5500	3.06	0.27	32079
125.5559	1.74	0.15	18287
127.4933	18.82	1.65	197343
129.4987	25.18	2.21	264031
130.4773	4.05	0.35	42479
137.4018	3.69	0.32	38687
140.3315	34.53	3.02	362079
141.3431	23.73	2.08	248847
142.3440	6.34	0.56	66479
143.3271	4.24	0.37	44511
144.3280	13.88	1.22	145519
151.3152	7.74	0.68	81151
155.2808	15.34	1.34	160815
156.2855	11.45	1.00	120063
157.2792	98.45	8.62	1032351
158.2689	10.55	0.92	110607
159.2761	5.35	0.47	56127
168.2507	2.54	0.22	26639
169.2514	3.80	0.33	39887
171.2228	3.05	0.27	31983
172.2314	16.54	1.45	173391
173.2359	14.05	1.23	147359
174.2279	1.96	0.17	20591
183.2418	10.32	0.90	108223
184.2383	2.18	0.19	22815
185.2448	30.75	2.69	322447
186.2538	3.69	0.32	38687
187.2663	1141.65	100.00	11971087
188.2729	104.76	9.18	1098511
189.2657	57.18	5.01	599615
190.2695	4.93	0.43	51711
196.2757	2.31	0.20	24239
197.2815	3.20	0.28	33599
199.3006	5.69	0.50	59615
200.3223	2.29	0.20	24031
210.3611	4.14	0.36	43359
211.3854	2.93	0.26	30703
216.4127	47.42	4.15	497231
217.4255	5.61	0.49	58863
218.4145	3.00	0.26	31407

IR spectrum



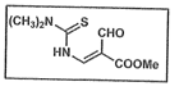
[コメント情報]
試料名
コメント
測定者
所属
会社　岩手大学　工学部

[データ情報]
作成日時　2014/10/31 13:33
データタイプ　等間隔データ
横軸　Wavenumber [cm-1]
縦軸　%T
スタート　399.193 cm-1
エンド　4600.36 cm-1
データ間隔　0.964233 cm-1
データ数　4358

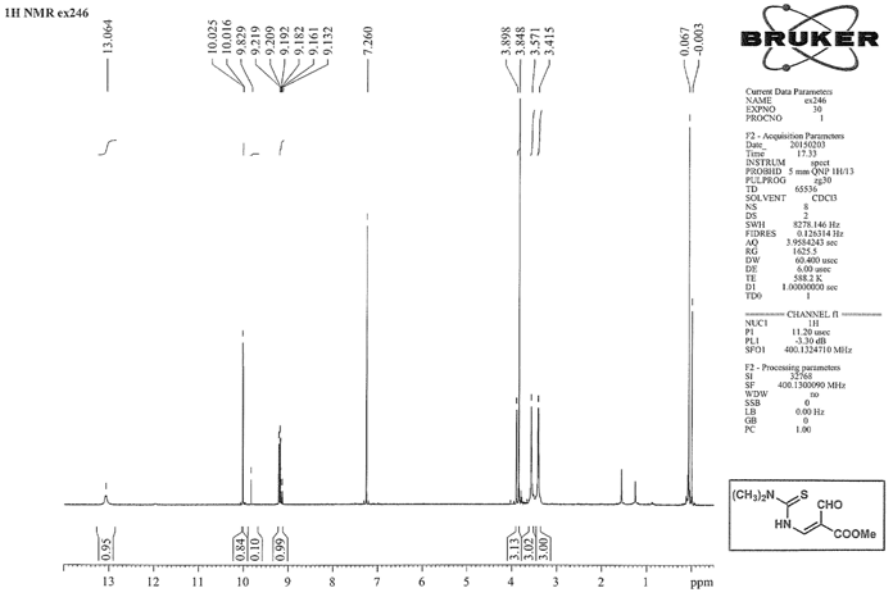
[測定情報]
機種名　FT/IR-4200typeA
シリアル番号　B061661018
光源　標準光源
検出器　TGS
積算回数　16
分解　4 cm-1
ゼロフィリング　On
アポダイゼーション　Cosine
ゲイン　Auto (128)
アパーチャー　Auto (7.1 mm)
スキャンスピード　Auto (2 mm/sec)
フィルタ　Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3636.1	79.5022	2	3596.6	76.4735	3	3561.9	76.409
4	3526.2	74.0133	5	3486.7	70.962	6	3440.4	71.5064
7	3396.0	74.0193	8	2949.6	68.7954	9	2877.3	73.9436
10	2377.8	68.9352	11	2340.2	73.2042	12	1716.3	52.2843
13	1653.7	61.4903	14	1594.8	59.3069	15	1532.2	57.8266
16	1435.7	71.676	17	1408.8	78.2575	18	1346.1	67.7895
19	1241.9	43.3935	20	1147.4	55.1518	21	1093.4	64.6627
22	984.5	75.9582	23	959.4	72.9685	24	899.6	73.4057
25	779.1	63.4479	26	475.4	77.9351			

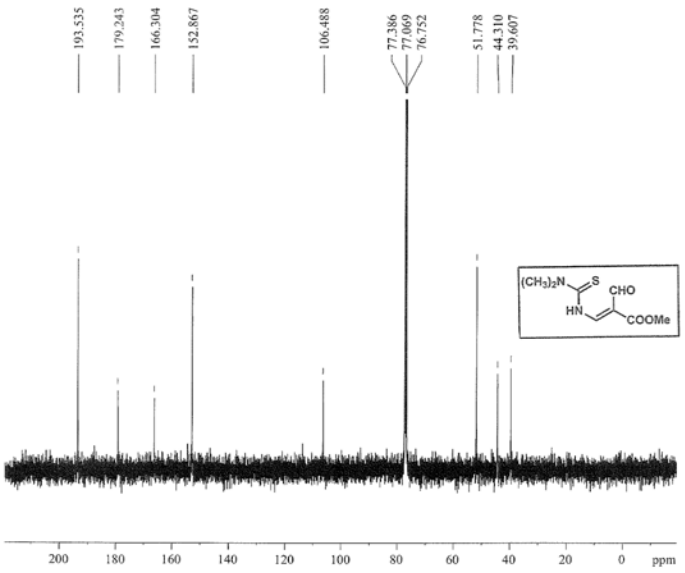


^{1}H NMR



^{13}C NMR

13C NMR ex246 CPD



Current Data Parameters
NAME ex246
EXPNO 6
PROCNO 1

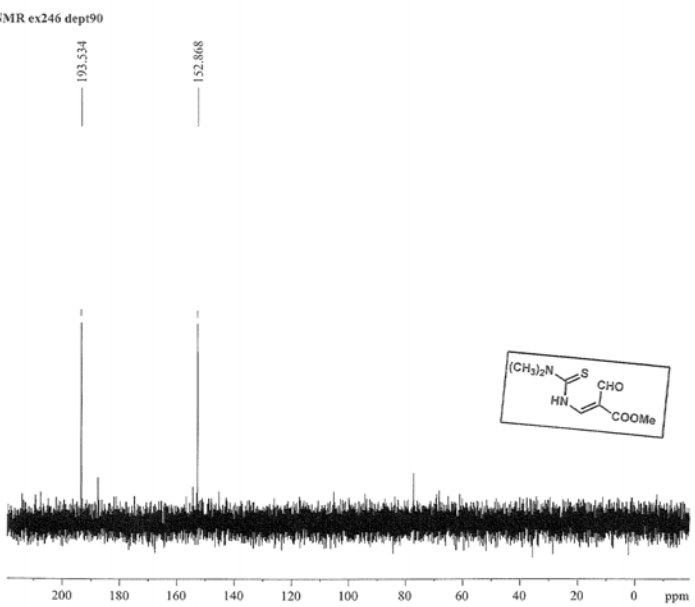
F2 - Acquisition Parameters
Date_ 20141030
Time 22.36
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 305
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 9195.2
DW 20.850 usec
DE 6.00 usec
TE 653.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR ex246 dept90



Current Data Parameters
NAME ex246
EXPNO 62
PROCNO 1

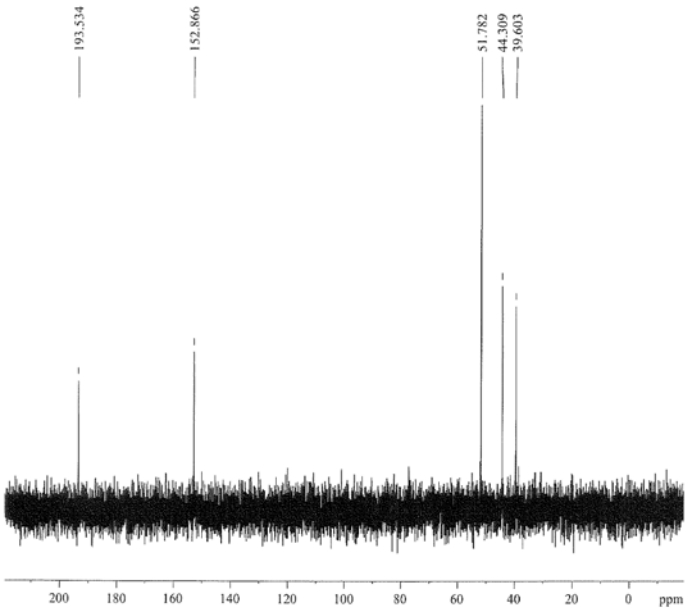
F2 - Acquisition Parameters
Date_ 20141030
Time 22.51
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 103
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 663.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR ex246 dept135



Current Data Parameters
NAME ex246
EXPNO 61
PROCNO 1

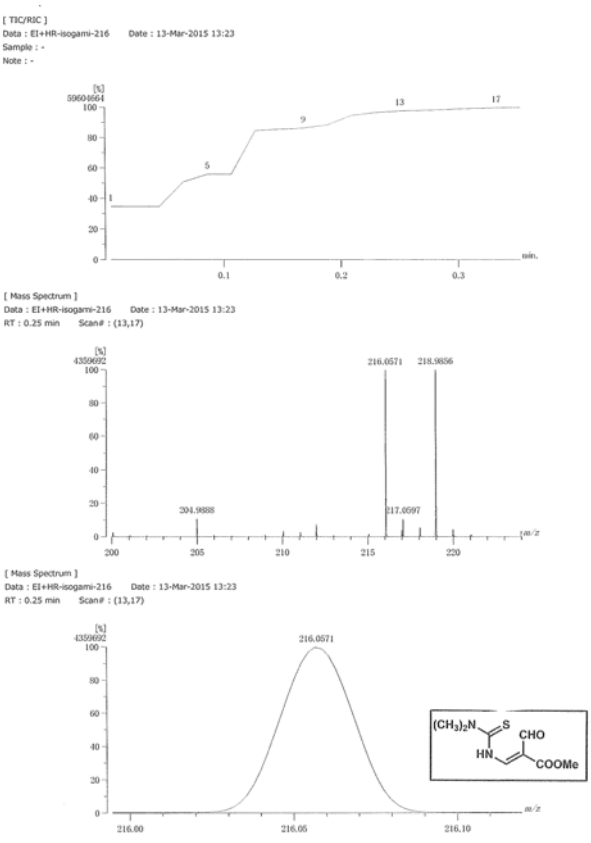
F2 - Acquisition Parameters
Date_ 20141030
Time 22.43
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 104
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 29193
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.70 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

HRMS



Data : EI+HR-isogami-216 Date : 13-Mar-2015 13:23
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.25 min Scan# : (13,17)
Elements : C 8/0, H 12/0, N 2/0, O 3/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 5.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	216.0571	99.74	+1.1 / +0.2	5.0	C8 H12 N2 O3 S

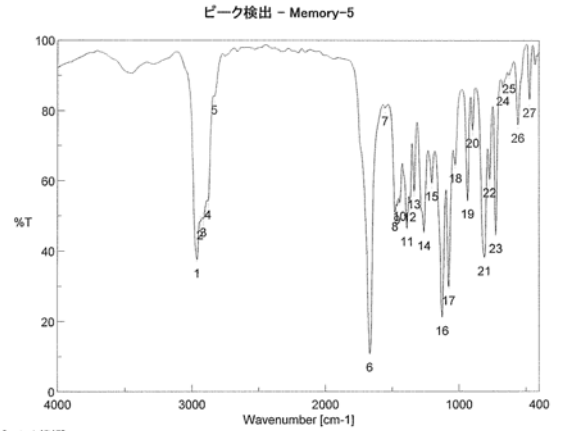
[Theoretical Ion Distribution]
Molecular Formula : C8 H12 N2 O3 S
(m/z 216.0569, MW 216.2609, U.S. 5.0)
Base Peak : 216.0569, Averaged MW : 216.2579(a), 216.2593(w)

m/z	INT.
216.0569	100.0000
217.0595	10.5361
218.0544	5.5332
219.0568	0.5092
220.0564	0.0709
221.0583	0.0053
222.0594	0.0004

(4) 5*H*-1,2,4-Oxathiazoles (13):

13a (R^1 = NMe_2, R^2 = *t*-C_4H_9):

IR Spectrum



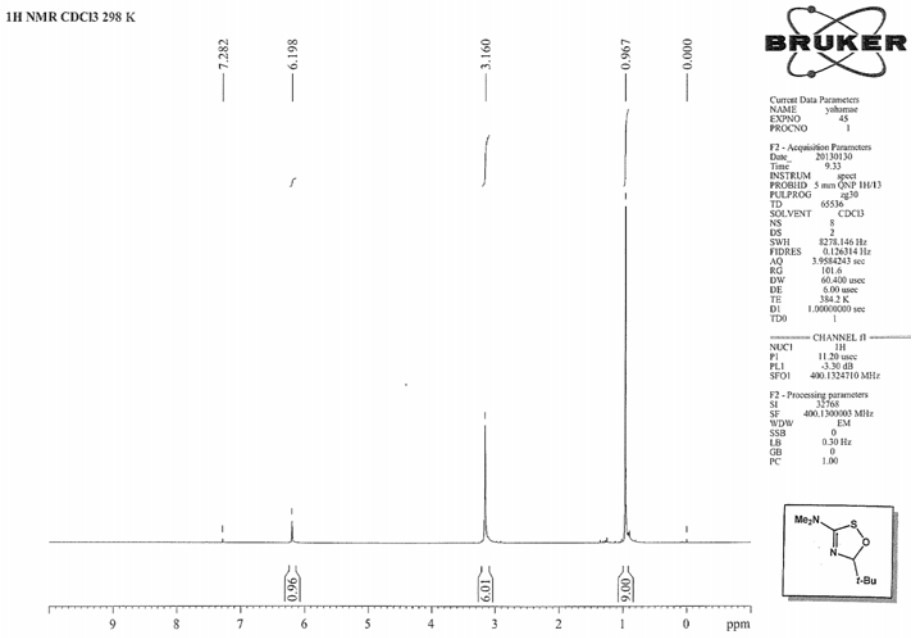
[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]		[測定情報]	
作成日時	2013/02/26 15:21	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	399.193 cm-1	積算回数	32
エンド	4000.6 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	3736	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2960.2	38	2	2935.1	48	3	2911.0	49
4	2876.3	54	5	2827.1	84	6	1668.1	11
7	1552.4	81	8	1478.2	51	9	1462.7	53
10	1442.5	54	11	1388.5	46	12	1367.3	53
13	1334.5	57	14	1261.2	45	15	1202.4	59
16	1126.2	21	17	1077.1	30	18	1026.9	64
19	935.3	54	20	896.7	75	21	809.0	38
22	770.4	60	23	724.1	44	24	669.2	87
25	622.9	90	26	557.3	76	27	470.6	83

^{1}H NMR



Current Data Parameters
NAME yahamae
EXPNO 45
PROCNO 1

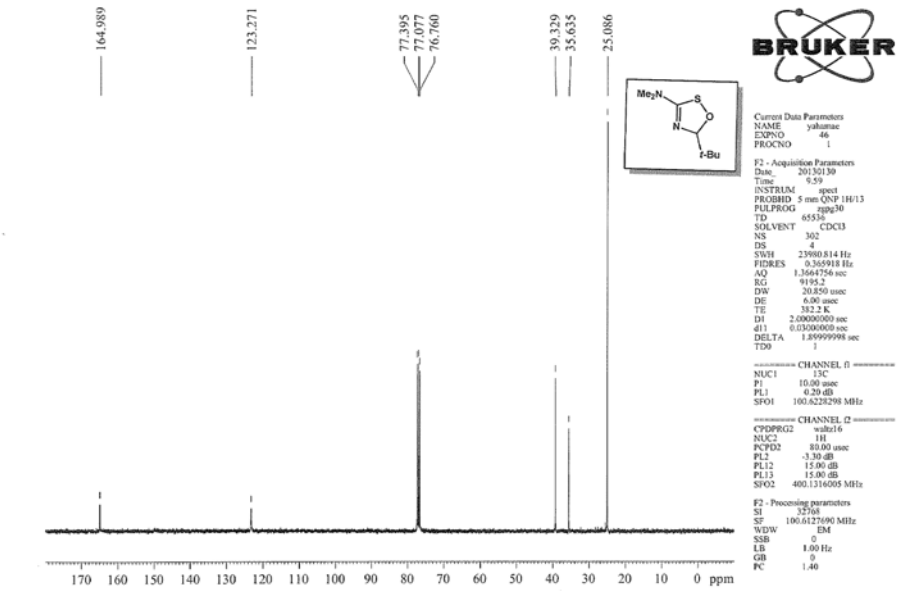
F2 - Acquisition Parameters
Date_ 20130130
Time 9.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 101.6
DW 60.400 usec
DE 6.00 usec
TE 384.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

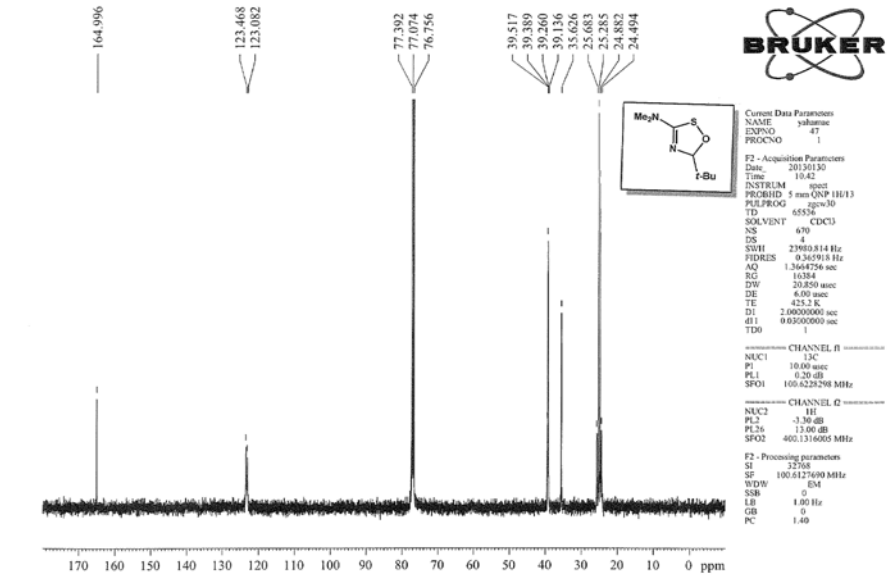
F2 - Processing parameters
SI 32768
SF 400.1300005 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR

13C NMR CDCl3 298 K CPD



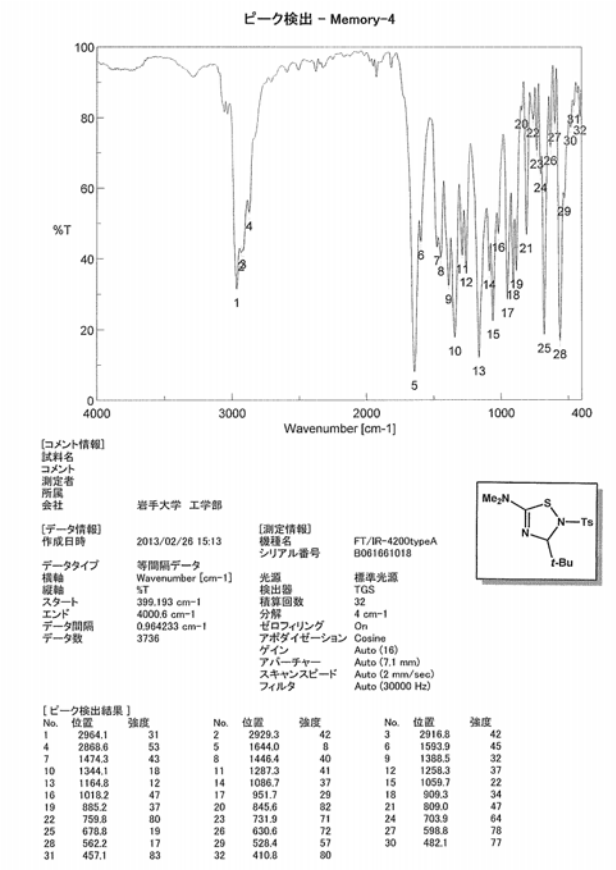
13C NMR CDCl3 298 K Off Resonance



(5) 2,3-Dihydro-1,2,4-thiadiazoles (15) and Amidinoamidine-C_6H_5-NMe_2-NTs (16)

15a (R^1 = NMe_2, R^2 = *t*-C_4H_9):

IR Spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2013/02/26 15:13

データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4000.6 cm-1
データ間隔 0.964233 cm-1
データ数 3736

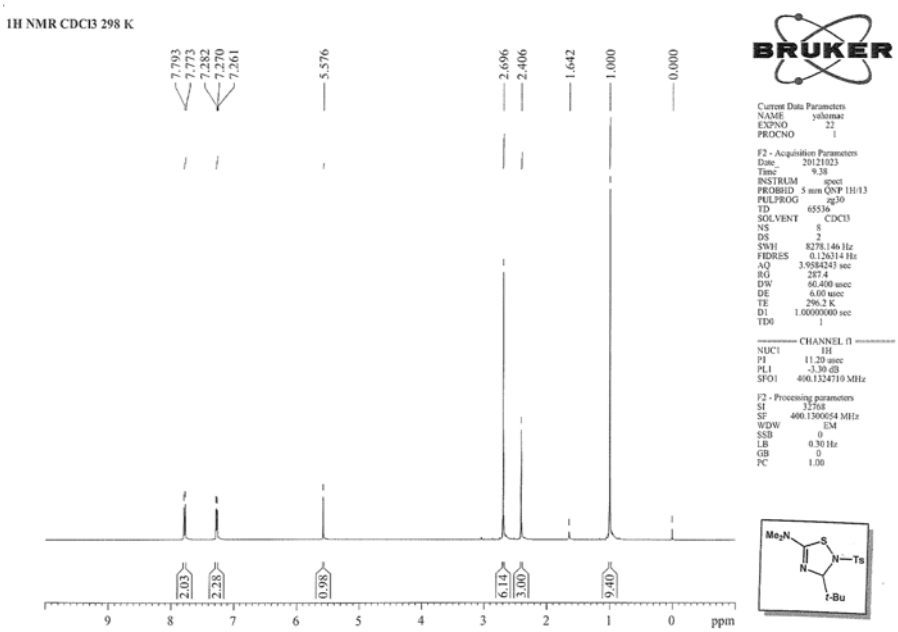
[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018

光源 標準光源
検出器 TGS
積算回数 32
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (16)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2964.1	31	2	2929.3	42	3	2916.8	42
4	2868.6	53	5	1644.0	8	6	1593.9	45
7	1474.3	43	8	1446.4	40	9	1388.5	32
10	1344.1	18	11	1287.3	41	12	1258.3	37
13	1164.8	12	14	1086.7	37	15	1059.7	22
16	1018.2	47	17	951.7	29	18	909.3	34
19	885.2	37	20	845.6	82	21	809.0	47
22	759.8	80	23	731.9	71	24	703.9	64
25	678.8	19	26	630.6	72	27	598.8	78
28	562.2	17	29	528.4	57	30	482.1	77
31	457.1	83	32	410.8	80			

