

## Supporting Information

### A protecting group-free divergent synthesis of natural benzofurans via one-pot synthesis of 2-bromo-6-hydroxybenzofurans

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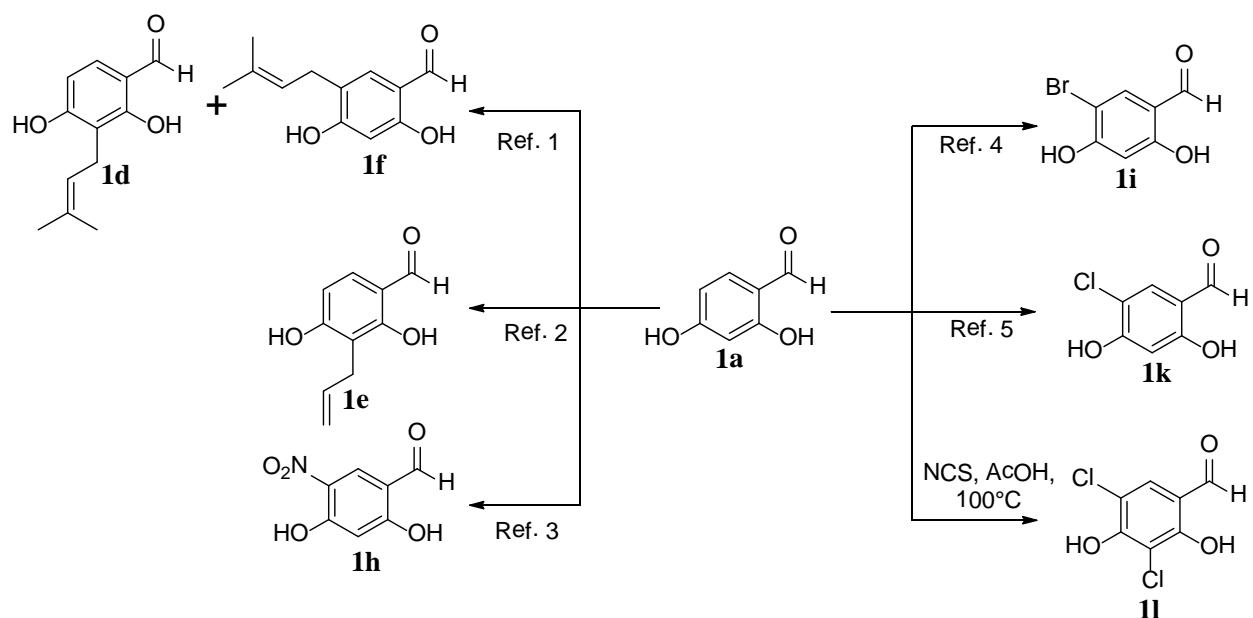
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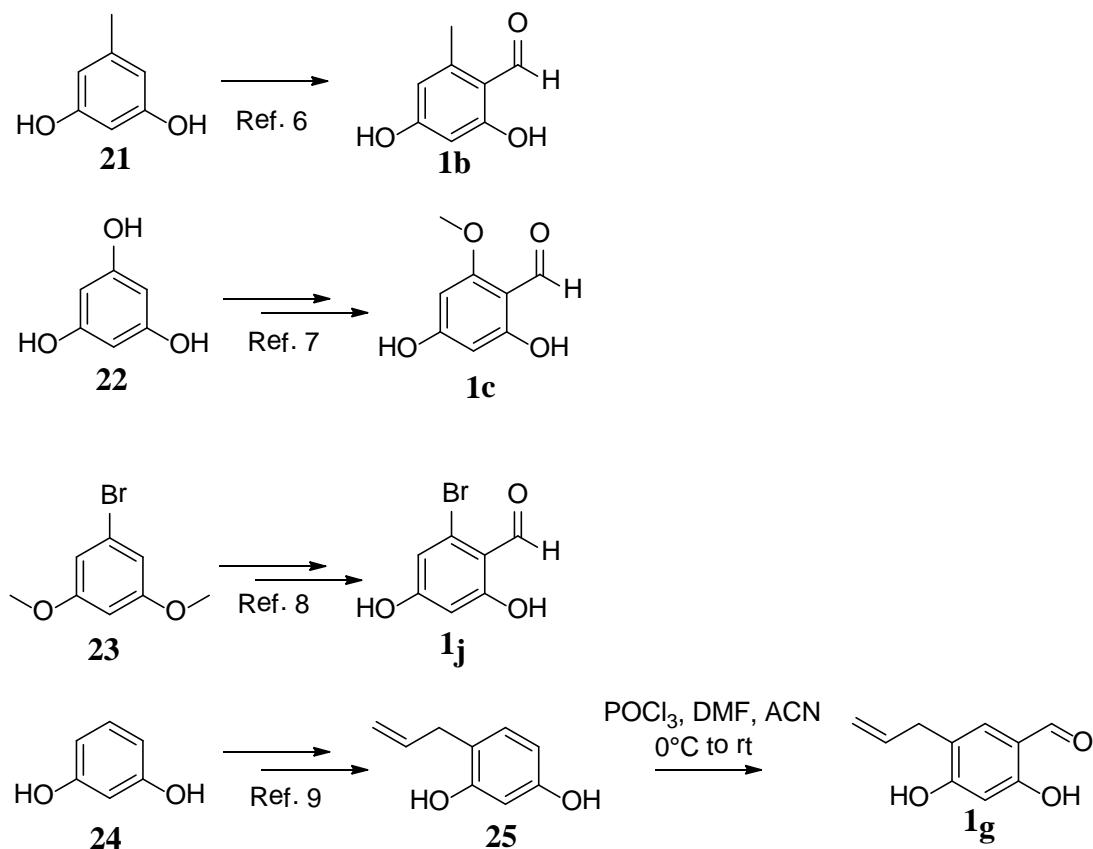
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**Scheme 1.** The synthesis of aldehydes **1d-f**, **1h**, **1i**, **1k**, and **1l** from **1a**

**Synthesis of 3,5-dichloro-2,4-dihydroxybenzaldehyde (1l).** To a solution of **1a** (1.00 g, 7.24 mmol) in AcOH was added NCS (2.40 g, 18.1 mmol) and reaction mixture was heated to 100 °C for 16 h. Reaction mass was cooled to rt and poured into crushed ice. The precipitated solid was filtered and dried under vacuum to give **1l** as light brown solid. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 11.48 (brs, 1H), 9.88 (s, 1H), 7.78 (s, 1H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 193.03, 157.34, 156.51, 131.24, 115.97, 113.70, 110.00; HRMS (ESI) *m/z* calcd for C<sub>7</sub>H<sub>5</sub>Cl<sub>2</sub>O<sub>3</sub> [M + H]<sup>+</sup> 206.9616; found 206.9606.



**Scheme 2.** The synthesis of aldehydes **1b**, **1c**, **1g**, and **1j**.

**Synthesis of 5-allyl-2,4-dihydroxybenzaldehyde (**1g**).** To a solution of **25** (3.00 g, 19.9 mmol) in ACN at 0 °C was added DMF (3.1 mL, 39.9 mmol) and  $\text{POCl}_