^{1}H NMR



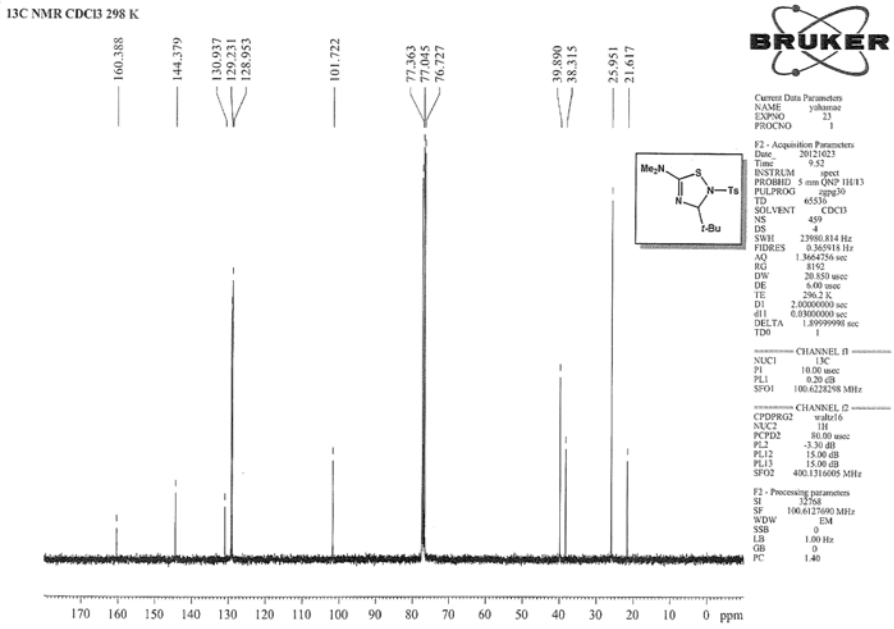
Current Data Parameters
NAME yahimac
EXPNO 22
PROCNO 1

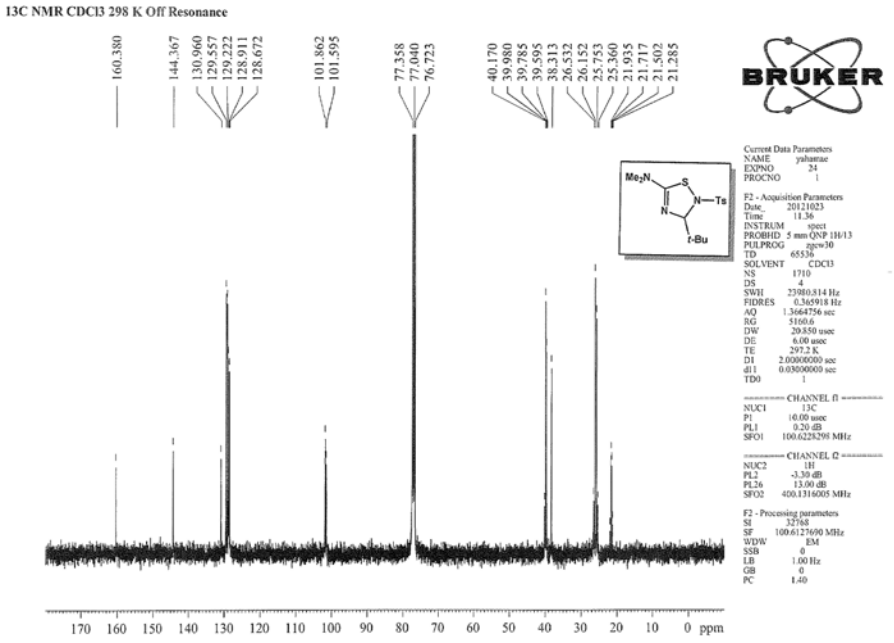
F2 - Acquisition Parameters
Date_ 20121023
Time 9.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

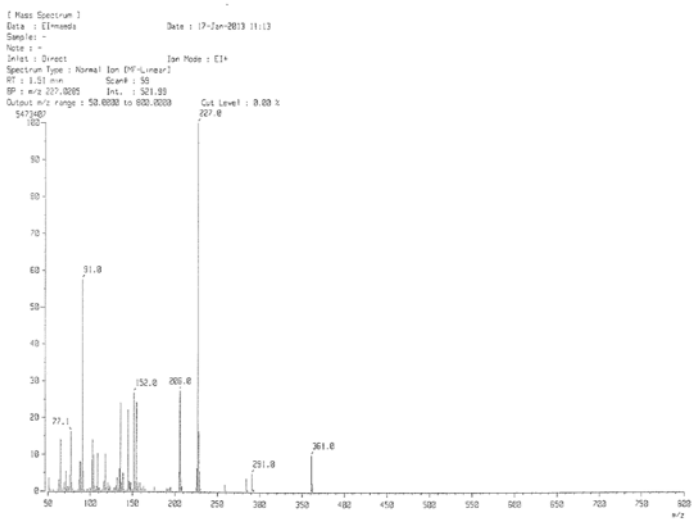
^{13}C NMR





15b ($R^1 = NMe_2$, $R^2 = C_6H_5$):

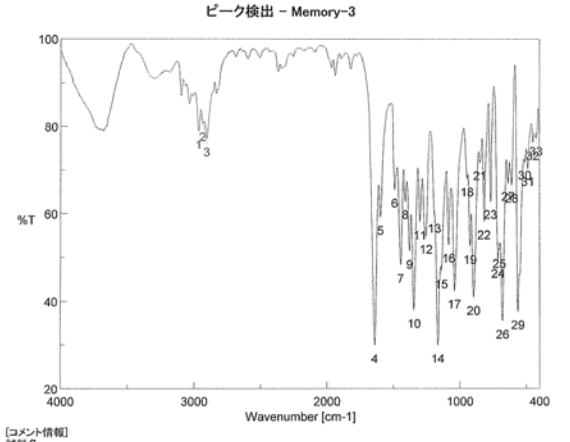
Mass Spectrum



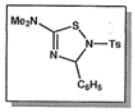
Data : EI+maeda Date : 17-Jan-2013 11:13
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.51 min Scan# : 59
BP : m/z 227.0285 Int. : 521.99
Output m/z range : 100.0000 to 800.0000 Cut Level : 0.00 %

m/z	Int.	Norm.	m/z	Int.	Norm.
100.9932	2.27	0.43	162.9906	6.91	1.32
101.9977	44.41	8.51	165.0313	3.15	0.60
103.0069	73.23	14.03	175.9981	5.99	1.15
104.0199	51.38	9.84	189.9889	3.99	0.76
105.0200	7.24	1.39	191.0324	2.01	0.38
106.0177	1.69	0.32	192.0061	3.95	0.76
107.0264	3.08	0.59	194.0571	4.77	0.91
107.9836	6.74	1.29	195.0542	5.56	1.06
108.9820	53.91	10.33	205.0126	27.82	5.33
109.9906	4.67	0.89	206.0273	143.44	27.48
110.9913	4.68	0.90	207.0284	19.49	3.73
113.9872	2.60	0.50	208.0306	7.28	1.40
116.0265	12.87	2.47	225.0229	5.57	1.07
117.0259	15.02	2.88	226.0285	33.11	6.34
118.0300	52.59	10.07	227.0285	521.99	100.00
119.0318	5.12	0.98	228.0297	86.44	16.56
120.9729	11.77	2.26	229.0242	29.04	5.56
121.9926	3.26	0.62	230.0298	3.69	0.71
122.9959	7.68	1.47	259.0035	10.16	1.95
123.9834	5.10	0.98	260.0023	2.50	0.48
128.0093	3.92	0.75	283.9854	19.19	3.68
129.0152	5.11	0.98	284.9890	3.02	0.58
130.0119	3.94	0.75	285.9658	1.84	0.35
131.0315	7.69	1.47	290.9803	25.86	4.95
132.0427	19.40	3.72	291.9655	4.80	0.92
133.0498	2.22	0.43	292.9827	3.05	0.58
133.9854	3.64	0.70	361.0136	51.28	9.82
134.9723	32.66	6.26	362.0178	11.85	2.27
135.9835	126.14	24.16	363.0328	6.09	1.17
136.9904	13.10	2.51			
137.9878	7.19	1.38			
138.9877	26.06	4.99			
139.9982	3.11	0.60			
143.0275	1.72	0.33			
144.0435	3.12	0.60			
145.0473	116.17	22.26			
146.0483	14.10	2.70			
147.0583	5.22	1.00			
147.9784	12.01	2.30			
149.0018	2.67	0.51			
150.0072	2.82	0.54			
151.9690	140.95	27.00			
152.9689	12.77	2.45			
153.9569	7.95	1.52			
154.9706	126.97	24.32			
155.9797	12.86	2.46			
156.9704	7.07	1.35			
159.0577	12.23	2.34			
160.0570	4.80	0.92			
160.9775	3.36	0.64			

IR Spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

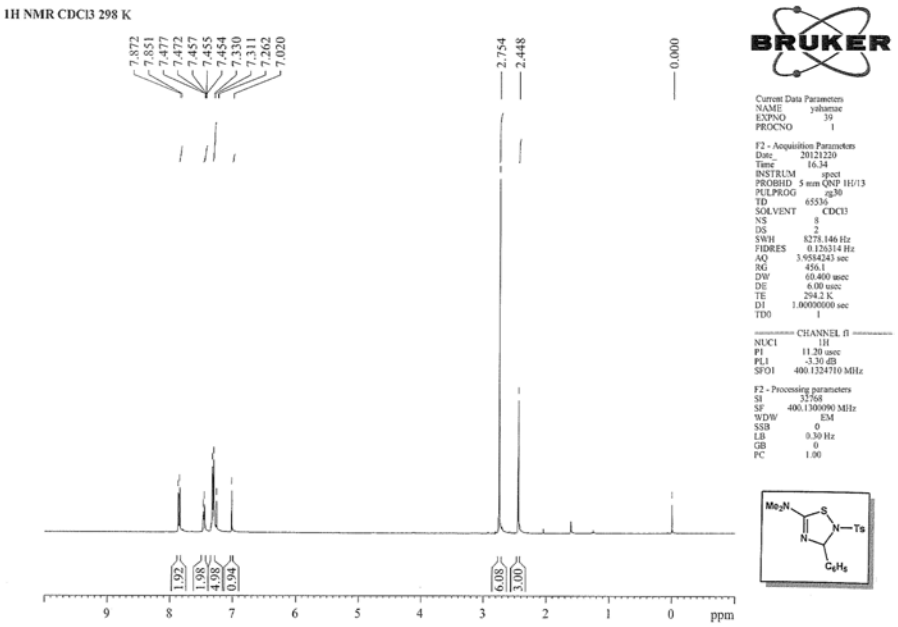


[データ情報]		[測定情報]	
作成日時	2013/02/26 14:58	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	399.193 cm-1	積算回数	32
エンド	4000.6 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	3736	アポダイゼーション	Cosine
		ゲイン	Auto (16)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

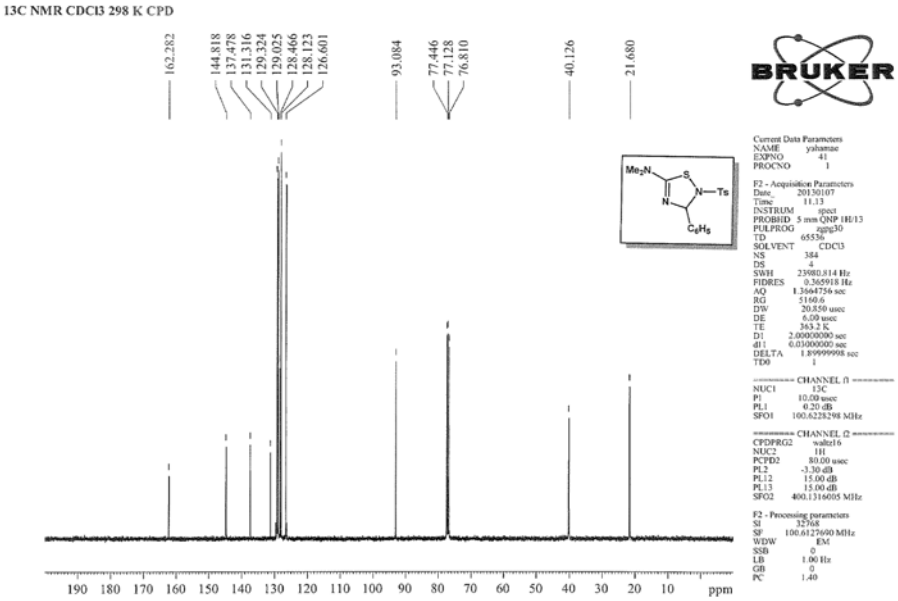
[ピーク検出結果]

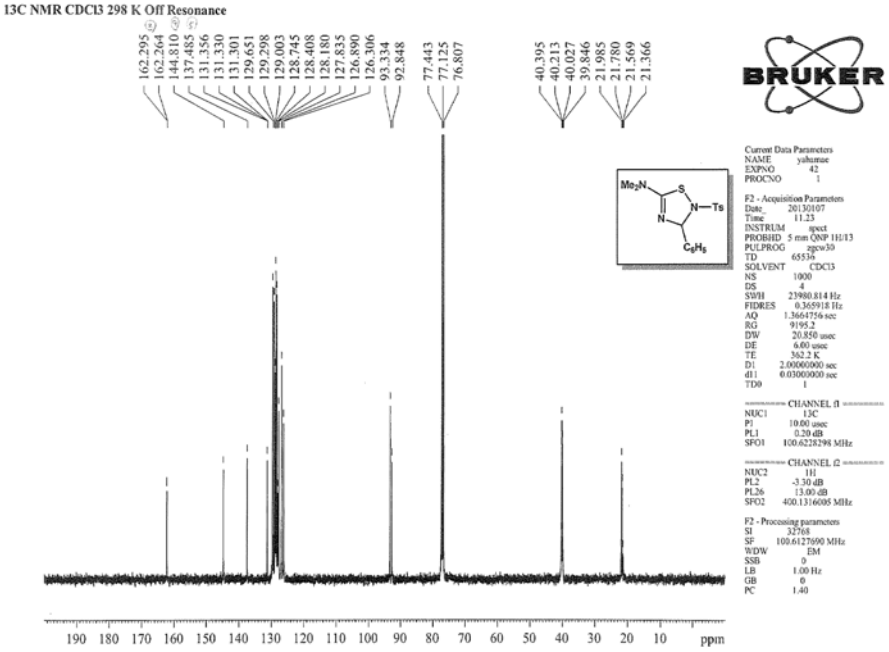
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2959.2	79	2	2927.4	81	3	2899.5	77
4	1641.1	30	5	1595.8	59	6	1488.8	65
7	1444.4	48	8	1408.8	63	9	1377.9	51
10	1345.1	38	11	1298.8	58	12	1253.5	55
13	1189.9	60	14	1166.7	30	15	1138.8	47
16	1082.8	53	17	1040.4	42	18	945.0	68
19	922.8	53	20	895.8	41	21	848.5	72
22	815.7	58	23	767.5	63	24	712.6	49
25	702.9	52	26	678.8	36	27	636.4	67
28	610.4	67	29	563.1	38	30	511.0	72
31	487.9	70	32	450.3	76	33	425.2	77

^{1}H NMR


1H NMR CDCl3 298 K
7.872
7.851
7.477
7.472
7.457
7.455
7.454
7.330
7.311
7.262
7.020
2.754
2.448
0.000
1.92
1.98
4.98
0.94
6.08
3.00
9
8
7
6
5
4
3
2
1
0
ppm
BRUKER
Current Data Parameters
NAME yahamae
EXPNO 39
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121220
Time 16.34
INSTRUM spect
PROBHD 5 mm QNP H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me2N
S
N
Ts
C6H5

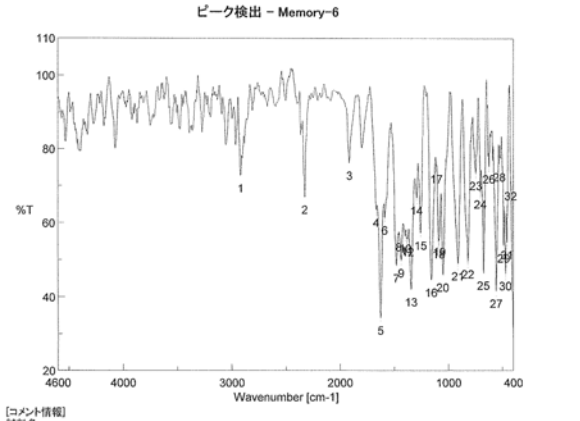
^{13}C NMR


13C NMR CDCl3 298 K CPD
162.282
144.818
137.478
131.316
129.324
129.025
128.466
128.123
126.601
93.084
77.446
77.128
76.810
40.126
21.680
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
BRUKER
Current Data Parameters
NAME yahamae
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130107
Time 11.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 384
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.00 usec
TE 363.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me2N
S
N
Ts
C6H5



15c (R^1 = NMe_2, R^2 = *p*-ClC_6H_4):

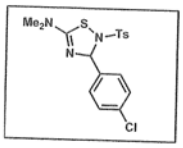
IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/11/17 13:58
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (128)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

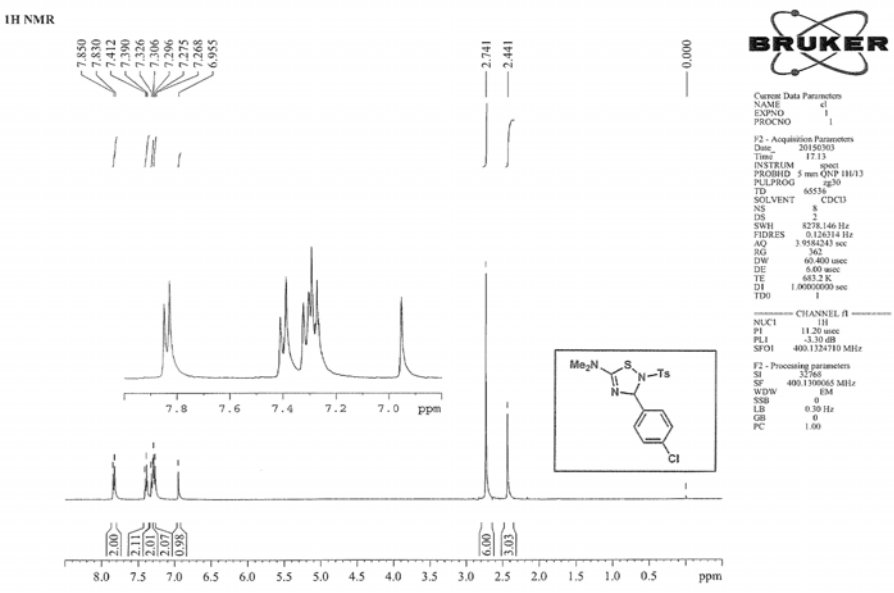


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2918.7	72.7401	2	2326.7	66.9318	3	1916.9	76.2024
4	1667.2	63.4634	5	1627.6	34.3387	6	1589.1	61.3925
7	1483.0	48.4886	8	1461.8	56.8598	9	1439.6	49.8638
10	1401.0	56.45	11	1385.6	55.8969	12	1377.9	55.557
13	1345.1	42.0377	14	1295.0	66.7349	15	1259.3	57.28
16	1160.0	44.5954	17	1111.8	75.3075	18	1091.5	54.9691
19	1084.8	55.6193	20	1052.0	45.9857	21	912.2	49.0383
22	820.6	49.5913	23	747.3	73.4138	24	704.9	68.4157
25	675.9	46.5093	26	624.8	75.2624	27	558.3	41.6226
28	530.3	75.7715	29	489.8	53.8971	30	473.4	46.4014
31	459.0	54.7237	32	424.3	70.7045			

^{1}H NMR

1H NMR



BRUKER

Current Data Parameters
NAME cl
EXPNO 1
PROCNO 1

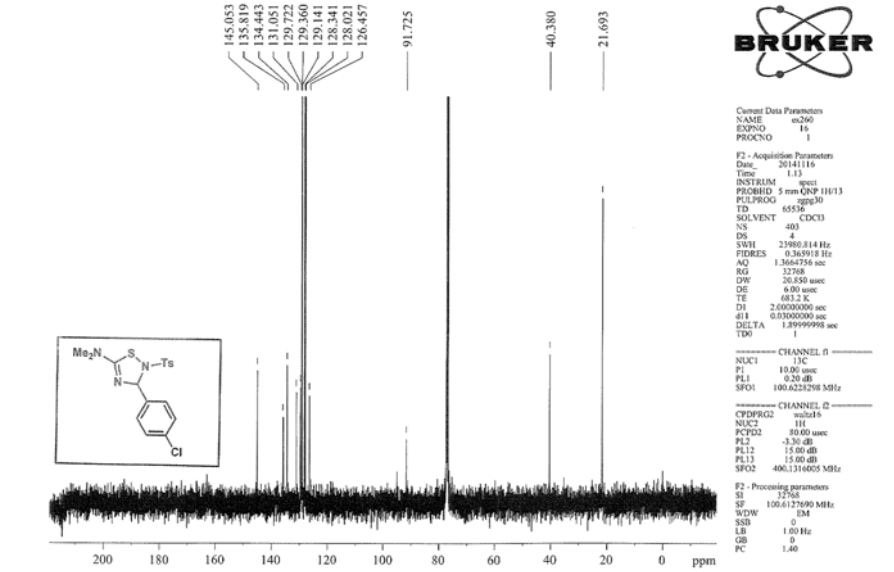
F2 - Acquisition Parameters
Date_ 20150303
Time 17.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR

13C NMR CPD



BRUKER

Current Data Parameters
NAME en260
EXPNO 16
PROCNO 1

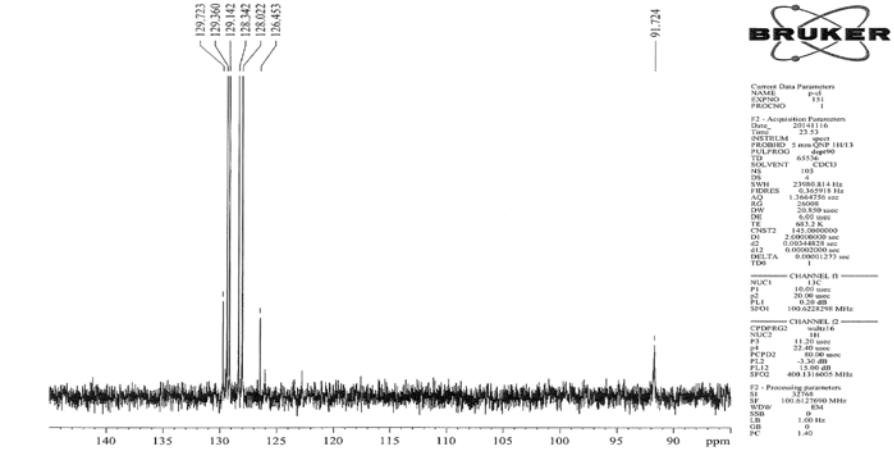
F2 - Acquisition Parameters
Date_ 20141116
Time 1.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 403
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 681.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6223298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept90



BRUKER

Current Data Parameters
NAME p-cl
EXPNO 131
PROCNO 1

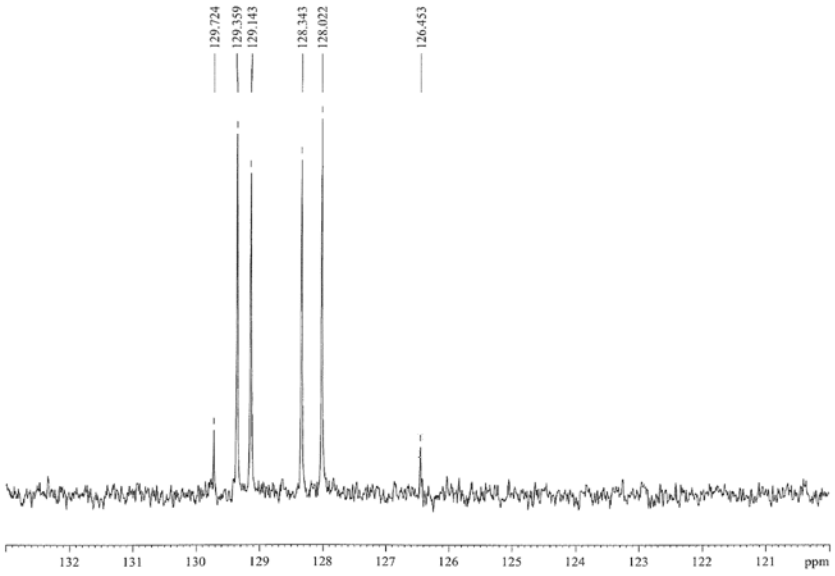
F2 - Acquisition Parameters
Date_ 20141116
Time 23.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 103
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 26608
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P3 10.00 usec
P4 20.00 usec
PL1 0.20 dB
SFO1 100.6223298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
P4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

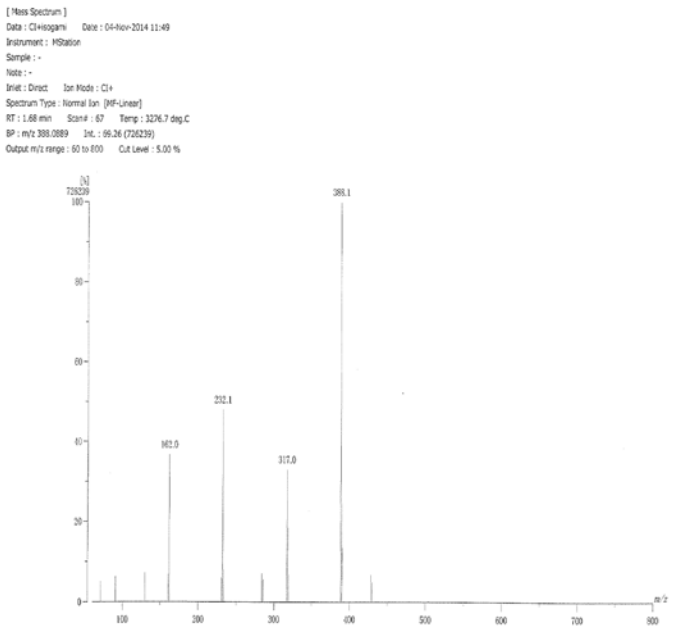
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C NMR dept135



15d ($R^1 = NMe_2$, $R^2 = CH{=}CHC_6H_5$):

Mass spectrum



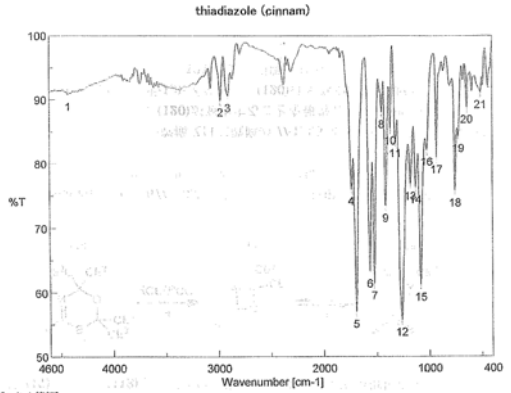
[Mass Spectrum]
Data : CI+isogami Date : 04-Nov-2014 11:49
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.68 min Scan# : 67 Temp : 3276.7 deg.C
BP : m/z 388.0889 Int. : 69.26 (726239)
Output m/z range : 60.0000 to 800.0000 Cut Level : 5.00 %

m/z	Int.	Norm.	
71.0303	3.58	5.17	37535
90.9620	4.43	6.40	46463
130.0110	5.11	7.38	53631
161.0038	4.83	6.97	50655
161.9793	25.51	36.84	267535
230.0376	4.22	6.09	44207
231.0287	4.15	5.99	43471
232.0555	33.31	48.10	349327
233.0588	5.58	8.05	58463
284.0523	5.05	7.29	52959
286.0317	3.98	5.74	41695
317.0257	22.89	33.05	240047
318.0539	12.87	18.59	134991
319.0309	4.84	6.98	50719
388.0889	69.26	100.00	726239
389.0833	17.13	24.74	179663
390.0890	9.47	13.68	99343
428.1177	4.80	6.94	50383
430.1343	3.47	5.02	36431

[Theoretical Ion Distribution]
Molecular Formula : C19 H22 N3 O2 S2
(m/z 388.1153, MW 388.5346, U.S. 12.5)
Base Peak : 388.1153, Averaged MW : 388.5294(a), 388.5309(w)

m/z	INT.
388.1153	100.0000
389.1181	23.8893
390.1137	11.9899
391.1152	2.3407
392.1129	0.5211
393.1135	0.0788
394.1136	0.0103
395.1142	0.0011
396.1151	0.0001

IR spectrum



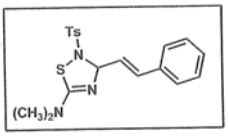
[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/10/27 19:19
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

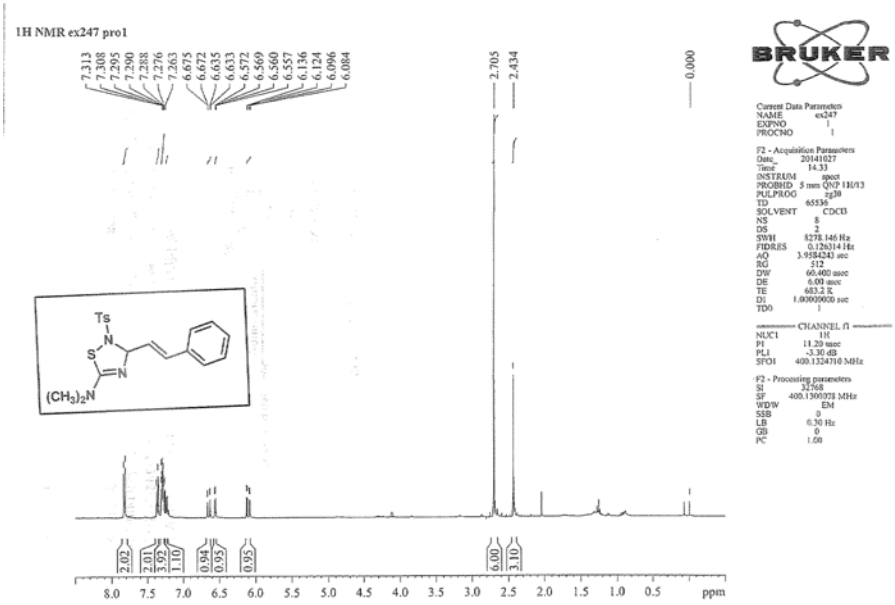
[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 16
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

[ピーク検出結果]

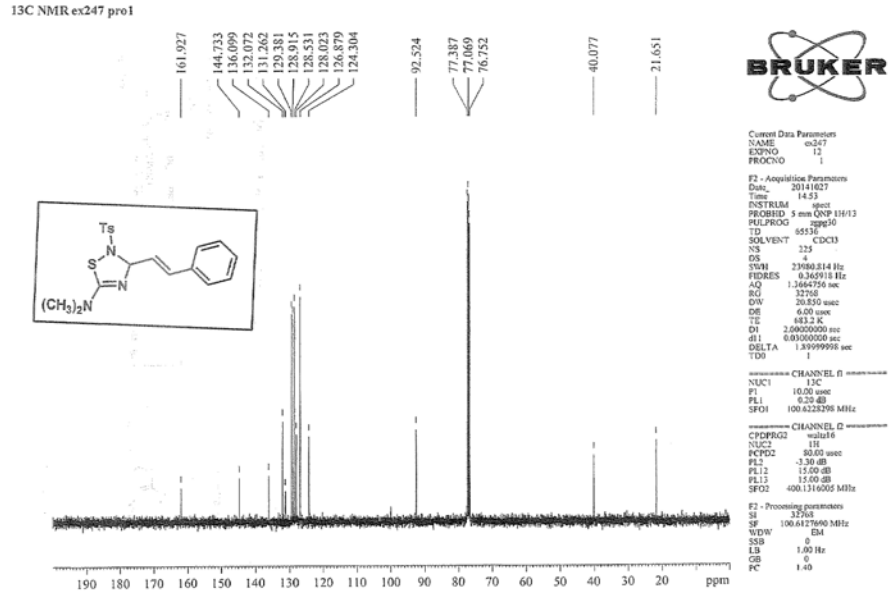
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	4422.9	90.8116	2	2984.3	89.9245	3	2913.0	90.6182
4	1738.5	76.1116	5	1694.2	56.9861	6	1564.0	63.3111
7	1522.5	61.4554	8	1452.1	68.0916	9	1414.5	73.4768
10	1370.2	85.5552	11	1322.0	93.5578	12	1261.2	55.7248
13	1179.3	76.8271	14	1130.1	76.2944	15	1081.9	61.2087
16	1022.1	82.1709	17	929.5	80.9554	18	755.0	75.8005
19	723.2	84.3101	20	641.2	88.8444	21	512.0	91.1632



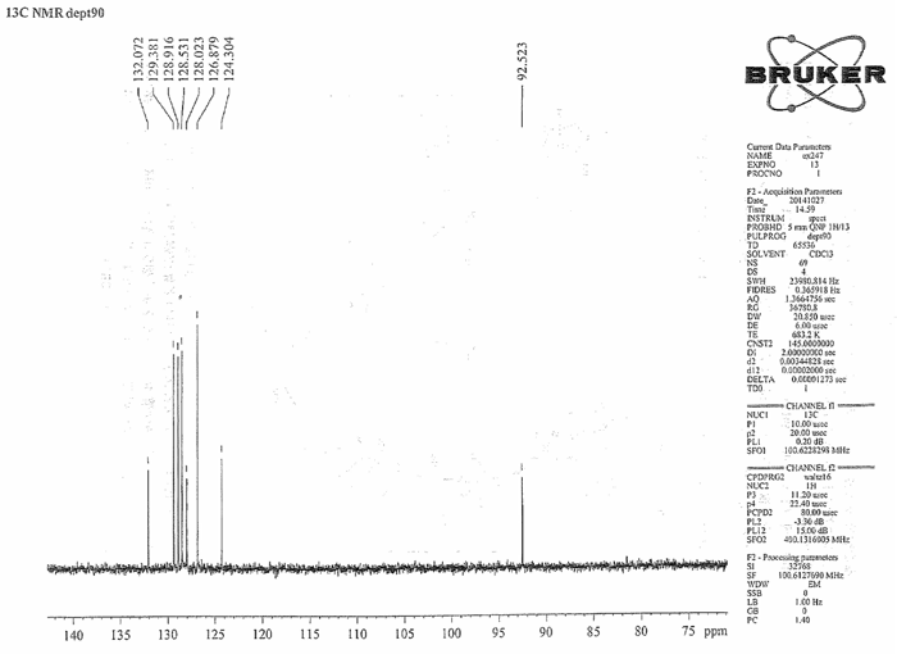
^{1}H NMR


1H NMR ex247 pro1
7.313
7.308
7.295
7.290
7.288
7.276
7.263
6.675
6.672
6.635
6.633
6.572
6.569
6.560
6.557
6.136
6.124
6.096
6.084
2.705
2.434
0.000
Ts
N
S
N
(CH3)2N
2.02
2.01
3.92
1.10
0.94
0.95
0.95
6.00
3.10
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
BRUKER
Current Data Parameters
NAME ex247
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141027
Time 14.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 512
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

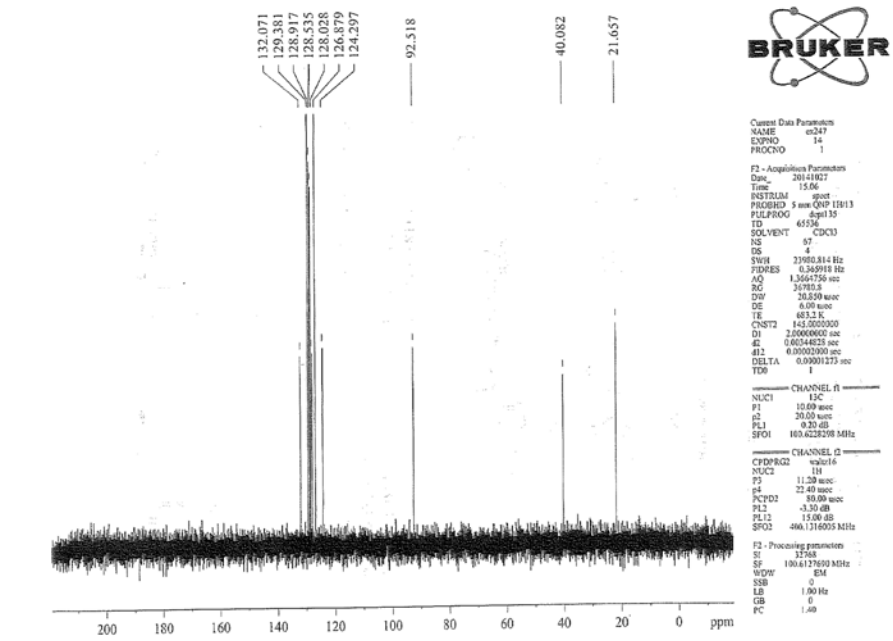
^{13}C NMR


13C NMR ex247 pro1
161.927
144.733
136.099
132.072
131.262
129.381
128.915
128.531
128.023
126.879
124.304
92.524
77.387
77.069
76.752
40.077
21.651
Ts
N
S
N
(CH3)2N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
BRUKER
Current Data Parameters
NAME ex247
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141027
Time 14.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 225
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

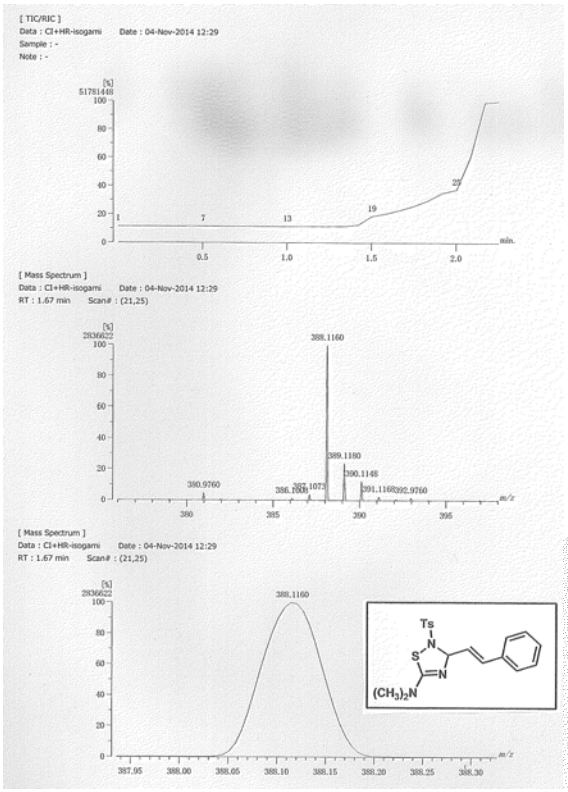
13C NMR dept90



13C NMR dept135



HRMS

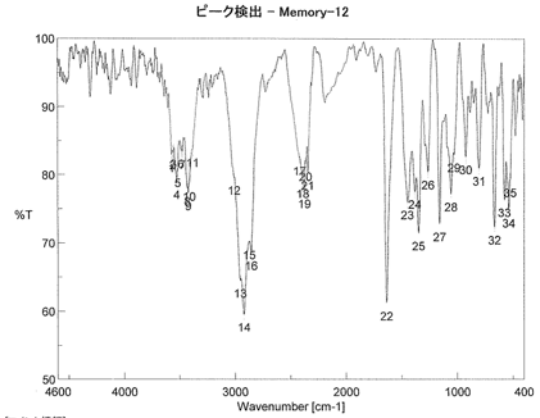


Data : CI+HR-isogami Date : 04-Nov-2014 12:29
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
RT : 1.67 min Scan# : (21,25)
Elements : C 19/0, H 22/0, N 3/0, O 2/0, S 2/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 12.5

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	388.1160	100.00	+1.7 / +0.7	12.5	C19 H22 N3 O2 S2

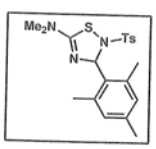
15e ($R^1 = NMe_2$, R^2 = Mes):

IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

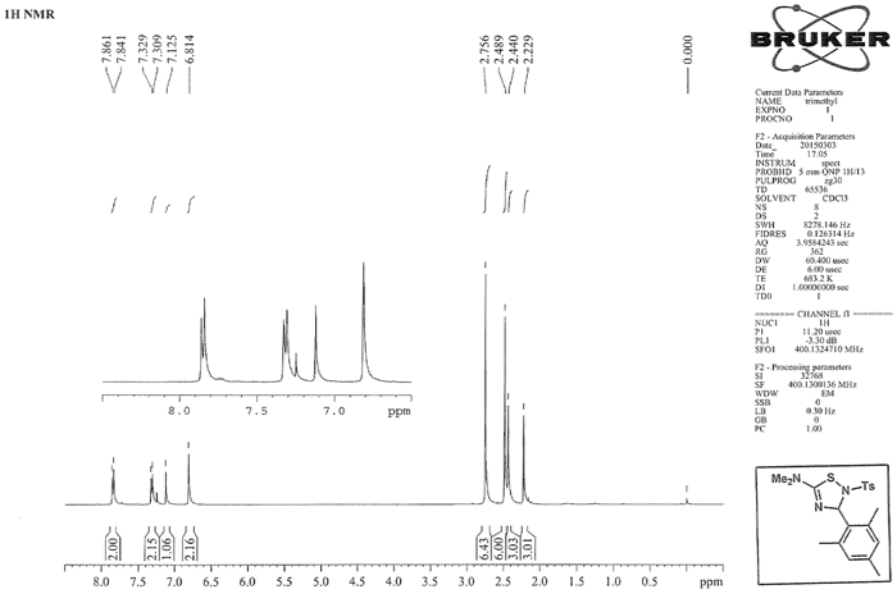
[データ情報]		[測定情報]	
作成日時	2014/11/17 14:20	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	399.193 cm-1	積算回数	16
エンド	4600.36 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	4358	アポダイゼーション	Cosine
		ゲイン	Auto (128)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)



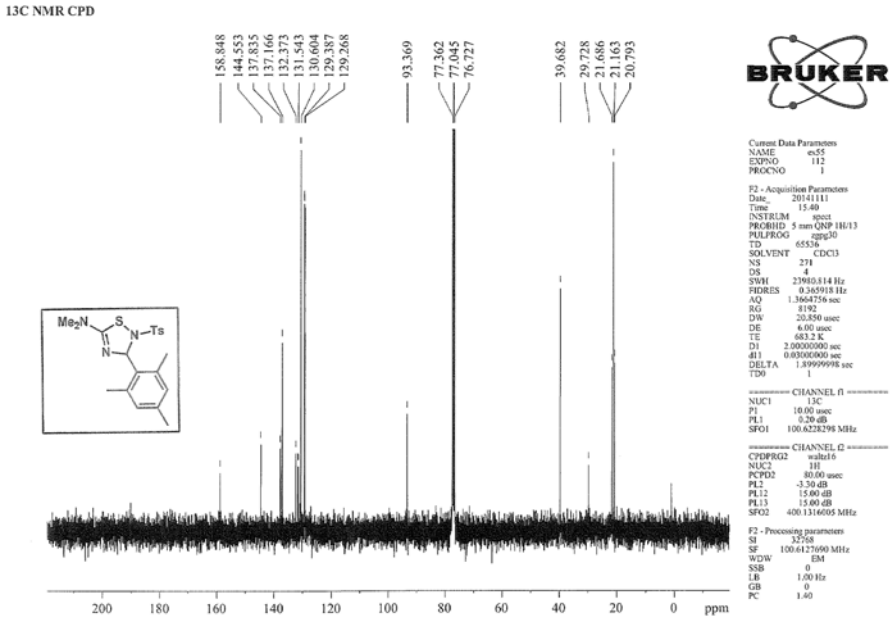
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3576.3	82.9071	2	3564.8	83.3012	3	3559.0	83.5075
4	3530.1	78.9446	5	3521.4	80.6998	6	3488.6	83.4832
7	3477.0	83.4066	8	3435.6	77.9915	9	3425.9	77.3057
10	3417.2	78.6729	11	3385.4	83.6578	12	3012.3	79.5884
13	2954.4	64.5339	14	2921.6	59.5714	15	2875.3	70.1382
16	2857.0	68.5648	17	2422.2	82.465	18	2393.2	79.1187
19	2379.7	77.6461	20	2368.2	81.6355	21	2347.9	80.3101
22	1637.3	61.2205	23	1450.2	75.988	24	1384.6	77.5579
25	1350.9	71.4641	26	1265.1	80.4091	27	1160.9	72.8028
28	1058.7	77.1761	29	1030.8	82.9472	30	925.7	82.6441
31	806.1	80.9601	32	666.3	72.3439	33	576.6	76.3435
34	538.0	74.8092	35	526.5	79.2877			

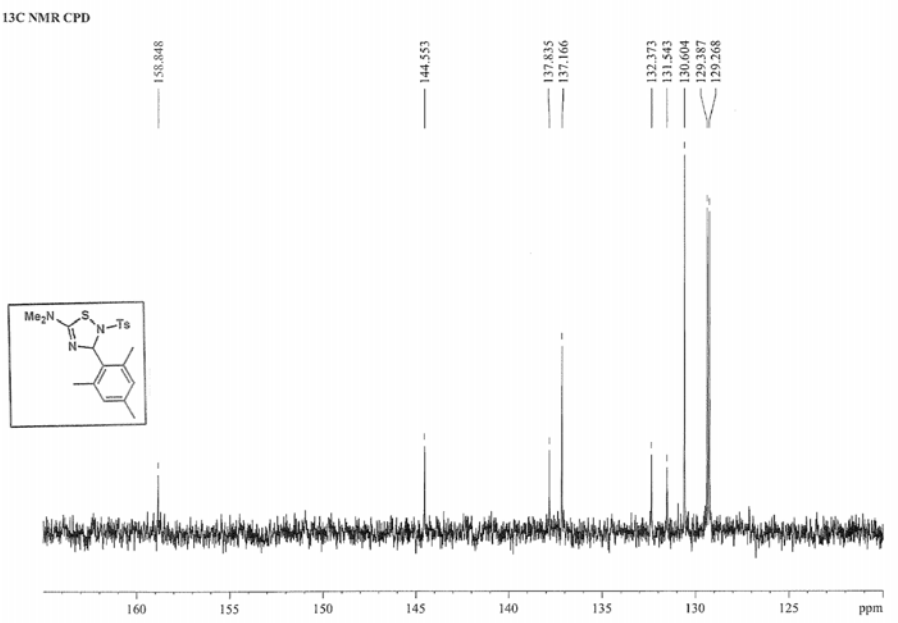
^{1}H NMR



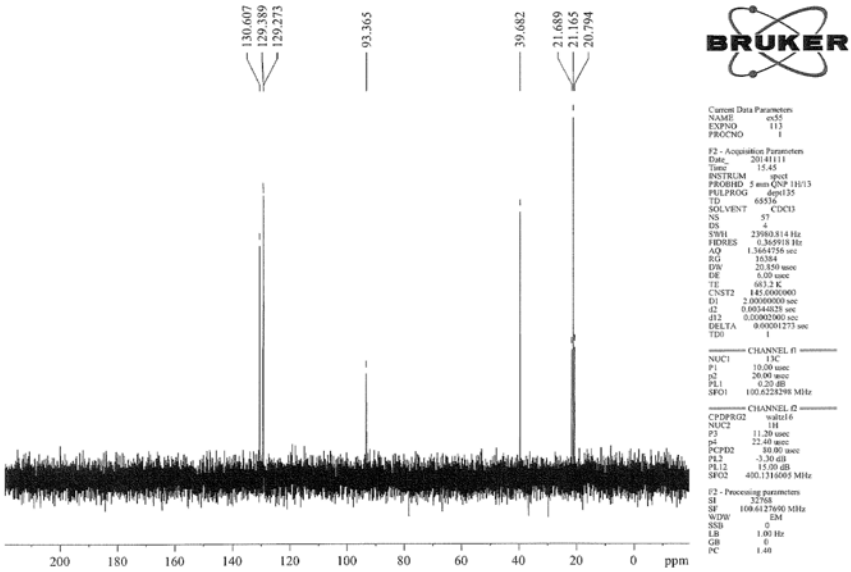
^{13}C NMR



13C NMR CPD



13C NMR dept135



BRUKER

Current Data Parameters
NAME ex55
EXPNO 113
PROCNO 1

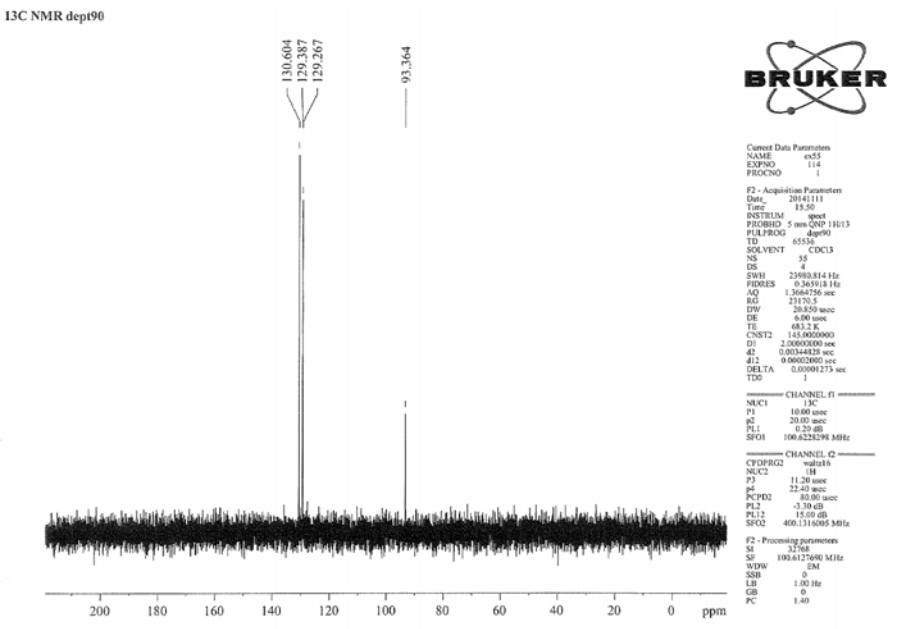
F2 - Acquisition Parameters
Date_ 20141111
Time 15.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 57
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept90



BRUKER

Current Data Parameters
NAME ex55
EXPNO 114
PROCNO 1

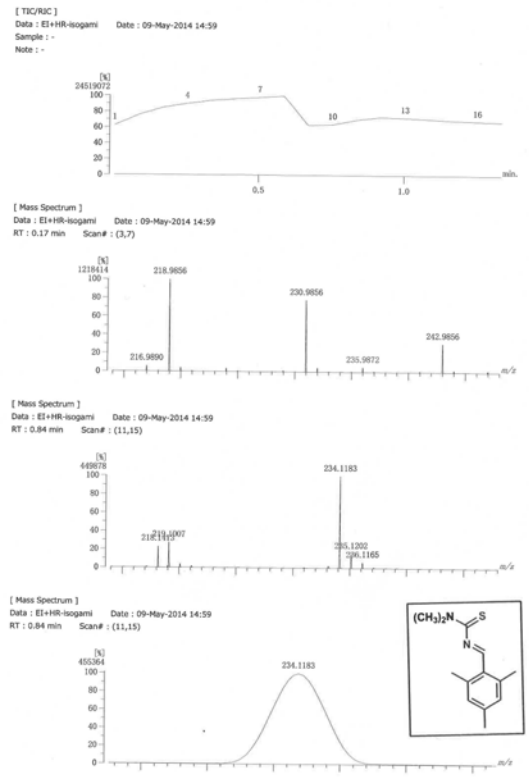
F2 - Acquisition Parameters
Date_ 20141111
Time 15.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 55
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 23170.5
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D0 2.00000300 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.29 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.39 dB
PL12 15.69 dB
SFO2 400.1316005 MHz

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

HRMS



Data : EI+HR-isogami Date : 09-May-2014 14:59
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.84 min Scan# : (11,15)
Elements : C 13/0, H 18/0, N 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 10.0

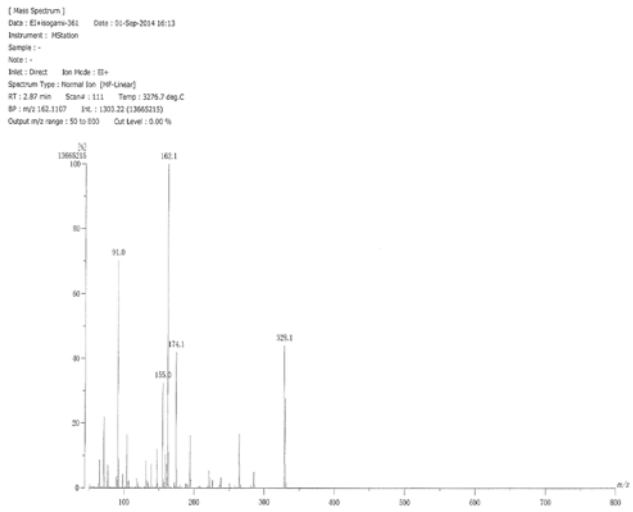
	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	234.1183	100.00	-3.3 / -0.8	7.0	C13 H18 N2 S

[Theoretical Ion Distribution]
Molecular Formula : C13 H18 N2 S
(m/z 234.1191, MW 234.3653, U.S. 7.0)
Base Peak : 234.1191, Averaged MW : 234.3622(a), 234.3635(w)

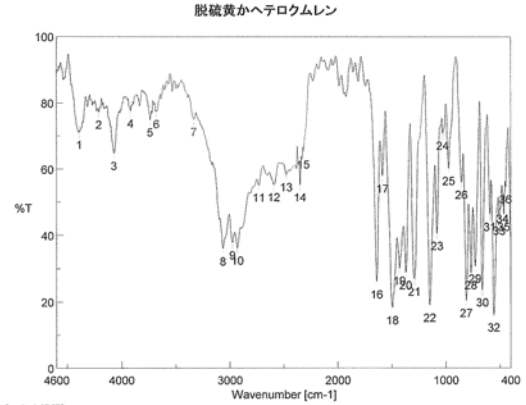
m/z	INT.
234.1191	100.0000
235.1219	15.9830
236.1170	5.6231
237.1186	0.7283
238.1191	0.0703
239.1199	0.0053
240.1216	0.0003

Amidinoamidine-C_6H_5-NMe_2-NTs (16)

Mass spectrum



IR spectrum

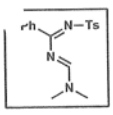


[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

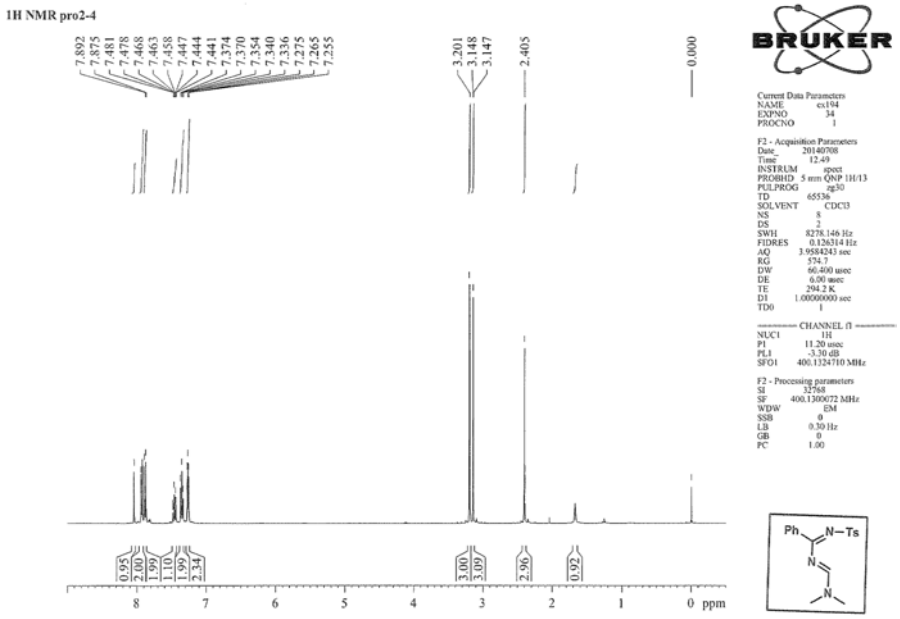
[データ情報]		[測定情報]	
作成日時	2014/09/08 17:22	機種名	FT/IR-4200typeA
更新日時	2014/09/08 17:23	シリアル番号	B061661018
データタイプ	等間隔データ	光源	標準光源
横軸	Wavenumber [cm-1]	検出器	TGS
縦軸	%T	積算回数	16
スタート	399.193 cm-1	分解	4 cm-1
エンド	4600.36 cm-1	ゼロフィリング	On
データ間隔	0.964233 cm-1	アポダイゼーション	Cosine
データ数	4358	ゲイン	Auto (128)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

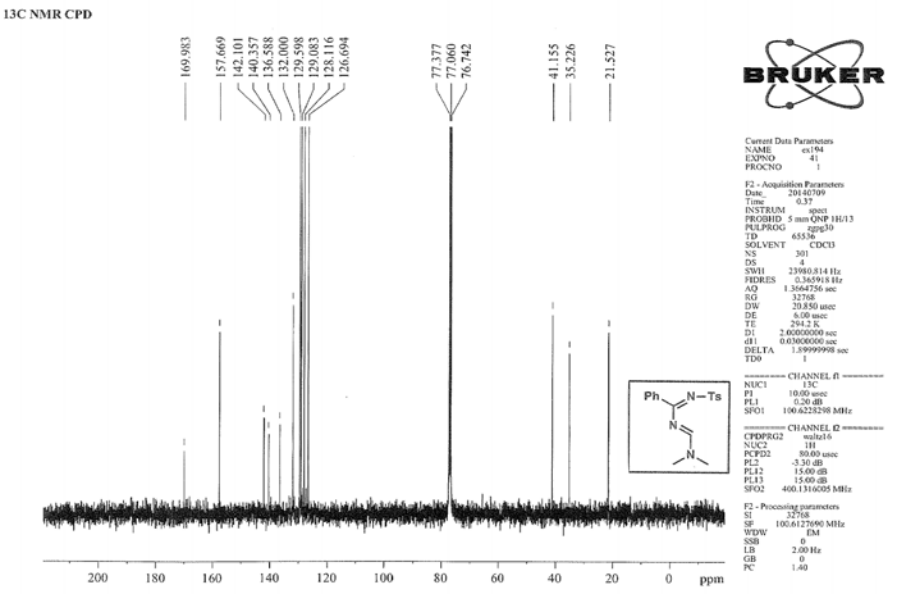
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	4389.2	71.1249	2	4208.9	77.2474	3	4069.1	64.7727
4	3914.8	77.6278	5	3734.5	74.9168	6	3676.6	77.4142
7	3330.5	75.0376	8	3065.3	36.024	9	2976.6	37.8437
10	2930.3	36.2699	11	2730.7	55.1987	12	2592.8	55.3043
13	2478.1	58.3411	14	2350.8	55.2951	15	2319.0	65.2412
16	1641.1	26.1231	17	1588.1	57.8838	18	1496.5	18.3149
19	1430.0	30.1806	20	1371.1	28.8634	21	1291.1	26.9715
22	1150.3	19.0389	23	1081.9	40.6533	24	1029.8	70.8868
25	973.9	60.2223	26	856.2	56.0464	27	811.9	20.4594
28	768.5	28.8799	29	729.9	30.8434	30	662.4	23.6699
31	592.0	46.4002	32	556.4	16.1003	33	506.2	45.1921
34	475.4	48.8275	35	462.8	46.4146	36	446.4	54.6787



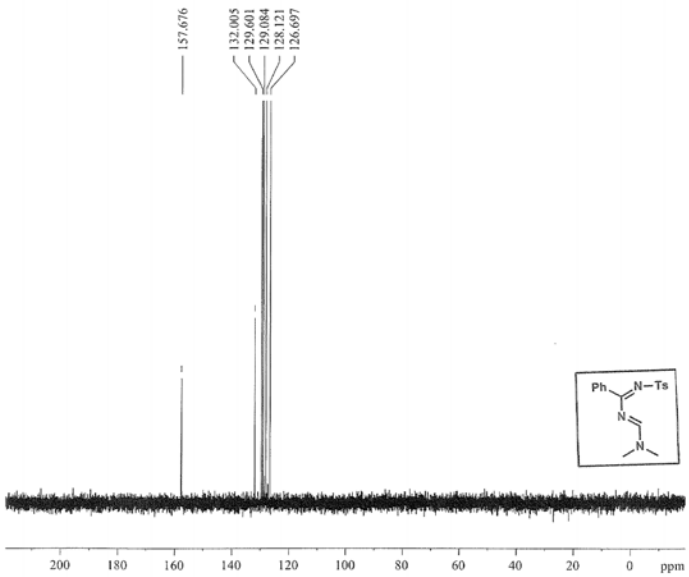
^{1}H NMR


1H NMR pro2-4
7.892
7.875
7.481
7.478
7.468
7.463
7.458
7.447
7.444
7.441
7.374
7.370
7.354
7.340
7.336
7.275
7.265
7.255
3.201
3.148
3.147
2.405
0.000
0.95
2.00
1.99
1.10
1.99
2.34
3.00
3.09
2.96
0.92
8
7
6
5
4
3
2
1
0 ppm
BRUKER
Current Data Parameters
NAME ex194
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date 20140708
Time 12.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9558243 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
N—Ts
N
N

^{13}C NMR


13C NMR CPD
169.983
157.669
142.101
140.357
136.588
132.000
129.598
129.083
128.116
126.694
77.377
77.060
76.742
41.155
35.226
21.527
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME ex194
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date 20140709
Time 0.37
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 301
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664736 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999908 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
Ph
N—Ts
N
N

13C NMR dept 90



Current Data Parameters
NAME ex194
EXPNO 42
PROCNO 1

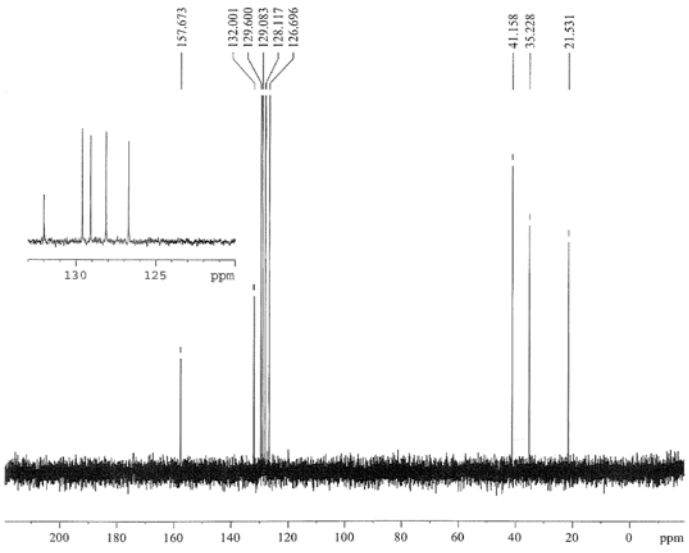
F2 - Acquisition Parameters
Date_ 20140709
Time 0.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 124
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
PC 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR dept135



Current Data Parameters
NAME ex194
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140709
Time 0.17
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 113
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

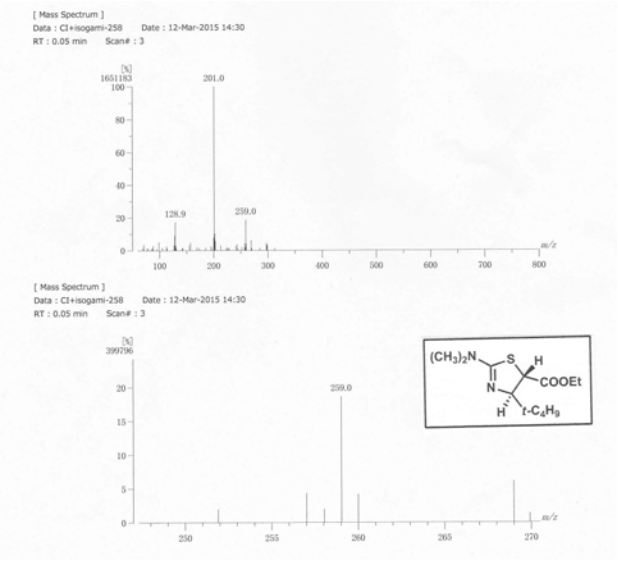
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

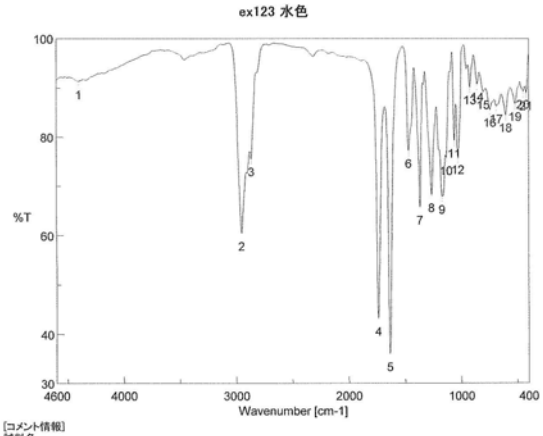
(6) 4,5-dihydro-1,3-thiazoles (18) and 1,3-thiazoles (19):

***trans*-18a ($R^1 = NMe_2$, $R^2 = t\text{-}C_4H_9$):**

Mass spectrum



IR Spectrum



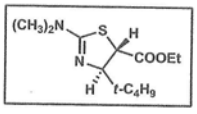
[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2014/02/21 18:17
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 399.193 cm-1
エンド 4600.36 cm-1
データ間隔 0.964233 cm-1
データ数 4358

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061661018
光源 標準光源
検出器 TGS
積算回数 18
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

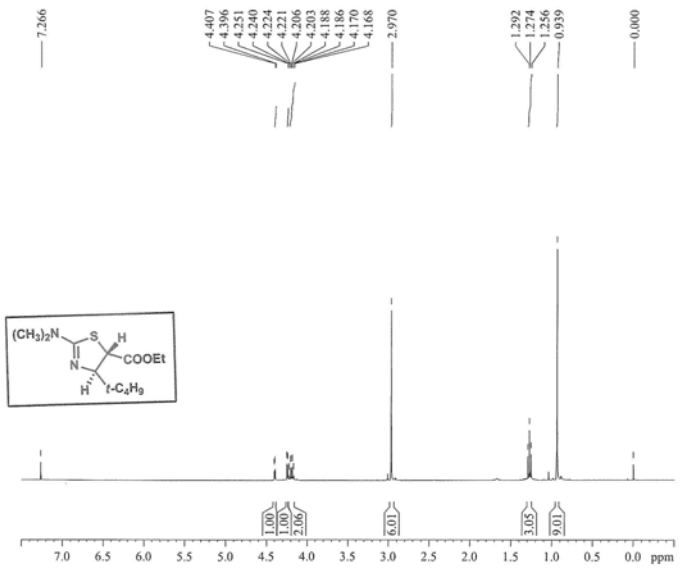
[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	4401.7	91.3048	2	2955.4	60.4548	3	2870.5	75.528
4	1739.5	43.2473	5	1635.3	36.0061	6	1470.5	77.2294
7	1368.3	65.7557	8	1266.0	68.2222	9	1171.5	67.8855
10	1135.9	75.7693	11	1062.6	79.3027	12	1030.8	75.991
13	923.7	90.1985	14	859.1	90.8073	15	804.2	89.2407
16	745.4	85.6005	17	688.5	86.3387	18	605.5	84.5126
19	522.6	86.8084	20	450.3	89.278	21	423.3	89.0342



^{1}H NMR

1H NMR ex318



BRUKER

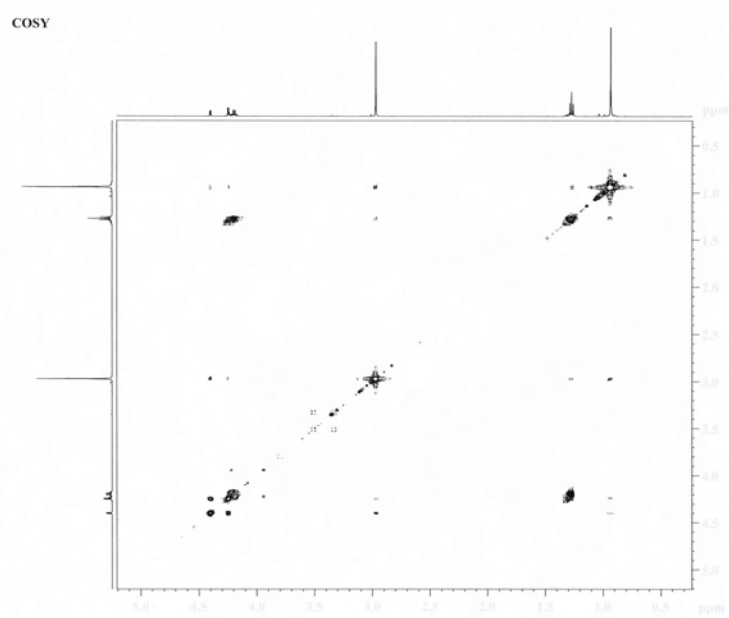
Current Data Parameters
NAME ex318
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150302
Time 21.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 724.1
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1309068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

COSY

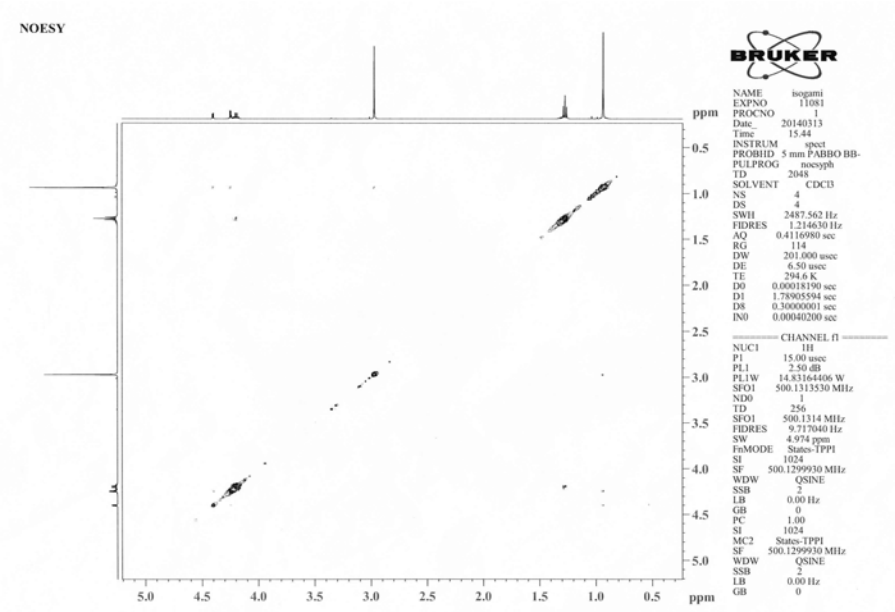


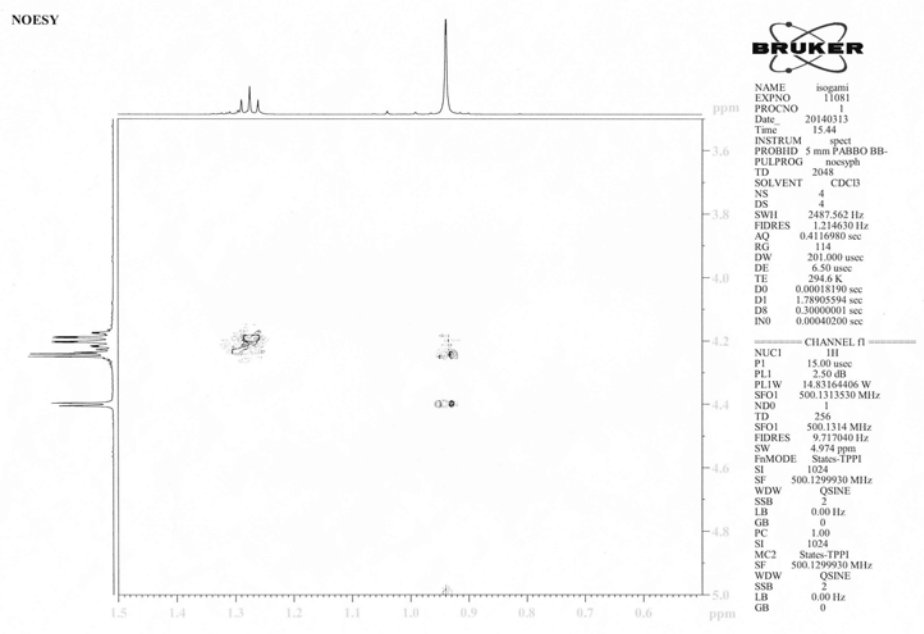
BRUKER

NAME isogami
EXPNO 11079
PROCNO 1
Date_ 20140313
Time 15.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpqf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 2487.562 Hz
FIDRES 1.214630 Hz
AQ 0.4116980 sec
RG 45.2
DW 201.000 usec
DE 6.50 usec
TE 294.5 K
D0 0.00000300 sec
D1 1.22843397 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00040200 sec

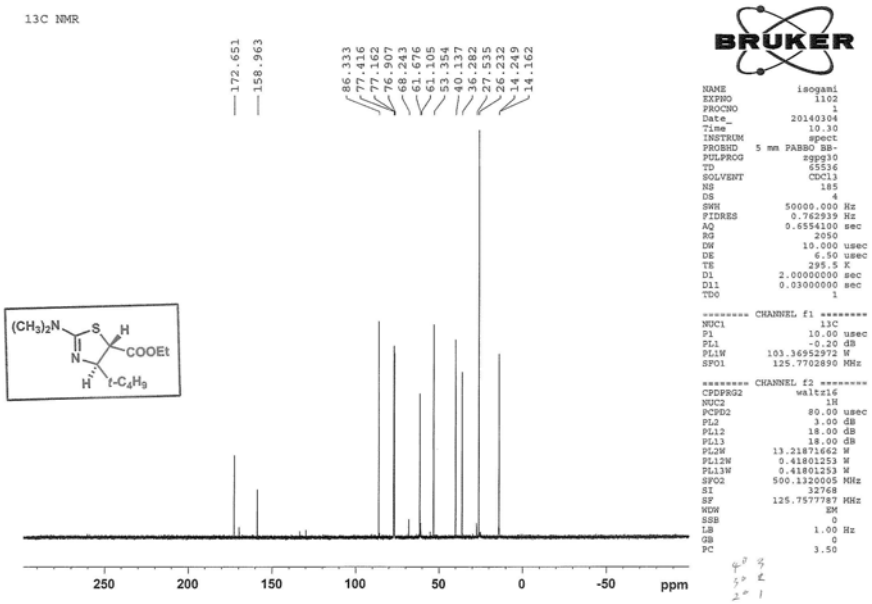
CHANNEL f1
NUC1 1H
P0 15.00 usec
P1 15.00 usec
PL1 2.50 dB
PL1W 14.83164406 W
SFO1 500.1313530 MHz

GRADIENT CHANNEL
GPNAM1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec
ND0 1
TD 128
SFO1 500.1314 MHz
FIDRES 19.434080 Hz
SW 4.974 ppm
FnMODE QF
SI 1024
SF 500.1299930 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 500.1299930 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

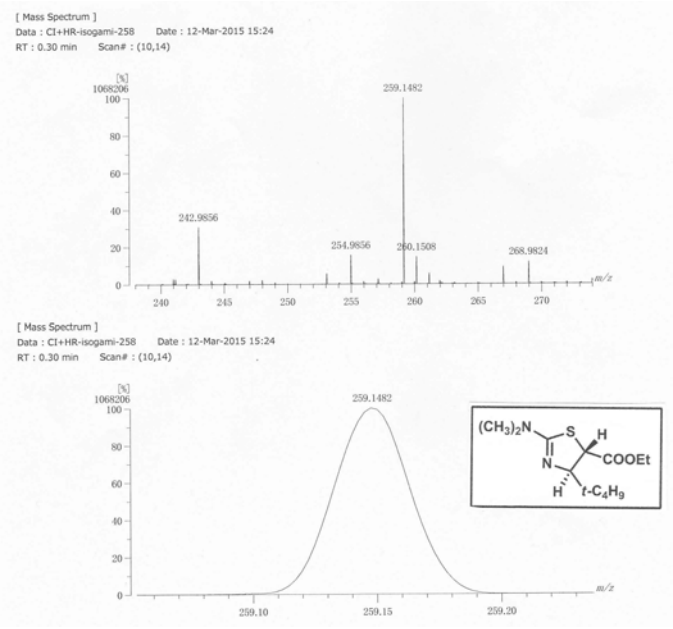

NOESY
BRUKER
NAME isogami
EXPNO 11081
PROCNO 1
Date_ 20140313
Time 15.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyph
TD 2048
SOLVENT CDCl3
NS 4
DS 4
SWH 2487.562 Hz
FIDRES 1.214630 Hz
AQ 0.4116980 sec
RG 114
DW 201.000 usec
DE 6.50 usec
TE 294.6 K
D0 0.00018190 sec
D1 1.78905594 sec
D8 0.30000001 sec
IN0 0.00040200 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PL1 2.50 dB
PL1W 14.83164406 W
SFO1 500.1313530 MHz
ND0 1
TD 256
SFO1 500.1314 MHz
FIDRES 9.717040 Hz
SW 4.974 ppm
FnMODE States-TPPI
SI 1024
SF 500.1299930 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 500.1299930 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
ppm
5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


NOESY
BRUKER
NAME isogami
EXPNO 11081
PROCNO 1
Date_ 20140313
Time 15.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyph
TD 2048
SOLVENT CDCl3
NS 4
DS 4
SWH 2487.562 Hz
FIDRES 1.214630 Hz
AQ 0.4116980 sec
RG 114
DW 201.000 usec
DE 6.50 usec
TE 294.6 K
D0 0.00018190 sec
D1 1.78905594 sec
D8 0.30000001 sec
IN0 0.00040200 sec
CHANNEL f1
NUC1 1H
P1 15.00 usec
PL1 2.50 dB
PL1W 14.83164406 W
SFO1 500.1313530 MHz
ND0 1
TD 256
SFO1 500.1314 MHz
FIDRES 9.717040 Hz
SW 4.974 ppm
FnMODE States-TPPI
SI 1024
SF 500.1299930 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 500.1299930 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
ppm
3.6 3.8 4.0 4.2 4.4 4.6 4.8 5.0
1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 ppm

^{13}C NMR

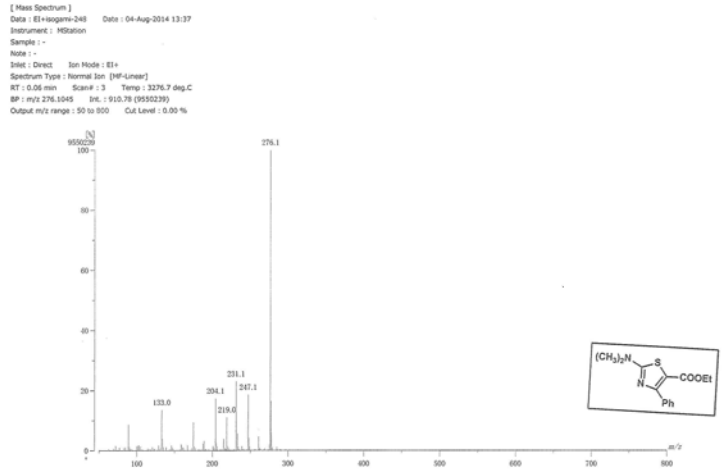


HRMS



19b ($R^1 = NMe_2$, $R^2 = C_6H_5$)

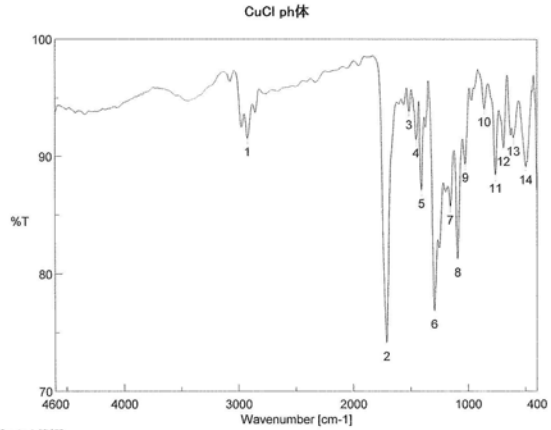
Mass spectrum



[Mass Spectrum]
Data : EI+isogami-248 Date : 04-Aug-2014 13:37
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.06 min Scan# : 3 Temp : 3276.7 deg.C
BP : m/z 276.1045 Int. : 910.78 (9550239)
Output m/z range : 50.0000 to 800.0000 Cut Level : 2.00 %

m/z	Int.	Norm.	
89.0439	80.08	8.79	839695
132.9940	123.94	13.61	1299615
133.9957	35.80	3.93	375423
159.0634	18.99	2.09	199151
175.0486	86.71	9.52	909215
188.0252	21.59	2.37	226367
189.0575	29.83	3.27	312767
204.0678	158.36	17.39	1660575
205.0628	24.42	2.68	256031
215.0279	35.96	3.95	377071
219.0378	101.48	11.14	1064095
231.0641	209.90	23.05	2200991
232.0731	32.67	3.59	342575
233.0488	52.30	5.74	548447
247.0684	169.77	18.64	1780127
248.0640	37.94	4.17	397791
261.0621	42.73	4.69	448031
276.1045	910.78	100.00	9550239
277.1048	150.38	16.51	1576863
278.0988	54.80	6.02	574591

IR spectrum

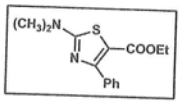


[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

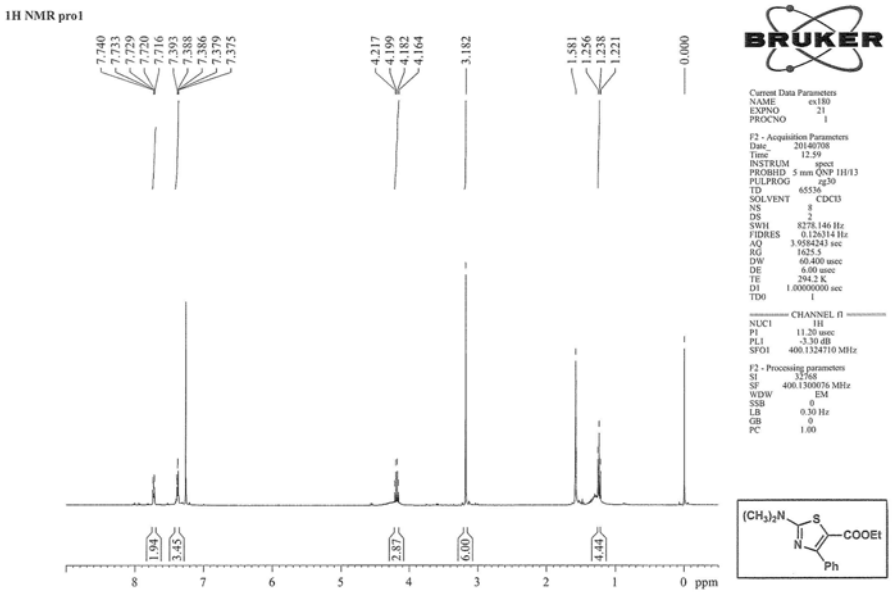
[データ情報]		[測定情報]	
作成日時	2014/09/08 14:46	機種名	FT/IR-4200typeA
更新日時	2014/09/08 14:46	シリアル番号	B061661018
データタイプ	等間隔データ	光源	標準光源
横軸	Wavenumber [cm-1]	検出器	TGS
縦軸	%T	積算回数	16
スタート	399.193 cm-1	分解	4 cm-1
エンド	4600.36 cm-1	ゼロフィリング	On
データ間隔	0.964233 cm-1	アポダイゼーション	Cosine
データ数	4358	ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2926.5	91.5462	2	1711.5	74.1559	3	1517.7	93.8671
4	1454.1	91.4511	5	1408.8	87.1358	6	1294.0	76.8907
7	1156.1	85.7237	8	1092.5	81.281	9	1025.9	89.3422
10	861.1	94.104	11	762.7	88.4322	12	691.4	90.7336
13	605.5	91.5991	14	497.5	89.1593			



^{1}H NMR



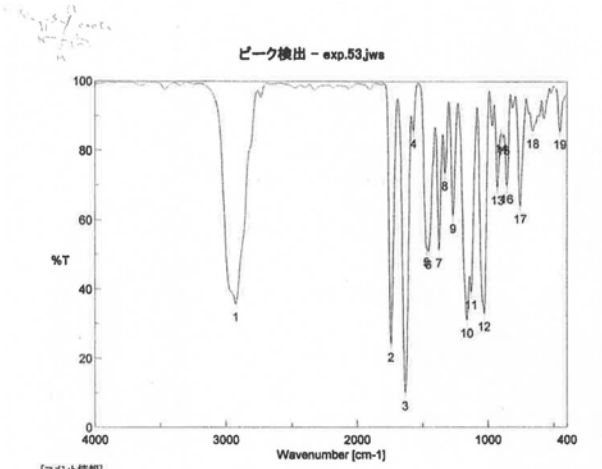
***cis*-18e (R^1 = NMe_2, R^2 = Mes)**

Mass spectrum

[Mass Spectrum]
Data : EI+nishinomiya-320-3 Date : 21-Feb-2017 16:43
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.33 min Scan# : 52 Temp : 3276.7 deg.C
BP : m/z 247.1086 Int. : 1404.92 (14731663)
Output m/z range : 50.0000 to 800.0000 Cut Level : 2.00 %

m/z	Int.	Norm.	
71.2028	32.04	2.28	335951
88.1702	389.76	27.74	4086911
91.1564	40.53	2.88	424975
103.9909	104.28	7.42	1093503
105.0000	78.28	5.57	820863
115.0072	67.30	4.79	705679
116.0202	42.51	3.03	445775
117.0300	41.39	2.95	434047
128.0253	85.02	6.05	891535
129.0313	86.17	6.13	903567
130.0407	55.83	3.97	585439
131.0468	72.77	5.18	763023
143.0470	75.72	5.39	793999
144.0489	75.89	5.40	795791
145.0535	57.22	4.07	600015
146.0546	98.99	7.05	1037967
147.0296	45.03	3.21	472223
157.0527	28.41	2.02	297855
158.0613	471.06	33.53	4939407
159.0661	91.08	6.48	955023
161.0084	40.55	2.89	425199
162.0216	84.95	6.05	890787
163.0226	39.33	2.80	412415
172.0714	36.73	2.61	385183
173.0377	29.45	2.10	308799
175.0253	67.23	4.79	704911
176.0312	93.40	6.65	979343
177.0391	45.12	3.21	473119
187.0913	206.70	14.71	2167439
188.0886	30.07	2.14	315295
190.0344	51.65	3.68	541599
201.0935	253.16	18.02	2654607
202.1082	68.59	4.88	719247
247.1086	1404.92	100.00	14731663
248.1064	230.43	16.40	2416271
249.1055	79.63	5.67	834959
275.1090	75.88	5.40	795711
305.1145	45.24	3.22	474415
320.1548	858.53	61.11	9002303
321.1561	170.00	12.10	1782591
322.1370	55.57	3.96	582735

IR spectrum

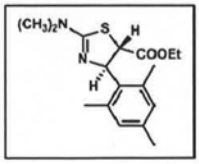


[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

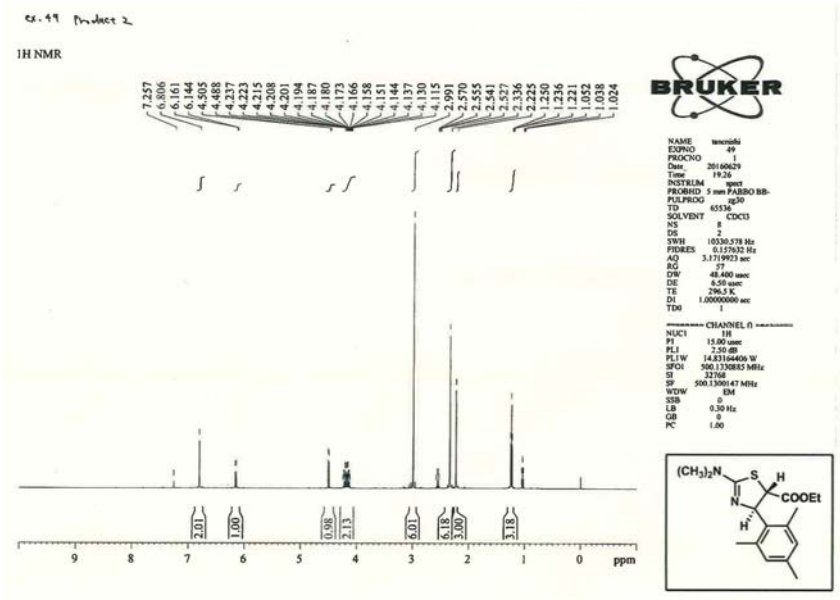
[データ情報]		[測定情報]	
作成日時	2016/11/18 20:31	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	349.053 cm-1	積算回数	Auto (100)
エンド	7800.85 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	7729	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2924.5	35.6989	2	1739.5	24.1485	3	1633.4	9.97121
4	1570.7	85.912	5	1468.5	51.8791	6	1453.1	50.9636
7	1373.1	51.3292	8	1328.7	73.5788	9	1266.0	61.3229
10	1160.0	31.0913	11	1127.2	39.1832	12	1028.8	32.9316
13	927.8	69.4498	14	899.6	84.4695	15	864.2	83.8891
16	856.2	69.8325	17	756.9	84.0566	18	660.5	85.8468
19	454.2	85.6775						



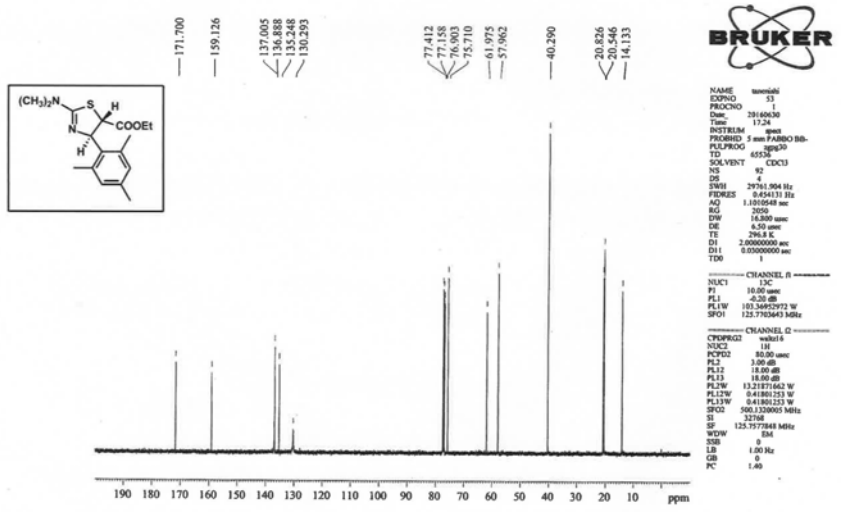
^{1}H NMR



^{13}C NMR

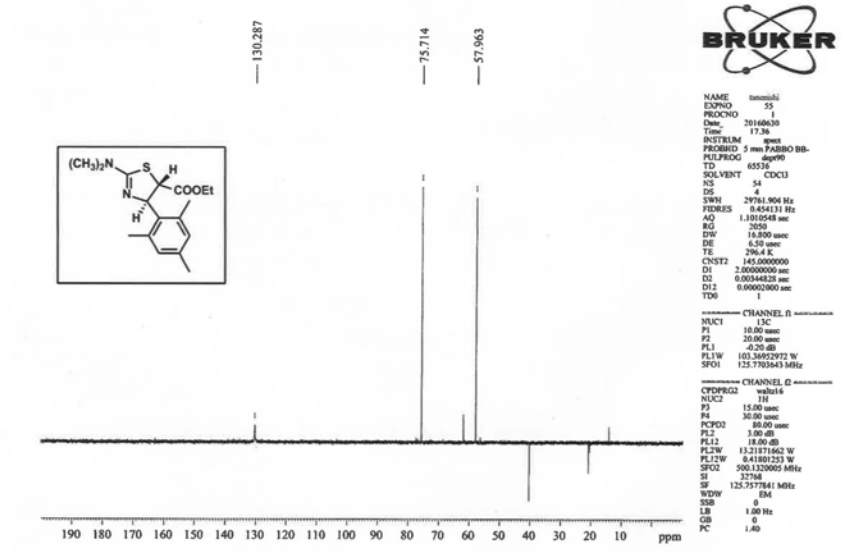
۹۵۰۹۹ (۲)

13C NMR CPD



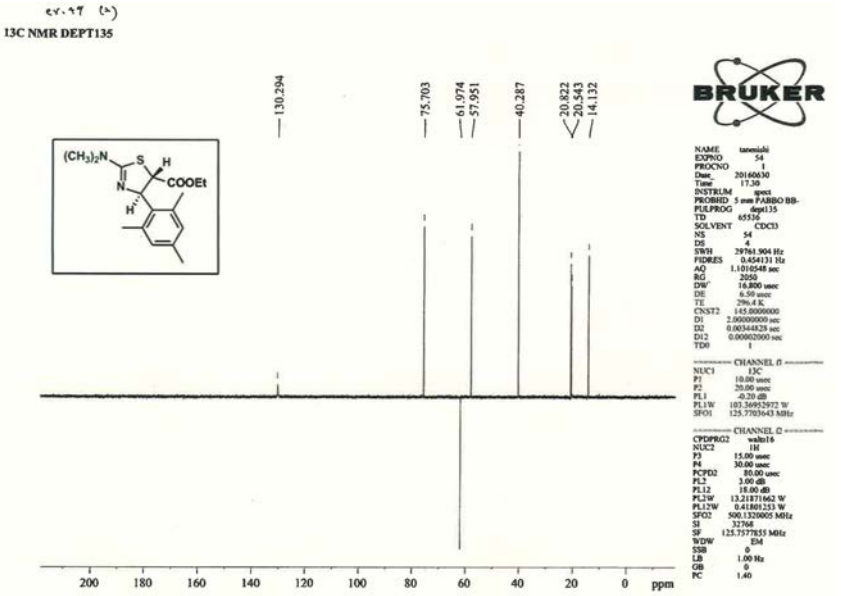
۶۷۰۹۹ (۲)

13C NMR DEPT90

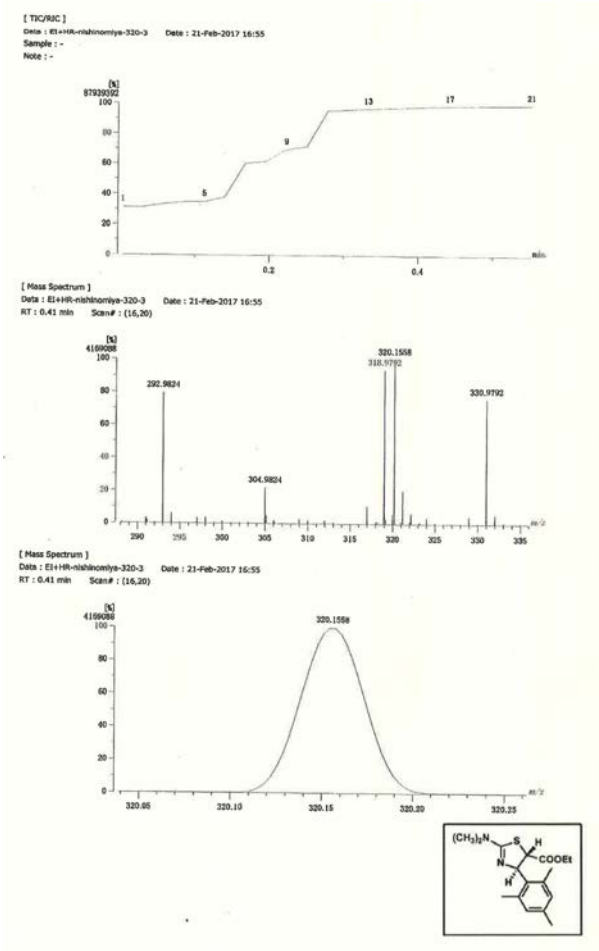


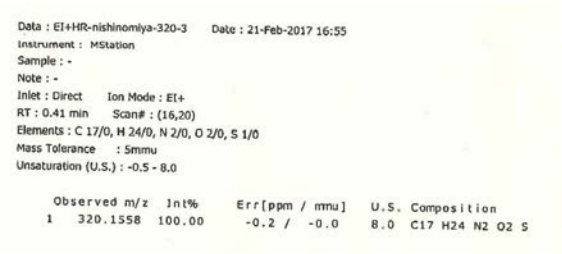
۶۷۰۹۹ (۲)

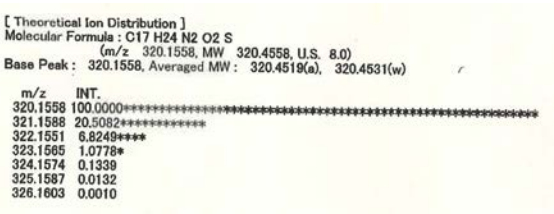
13C NMR DEPT135



HRMS

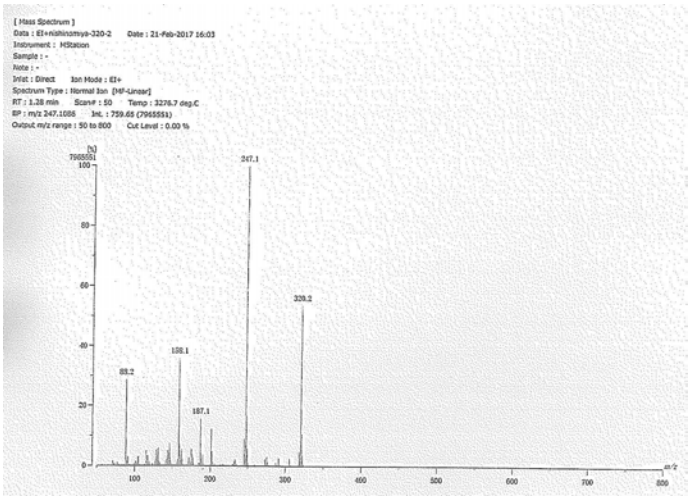






***trans*-18e ($R^1 = NMe_2$, $R^2 = Mes$)**

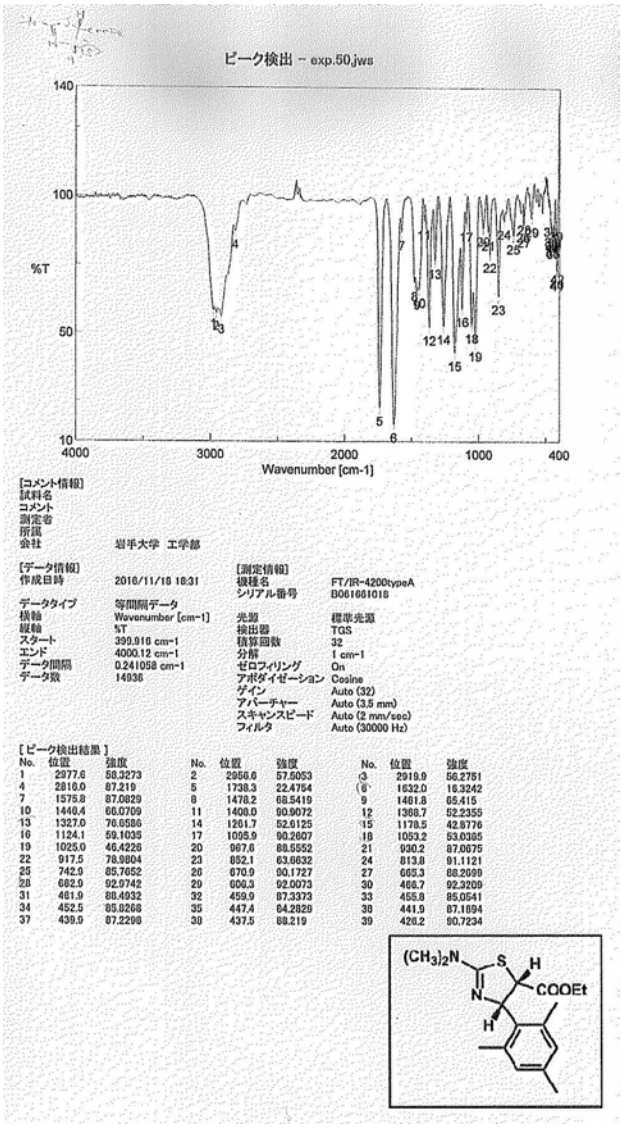
Mass spectrum



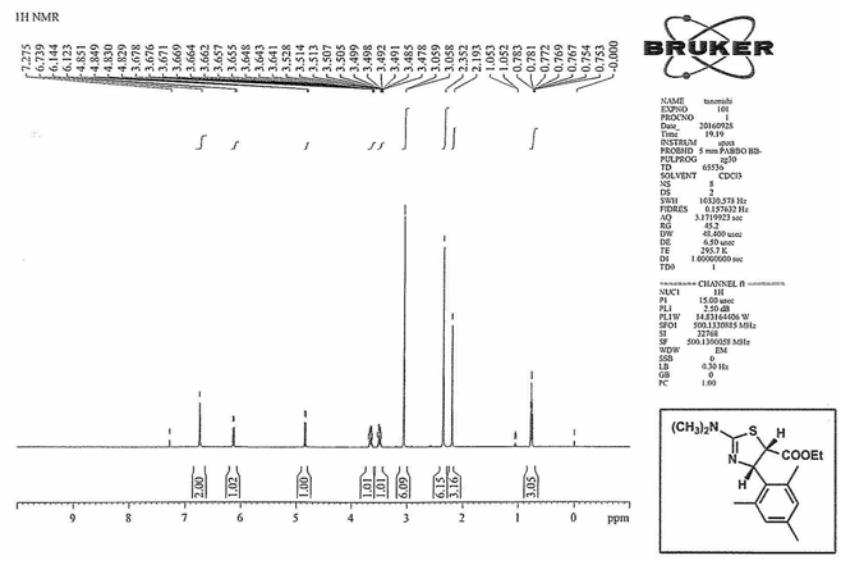
[Mass Spectrum]
Data : EI+nishinomiya-320-2 Date : 21-Feb-2017 16:03
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.28 min Scan# : 50 Temp : 3276.7 deg.C
BP : m/z 247.1086 Int. : 759.65 (7965551)
Output m/z range : 50.0000 to 800.0000 Cut Level : 2.00 %

m/z	Int.	Norm.	
88.1758	218.44	28.76	2290527
91.1620	24.74	3.26	259423
103.9969	23.06	3.04	241807
105.0061	23.45	3.09	245903
115.0137	38.96	5.13	408479
116.0202	25.45	3.35	266847
117.0365	25.30	3.33	265263
128.0320	39.69	5.22	416159
129.0380	40.48	5.33	424431
130.0407	28.65	3.77	300399
131.0536	46.41	6.11	486639
142.0424	16.19	2.13	169759
143.0541	37.36	4.92	391775
144.0560	39.68	5.22	416063
145.0607	32.42	4.27	339983
146.0617	57.76	7.60	605679
147.0153	19.89	2.62	208543
157.0527	17.37	2.29	182159
158.0687	273.35	35.96	2866271
159.0736	52.95	6.97	555183
161.0084	19.19	2.53	201247
162.0216	41.70	5.49	437279
163.0301	17.51	2.31	183615
172.0714	21.77	2.87	228303
175.0331	42.38	5.58	444367
176.0390	28.18	3.71	295487
177.0391	19.97	2.63	209359
187.0994	119.61	15.75	1254239
188.0967	18.20	2.40	190847
190.0508	29.34	3.86	307663
201.1101	94.13	12.39	986975
202.1165	37.44	4.93	392607
233.1033	18.21	2.40	190943
245.0922	69.46	9.15	728687
246.1038	20.17	2.66	211487
247.1086	759.65	100.00	7965551
248.1156	127.33	16.76	1335151
249.1147	44.03	5.80	461727
273.0980	18.30	2.41	191935
275.1186	23.54	3.10	246815
291.1122	20.32	2.67	213023
305.1346	19.83	2.61	207983
318.1464	36.62	4.82	383967
319.1442	21.31	2.81	223471
320.1548	407.32	53.62	4271007
321.1664	80.92	10.65	848543
322.1474	26.89	3.54	281999

IR spectrum

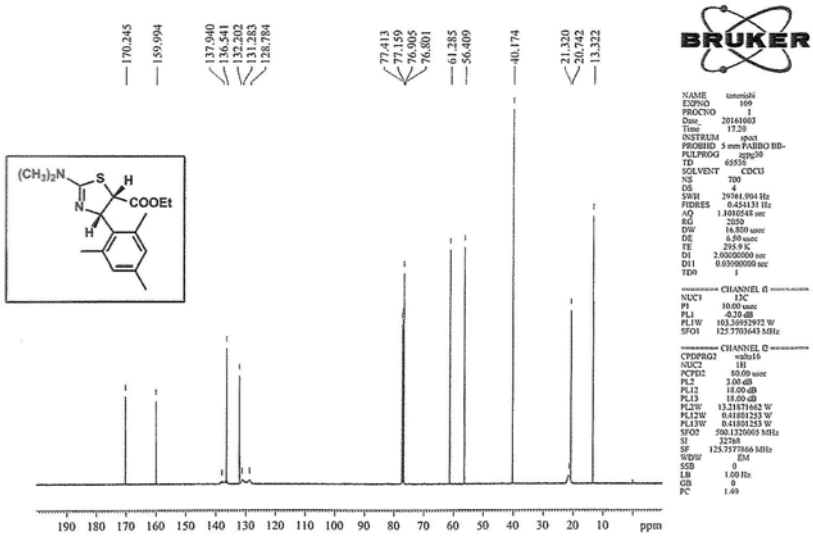


^{1}H NMR



^{13}C NMR

13C NMR CPD



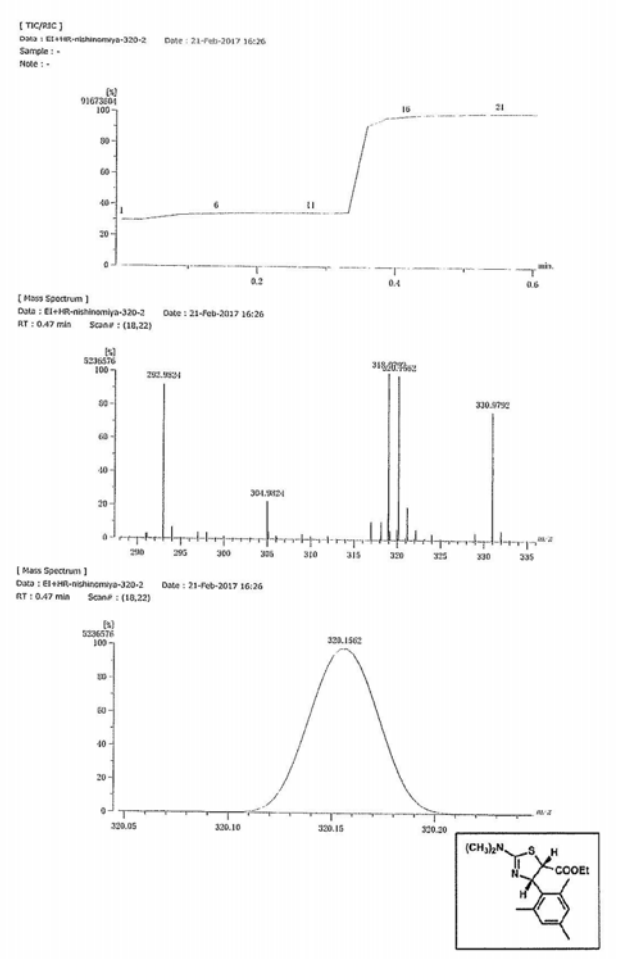
BRUKER

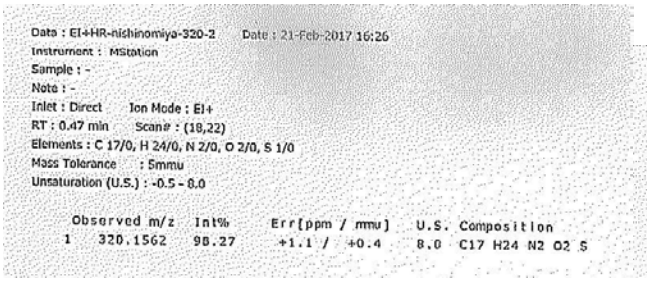
NAME tanemishi
EXPNO 109
PROCNO 1
Date_ 20161003
Time 17.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1030545 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -0.20 dB
PL1W 103.36952972 W
SFO1 125.77033643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 18.00 dB
PL13 18.00 dB
PL2W 13.21671662 W
PL12W 0.41801253 W
PL13W 0.41801253 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577866 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

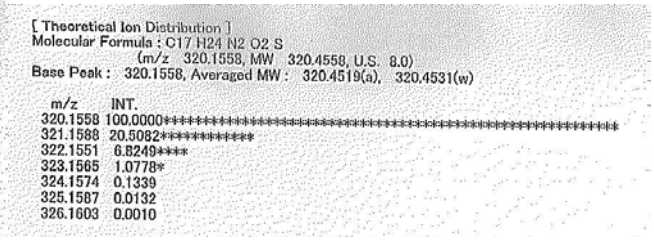
HRMS





Data : EI+HR-nishinomiya-320-2 Date : 21-Feb-2017 16:26
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.47 min Scan# : (18,22)
Elements : C 17/0, H 24/0, N 2/0, O 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 8.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	320.1562	98.27	+1.1 / +0.4	8.0	C17 H24 N2 O2 S

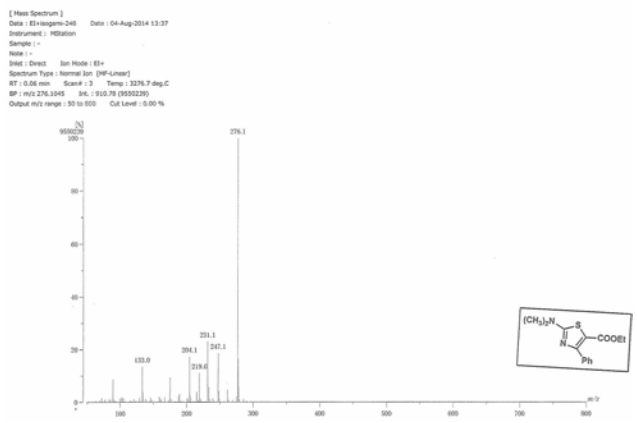


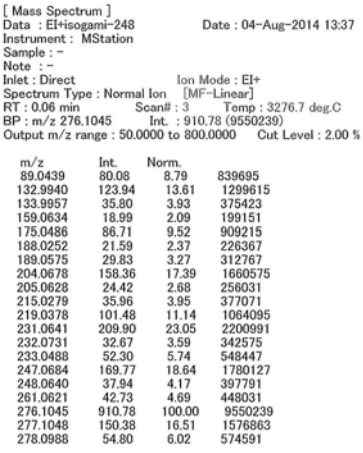
[Theoretical Ion Distribution]
Molecular Formula : C17 H24 N2 O2 S
(m/z 320.1558, MW 320.4558, U.S. 8.0)
Base Peak : 320.1558, Averaged MW : 320.4519(a), 320.4531(w)

m/z	INT.
320.1558	100.0000
321.1588	20.5082
322.1551	6.8249
323.1565	1.0778
324.1574	0.1339
325.1587	0.0132
326.1603	0.0010

19b ($R^1 = NMe_2$, $R^2 = C_6H_5$, $R^3 = CO_2Me$)[16]:

Mass spectrum

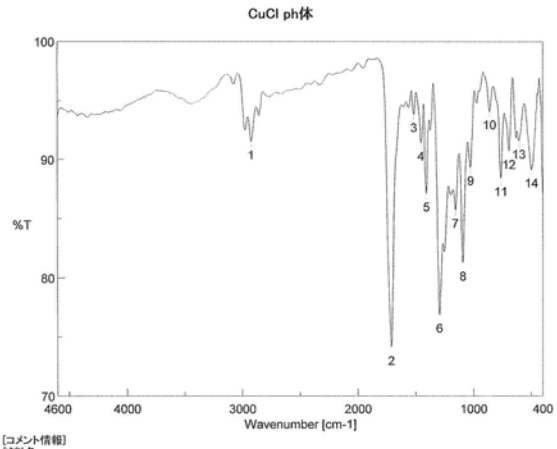




[Mass Spectrum]
Data : EI+isogami-248 Date : 04-Aug-2014 13:37
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.06 min Scan# : 3 Temp : 3276.7 deg.C
BP : m/z 276.1045 Int. : 910.78 (9550239)
Output m/z range : 50.0000 to 800.0000 Cut Level : 2.00 %

m/z	Int.	Norm.	
89.0439	80.08	8.79	839695
132.9940	123.94	13.61	1299615
133.9957	35.80	3.93	375423
159.0634	18.99	2.09	199151
175.0486	86.71	9.52	909215
188.0252	21.59	2.37	226367
189.0575	29.83	3.27	312767
204.0678	158.36	17.39	1660575
205.0628	24.42	2.68	256031
215.0279	35.96	3.95	377071
219.0378	101.48	11.14	1064095
231.0641	209.90	23.05	2200991
232.0731	32.67	3.59	342575
233.0488	52.30	5.74	548447
247.0684	169.77	18.64	1780127
248.0640	37.94	4.17	397791
261.0621	42.73	4.69	448031
276.1045	910.78	100.00	9550239
277.1048	150.38	16.51	1576863
278.0988	54.80	6.02	574591

IR spectrum

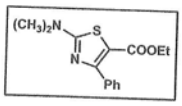


[コメント情報]
試料名
コメント
測定者
所属
会社　岩手大学　工学部

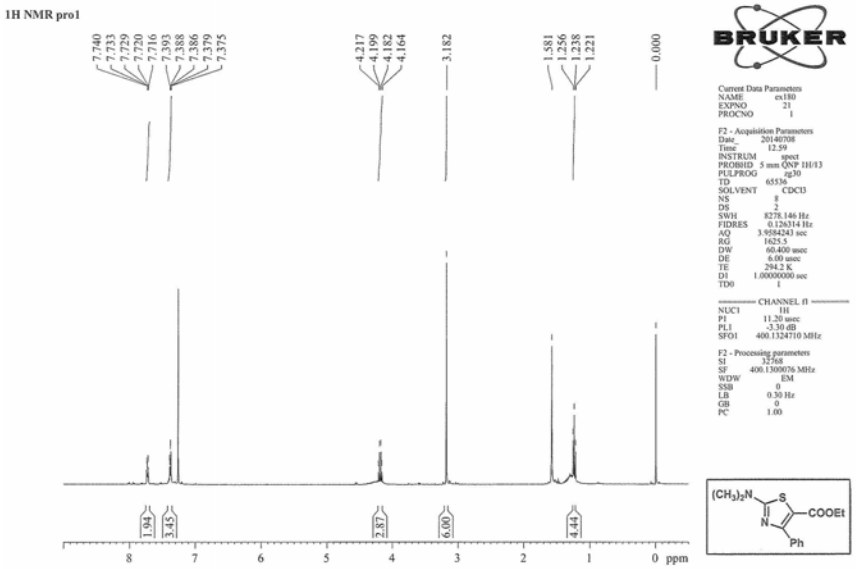
[データ情報]		[測定情報]	
作成日時	2014/09/08 14:46	機種名	FT/IR-4200typeA
更新日時	2014/09/08 14:46	シリアル番号	B061661018
データタイプ	等間隔データ	光源	標準光源
横軸	Wavenumber [cm-1]	検出器	TGS
縦軸	%T	積算回数	16
スタート	399.193 cm-1	分解	4 cm-1
エンド	4600.36 cm-1	ゼロフィリング	On
データ間隔	0.964233 cm-1	アポダイゼーション	Cosine
データ数	4358	ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2926.5	91.5462	2	1711.5	74.1559	3	1517.7	93.8671
4	1454.1	91.4511	5	1408.8	87.1358	6	1294.0	76.8907
7	1156.1	85.7237	8	1092.5	81.281	9	1025.9	89.3422
10	861.1	94.104	11	762.7	88.4322	12	691.4	90.7336
13	605.5	91.5991	14	497.5	89.1593			

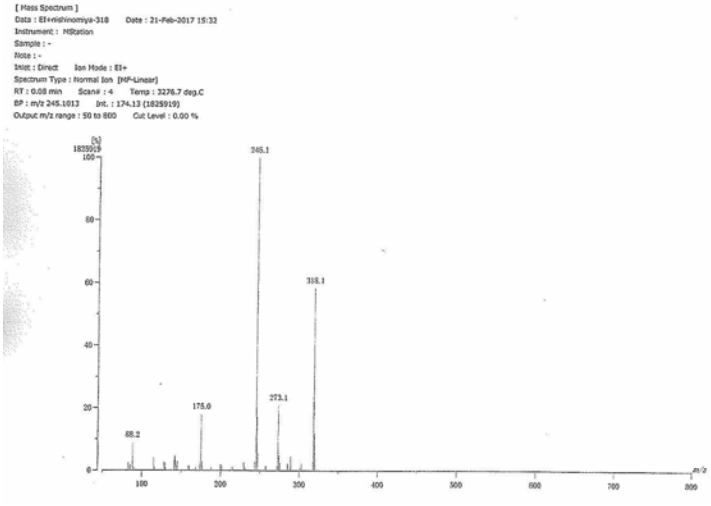


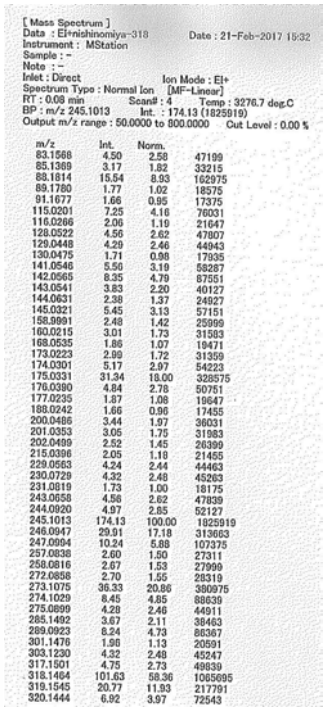
^{1}H NMR



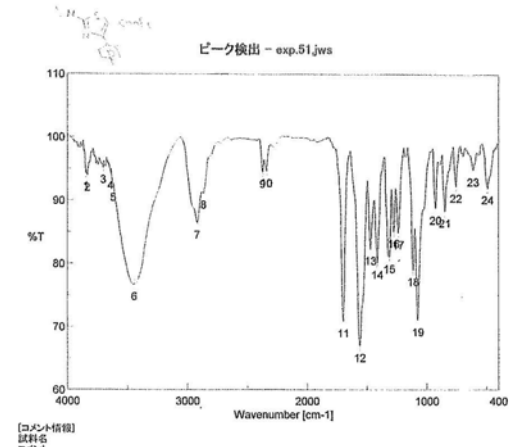
19e (R^1 = NMe_2, R^2 = Mes, R^3 = CO_2Me):

Mass spectrum





IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]
作成日時 2018/11/18 10:19

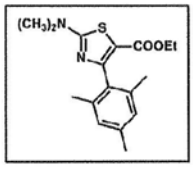
データタイプ 等間隔データ
横軸 Wavenumber [cm-1]
縦軸 %T
スタート 349.053 cm-1
エンド 7800.05 cm-1
データ間隔 0.964233 cm-1
データ数 7729

[測定情報]
機種名 FT/IR-4200typeA
シリアル番号 B061061016

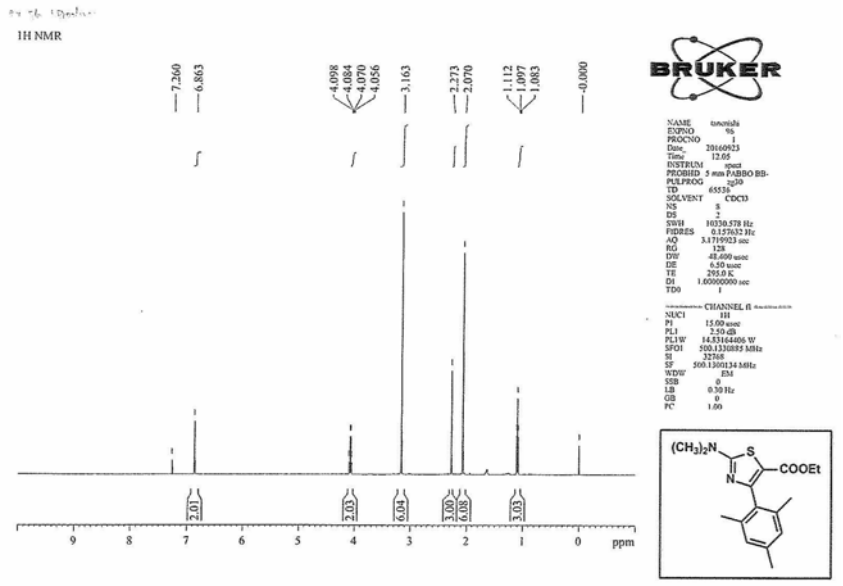
光源 標準光源
検出器 TGS
積算回数 Auto (124)
分解 4 cm-1
ゼロフィリング On
アポダイゼーション Cosine
ゲイン Auto (8)
アパーチャー Auto (7.1 mm)
スキャンスピード Auto (2 mm/sec)
フィルタ Auto (30000 Hz)

[ピーク検出結果]

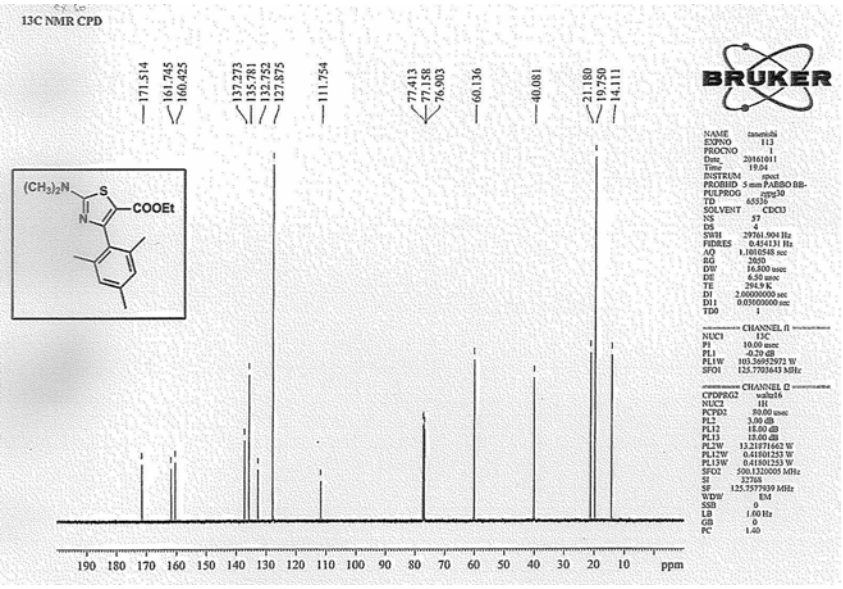
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3845.4	94.1535	2	3634.8	93.9205	3	3702.7	95.1775
4	3641.0	94.2503	5	3620.7	92.3711	6	3443.3	78.6935
7	2917.8	86.4279	8	2865.7	91.17	9	2372.0	94.5243
10	2339.2	94.6345	11	1698.0	70.8792	12	1560.1	66.9732
13	1469.5	92.3744	14	1412.6	80.1808	15	1312.3	91.067
16	1275.7	85.0921	17	1238.1	84.9021	18	1113.7	79.0476
19	1075.1	71.0507	20	926.6	88.761	21	848.5	88.3009
22	756.0	92.2374	23	611.3	94.8438	24	491.8	92.0046



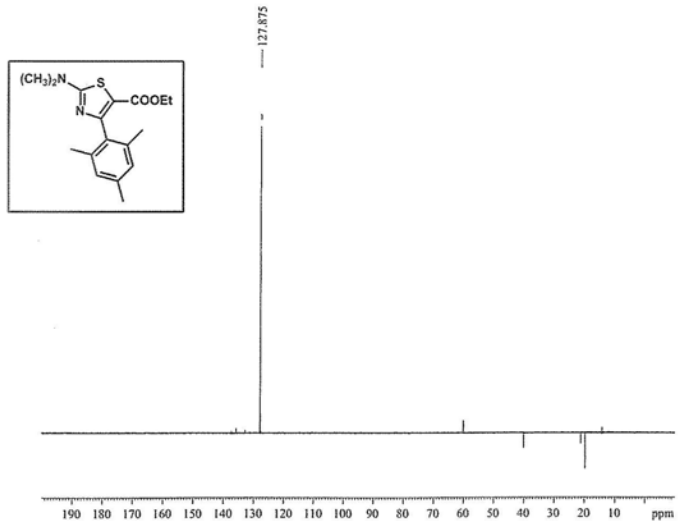
^{1}H NMR


1H NMR
7.260
6.863
4.098
4.084
4.070
4.056
3.163
2.273
2.070
1.112
1.097
1.083
0.000
2.01
2.05
6.04
3.00
6.08
3.03
9 8 7 6 5 4 3 2 1 0 ppm
BRUKER
(CH3)2N
S
N
COOEt

^{13}C NMR


13C NMR CPD
171.514
161.745
160.425
137.273
135.781
132.752
127.875
111.754
77.413
77.158
76.903
60.136
40.081
21.180
19.750
14.111
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
(CH3)2N
S
N
COOEt

13C NMR DEPT90



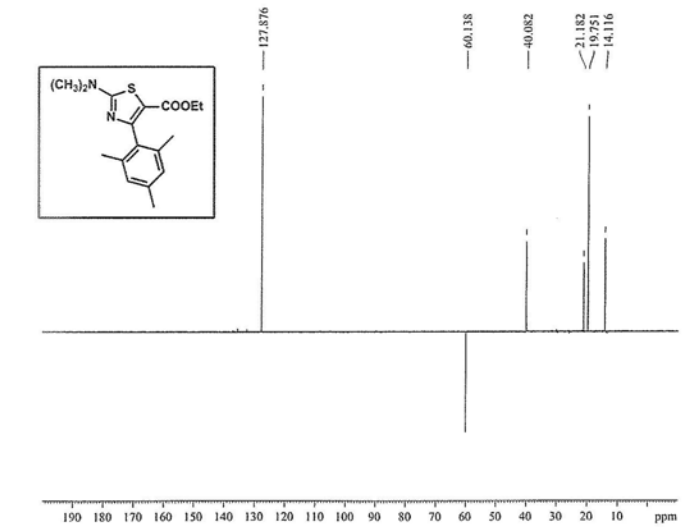
BRUKER

NAME tanavishi
EXPNO 115
PROCNO 1
Date_ 20161011
Time 19.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 20
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 294.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PL1 -0.20 dB
PL1W 103.36952972 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PL2 3.00 dB
PL12 18.00 dB
PL2W 13.21871662 W
PL12W 0.41801253 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577939 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C NMR DEPT135



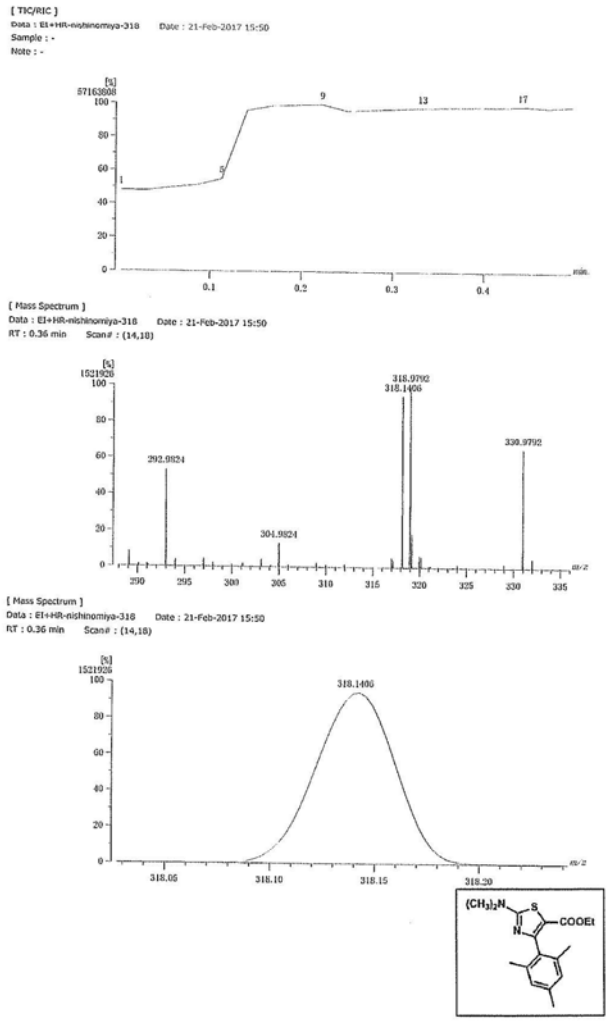
BRUKER

NAME tanavishi
EXPNO 114
PROCNO 1
Date_ 20161011
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 50
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 294.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PL1 -0.20 dB
PL1W 103.36952972 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PL2 3.00 dB
PL12 18.00 dB
PL2W 13.21871662 W
PL12W 0.41801253 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577939 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS



Data : EI+HR-nishinomiya-318 Date : 21-Feb-2017 15:50
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.36 min Scan# : (14,18)
Elements : C 17/0, H 22/0, N 2/0, O 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 9.0

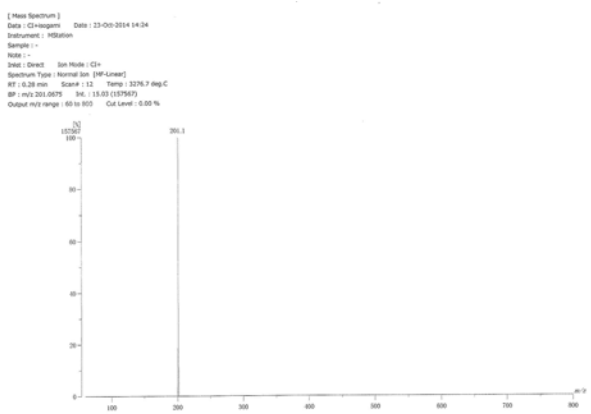
	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	318.1406	94.64	+1.3 / +0.4	9.0	C17 H22 N2 O2 S

[Theoretical Ion Distribution]
Molecular Formula : C17 H22 N2 O2 S
(m/z 318.1402, MW 318.4399, U.S. 9.0)
Base Peak : 318.1402, Averaged MW : 318.4362(a), 318.4374(w)

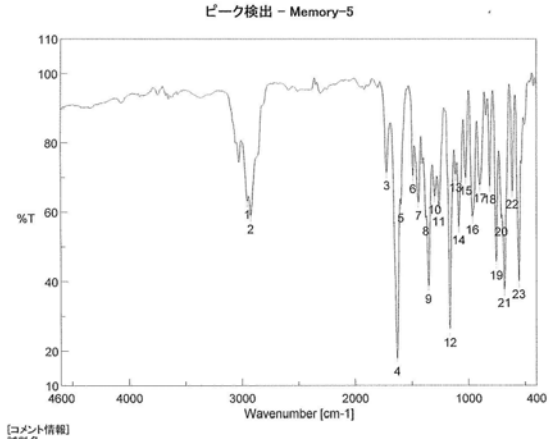
m/z	INT.
318.1402	100.0000
319.1432	20.5082
320.1395	6.8249
321.1409	1.0778
322.1417	0.1339
323.1430	0.0132
324.1447	0.0010

19f ($R^1 = NMe_2$, $R^2 = H$, $R^3 = CO_2Me$):

Mass spectrum

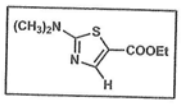


IR spectrum



[コメント情報]
試料名
コメント
測定者
所属
会社 岩手大学 工学部

[データ情報]		[測定情報]	
作成日時	2014/10/27 19:09	機種名	FT/IR-4200typeA
		シリアル番号	B061661018
データタイプ	等間隔データ		
横軸	Wavenumber [cm-1]	光源	標準光源
縦軸	%T	検出器	TGS
スタート	399.193 cm-1	積算回数	16
エンド	4600.36 cm-1	分解	4 cm-1
データ間隔	0.964233 cm-1	ゼロフィリング	On
データ数	4358	アポダイゼーション	Cosine
		ゲイン	Auto (8)
		アパーチャー	Auto (7.1 mm)
		スキャンスピード	Auto (2 mm/sec)
		フィルタ	Auto (30000 Hz)

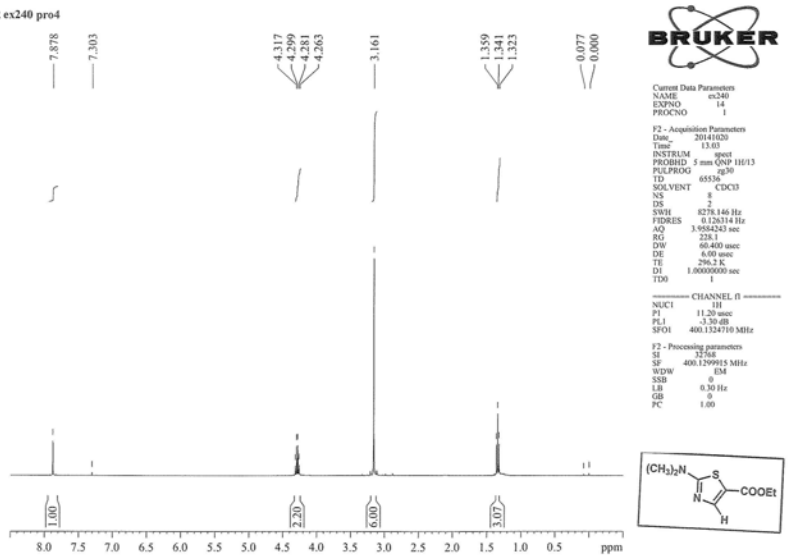


[ピーク検出結果]

No.	位置	強度	No.	位置	強度	No.	位置	強度
1	2956.3	63.1268	2	2925.5	58.9367	3	1724.1	71.4898
4	1630.5	17.9949	5	1598.7	62.1295	6	1491.7	70.5143
7	1443.5	62.8238	8	1377.9	58.3675	9	1353.8	38.8529
10	1299.8	64.5528	11	1261.2	61.0764	12	1164.8	26.3175
13	1114.7	70.9133	14	1086.7	55.8016	15	1025.0	69.9874
16	965.2	58.7593	17	900.6	67.8387	18	813.8	67.4737
19	756.0	45.634	20	710.6	58.1548	21	682.7	37.765
22	614.2	66.0755	23	554.4	40.2036			

^{1}H NMR

1H NMR ex240 pro4



BRUKER

Current Data Parameters
NAME ex240
EXPNO 14
PROCNO 1

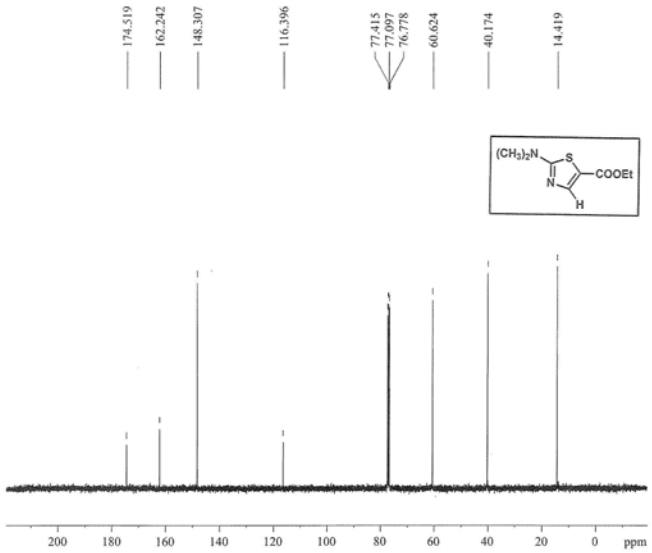
F2 - Acquisition Parameters
Date_ 20141020
Time 13.03
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 228.1
DW 60.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

========== CHANNEL f1 ==========
NUC1 1H
P1 11.20 usec
PL1 -3.30 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299915 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR

13C NMR ex240 CPD



BRUKER

Current Data Parameters
NAME ex240
EXPNO 21
PROCNO 1

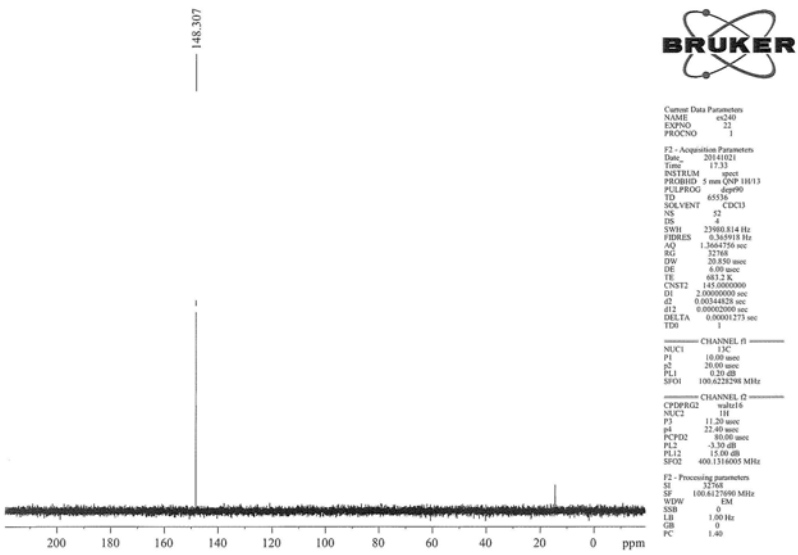
F2 - Acquisition Parameters
Date_ 20141021
Time 17.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 231
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

========== CHANNEL f1 ==========
NUC1 13C
P1 10.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR ex240 dept90



Current Data Parameters
NAME ex240
EXPNO 22
PROCNO 1

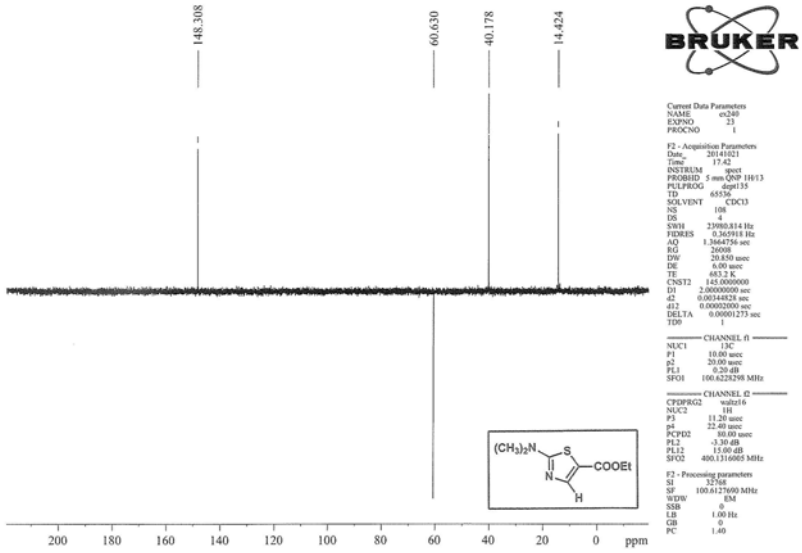
F2 - Acquisition Parameters
Date_ 20141021
Time 17.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 52
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

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

13C NMR ex240 dept135



Current Data Parameters
NAME ex240
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141021
Time 17.42
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 108
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 26000
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001273 sec
TD0 1

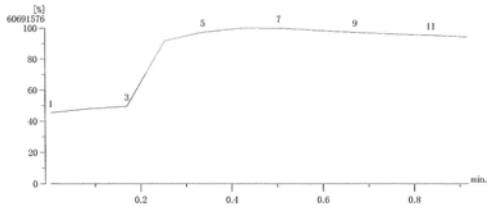
CHANNEL f1
NUC1 13C
P1 10.00 usec
p2 20.00 usec
PL1 0.20 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 11.20 usec
p4 22.40 usec
PCPD2 80.00 usec
PL2 -3.30 dB
PL12 15.00 dB
SFO2 400.1316005 MHz

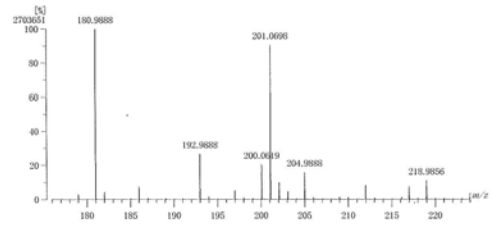
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS

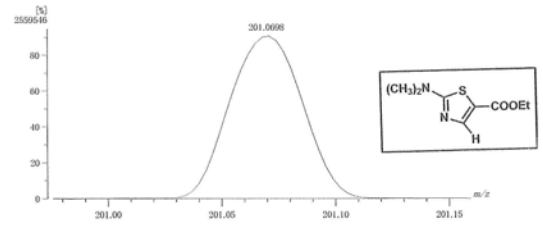
[TIC/RIC]
Data : CI+HR-isogami Date : 23-Oct-2014 15:07
Sample : -
Note : -



[Mass Spectrum]
Data : CI+HR-isogami Date : 23-Oct-2014 15:07
RT : 0.50 min Scan# : (7,11)



[Mass Spectrum]
Data : CI+HR-isogami Date : 23-Oct-2014 15:07
RT : 0.50 min Scan# : (7,11)



Data : CI+HR-isogami Date : 23-Oct-2014 15:07
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : CI+
RT : 0.50 min Scan# : (7,11)
Elements : C 8/0, H 13/0, N 2/0, O 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 10.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	201.0698	90.62	+0.1 / +0.0	4.5	C8 H13 N2 O2 S

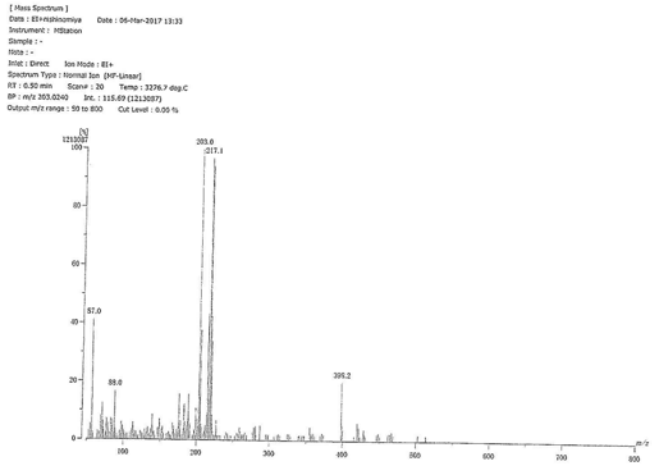
[Theoretical Ion Distribution]
Molecular Formula : C8 H13 N2 O2 S
(m/z 201.0698, MW 201.2694, U.S. 4.5)
Base Peak : 201.0698, Averaged MW : 201.2665(a), 201.2679(w)

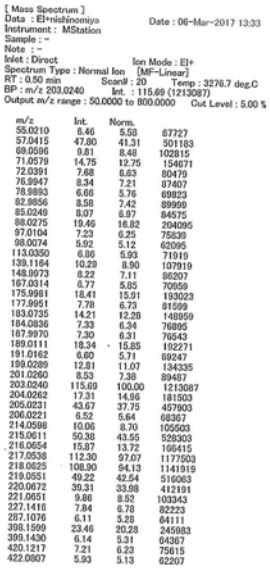
m/z	INT.
201.0698	100.0000**********
202.0724	10.4981******
203.0671	5.3287***
204.0694	0.4861
205.0689	0.0601
206.0707	0.0043
207.0719	0.0003

(7) 5-Chloro-1,3-thiazoles (20):

20a (R^1 = NMe_2, R^2 = *t*-C_4H_9)

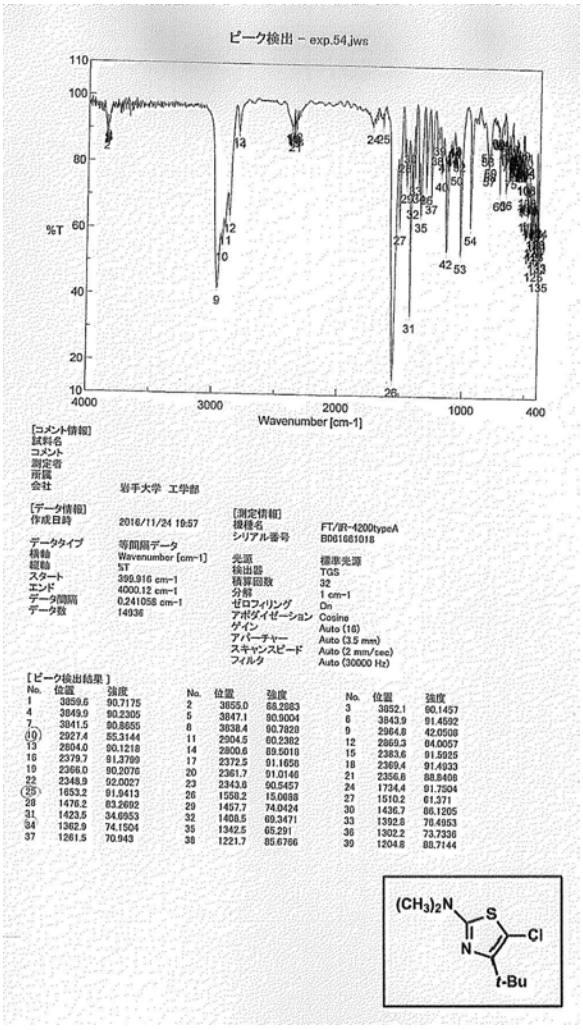
Mass spectrum





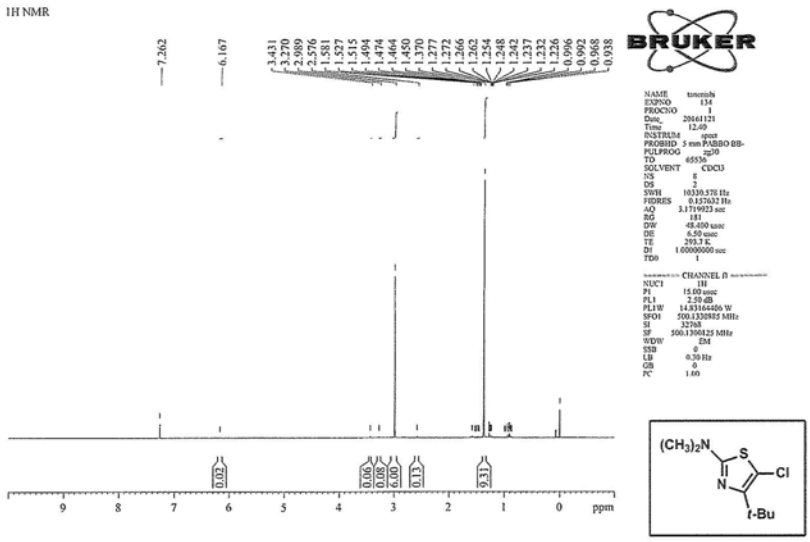
m/z	Int.	Norm.	
55.0210	6.46	5.58	67727
57.0415	47.80	41.31	501183
69.0596	9.81	8.48	102815
71.0579	14.75	12.75	154671
72.0391	7.68	6.63	80479
76.9947	8.34	7.21	87407
78.9893	6.66	5.76	69823
82.9856	8.58	7.42	89999
85.0246	8.07	6.97	84575
98.0275	19.46	16.82	204095
97.0104	7.23	6.25	75839
98.0074	5.92	5.12	62095
113.0350	6.86	5.93	71919
139.1164	10.29	8.90	107919
148.9973	8.22	7.11	86207
167.0314	6.77	5.85	70959
175.9981	18.41	15.91	193023
177.9951	7.78	6.73	81599
183.0735	14.21	12.28	148959
184.0836	7.33	6.34	76895
187.9970	7.30	6.31	76543
189.0111	18.34	15.85	192271
191.0162	6.60	5.71	69247
199.0289	12.81	11.07	134335
201.0260	8.53	7.38	89487
203.0240	115.69	100.00	1213087
204.0262	17.31	14.96	181503
205.0231	43.67	37.75	457903
206.0221	6.52	5.64	68367
214.0598	10.06	8.70	105503
215.0611	50.38	43.55	528303
216.0654	15.87	13.72	166415
217.0538	112.30	97.07	1177503
218.0625	108.90	94.13	1141919
219.0551	49.22	42.54	516063
220.0672	39.31	33.98	412191
221.0651	9.86	8.52	103343
227.1416	7.84	6.78	82223
287.1076	6.11	5.28	64111
398.1599	23.46	20.28	245983
399.1430	6.14	5.31	64367
420.1217	7.21	6.23	75615
422.0807	5.93	5.13	62207

IR spectrum

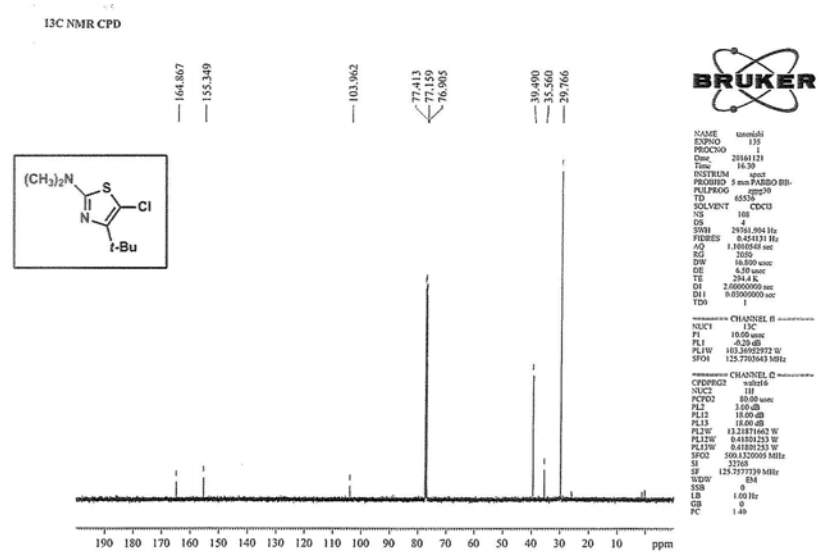


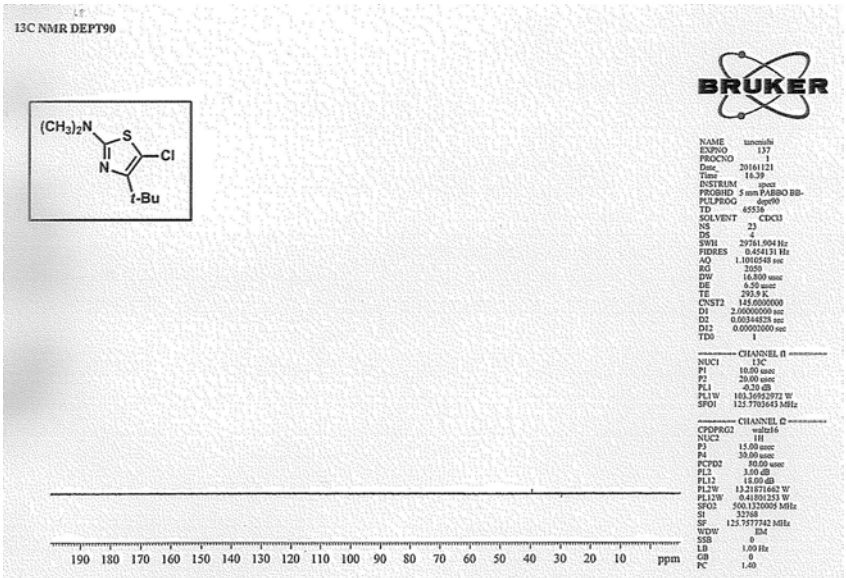
No.	位置	強度	No.	位置	強度	No.	位置	強度
1	3859.6	90.7175	2	3855.0	68.2883	3	3852.1	90.1457
4	3849.9	90.2305	5	3847.1	90.9004	6	3843.9	91.4592
7	3841.5	90.8655	8	3838.4	90.7828	9	2964.8	42.0508
10	2927.4	55.3144	11	2904.5	60.2362	12	2869.3	64.0057
13	2804.0	90.1218	14	2800.6	89.5018	15	2383.6	91.5925
16	2379.7	91.3799	17	2372.5	91.1656	18	2369.4	91.4933
19	2366.0	90.2076	20	2361.7	91.0146	21	2356.8	88.8408
22	2348.9	92.0027	23	2343.0	90.5457	24	1734.4	91.7504
25	1653.2	91.9413	26	1558.2	15.0688	27	1510.2	61.371
28	1476.2	83.2692	29	1457.7	74.0424	30	1436.7	86.1205
31	1423.5	34.6953	32	1408.5	69.3471	33	1392.8	76.4953
34	1362.9	74.1504	35	1342.5	65.291	36	1302.2	73.7336
37	1261.5	70.943	38	1221.7	85.6766	39	1204.8	88.7144

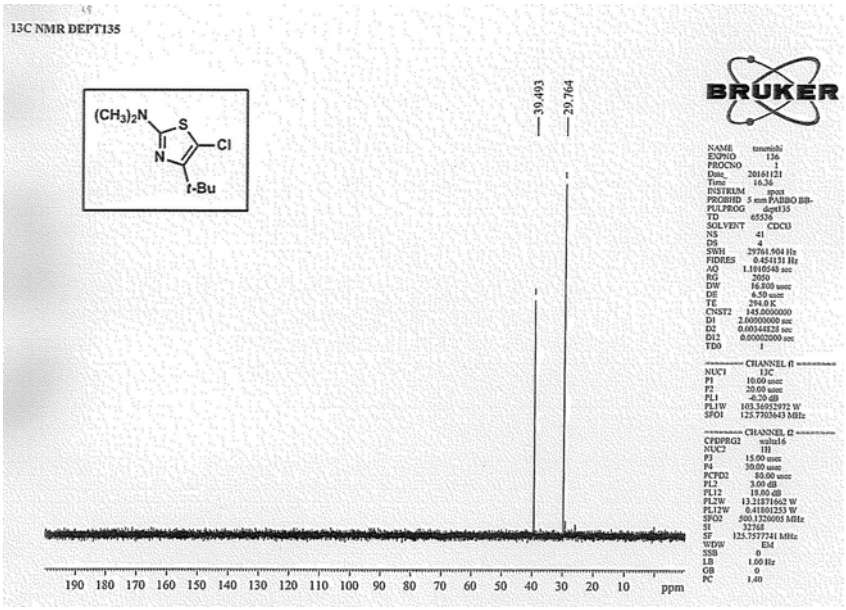
^{1}H NMR



^{13}C NMR

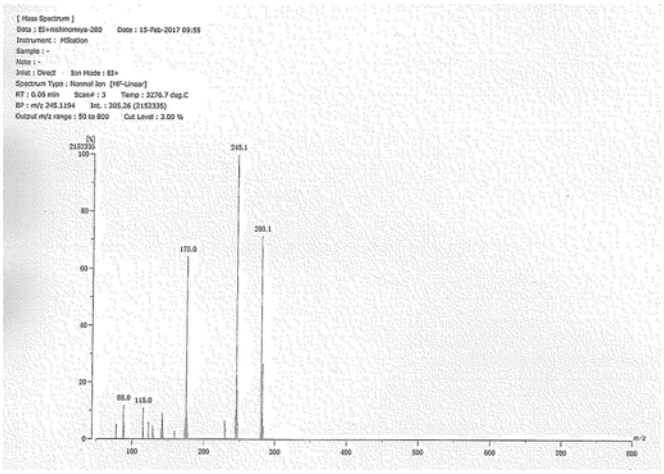






20e (R^1 = NMe_2, R^2 = Mes)

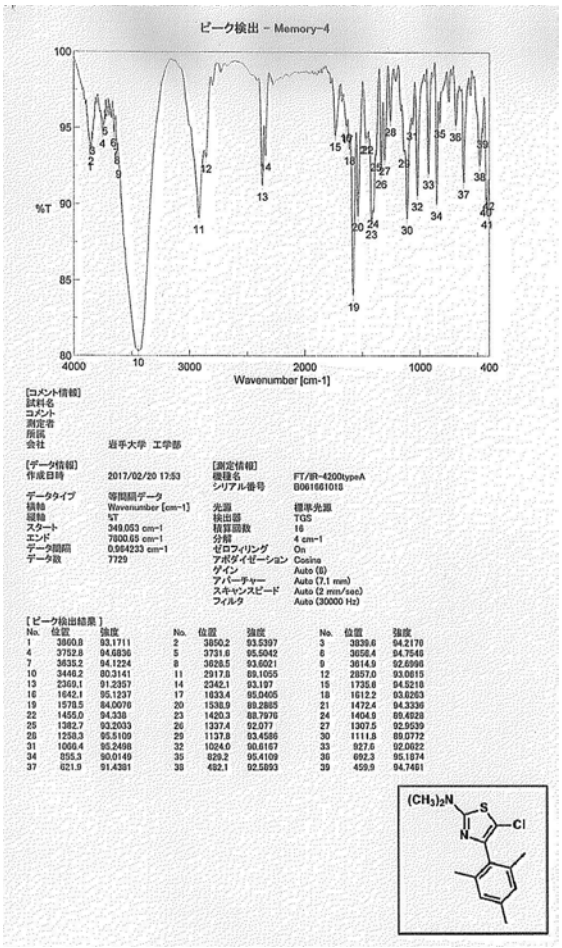
Mass spectrum



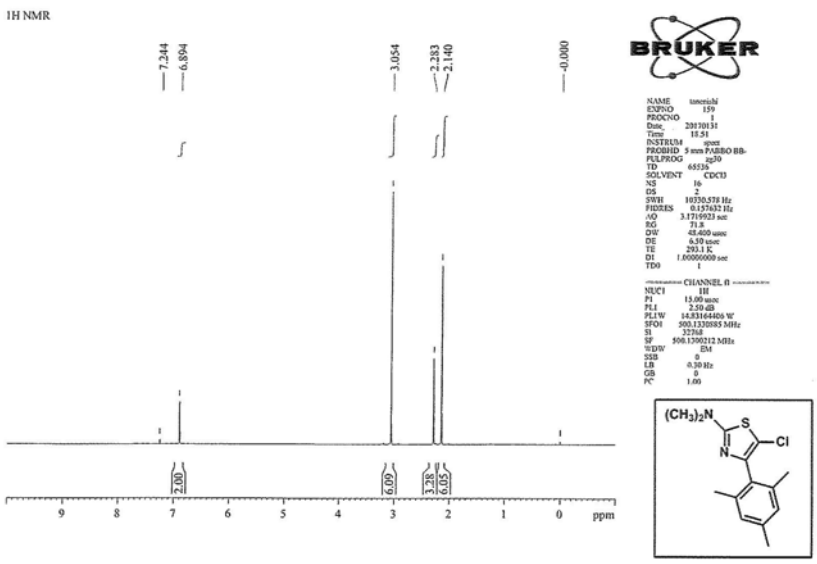
[Mass Spectrum]
Data : EI+nishinomiya-280 Date : 15-Feb-2017 09:55
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.06 min Scan# : 3 Temp : 3276.7 deg.C
BP : m/z 245.1194 Int. : 205.26 (2152335)
Output m/z range : 50.0000 to 800.0000 Cut Level : 3.00 %

m/z	Int.	Norm.	
77.9162	10.79	5.26	113135
88.0345	24.62	12.00	258175
115.0481	22.80	11.11	239039
122.5457	12.55	6.11	131551
128.0531	9.90	4.82	103791
129.0726	7.04	3.43	73823
140.0351	7.14	3.48	74847
141.0484	14.14	6.89	148303
142.0645	19.16	9.33	200879
143.0842	7.84	3.82	82207
159.0056	6.34	3.09	66463
173.0097	6.37	3.10	66815
174.0252	14.79	7.21	155135
175.0350	132.00	64.31	1384079
176.0410	18.88	9.20	197999
177.0411	11.33	5.52	118767
229.0771	13.47	6.56	141247
230.0739	8.15	3.97	85455
244.0930	17.30	8.43	181391
245.1194	205.26	100.00	2152335
246.1116	35.15	17.12	368543
247.1061	12.15	5.92	127439
280.0798	146.40	71.32	1535119
281.0872	27.32	13.31	286431
282.0571	54.39	26.50	570335
283.0875	9.84	4.79	103183

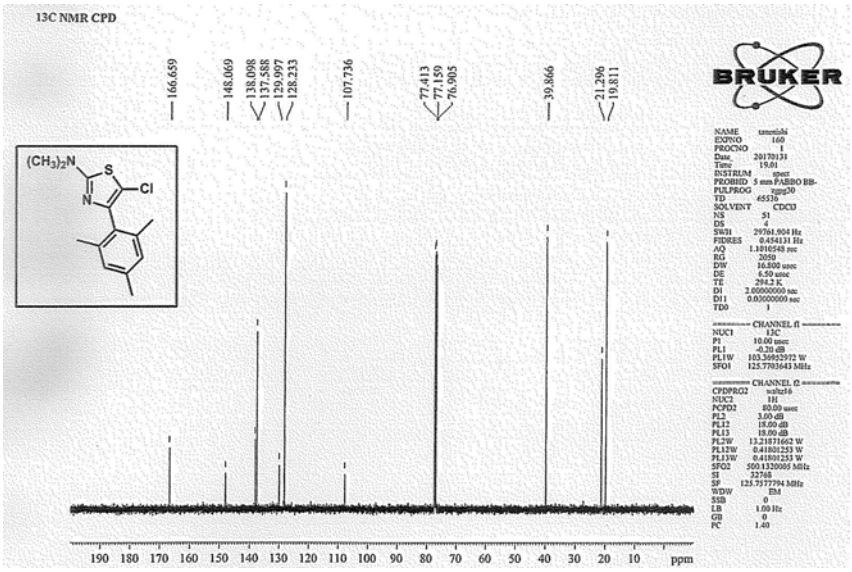
IR spectrum

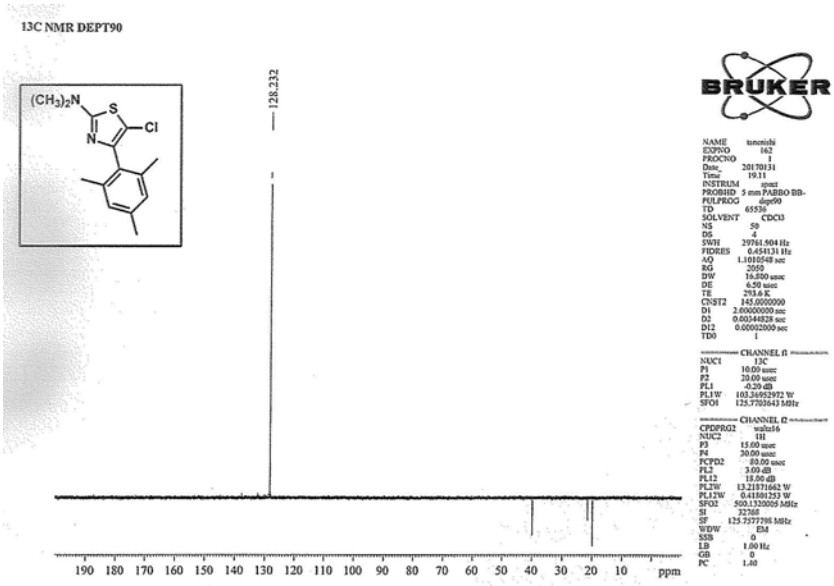


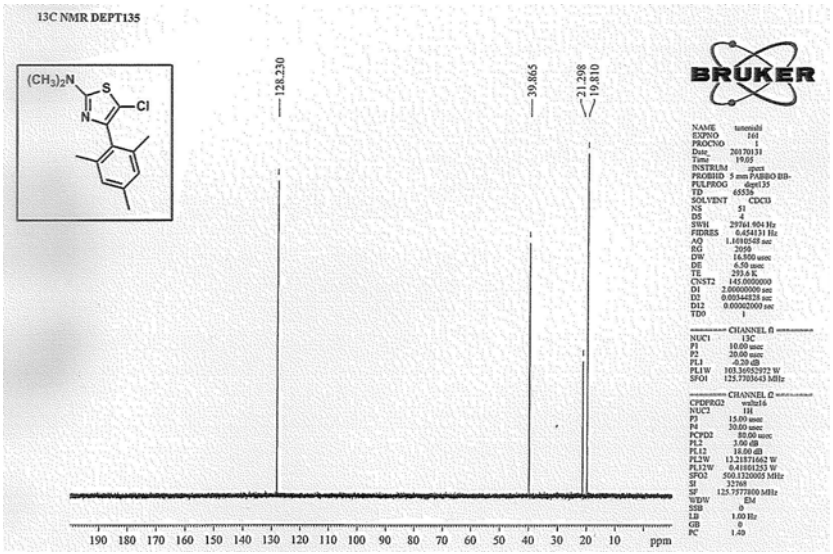
^{1}H NMR



^{13}C NMR

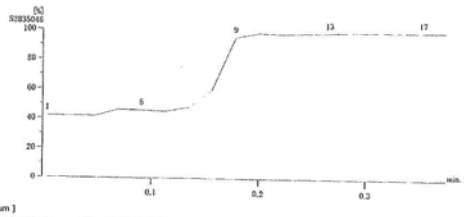

13C NMR CPD
166.659
148.069
138.098
137.588
130.997
128.233
107.736
77.413
77.150
76.905
39.866
21.296
19.811
BRUKER
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


13C NMR DEPT90
128.232
BRUKER
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

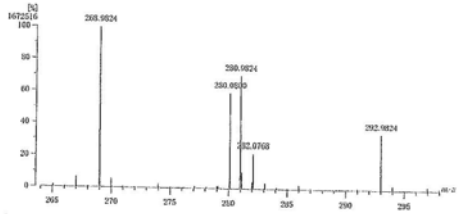

13C NMR DEPT135
128.230
39.865
21.298
19.810
BRUKER
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

HRMS

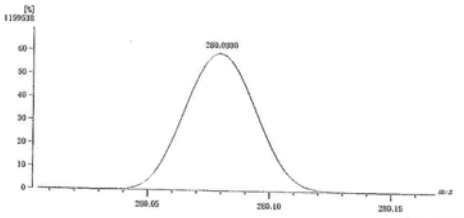
[TIC/BIC]
Data : EI+HR-nishinomiya-280 Date : 15-Feb-2017 10:39
Sample : -
Note : -

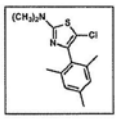


[Mass Spectrum]
Data : EI+HR-nishinomiya-280 Date : 15-Feb-2017 10:39
RT : 0.20 min Scan# : (10,14)



[Mass Spectrum]
Data : EI+HR-nishinomiya-280 Date : 15-Feb-2017 10:39
RT : 0.20 min Scan# : (10,14)





Data : EI+HR-nishinomiya-280 Date : 15-Feb-2017 10:39
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.20 min Scan# : (10,14)
Elements : C 14/0, H 17/0, 35Cl 1/0, 37Cl 1/0, N 2/0, S 1/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 8.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	280.0800	59.42	-0.4 / -0.1	8.0	C14 H17 35Cl N2 S

[Theoretical Ion Distribution]
Molecular Formula : C14 H17 N2 S Cl
(m/z 280.0801, MW 280.8214, U.S. 8.0)
Base Peak : 280.0801, Averaged MW : 280.8181(a), 280.8219(w)

m/z	INT.
280.0801	100.0000
281.0830	17.0953
282.0773	37.7792
283.0800	6.2576
284.0755	1.9334
285.0770	0.2590
286.0776	0.0254
287.0784	0.0020
288.0799	0.0001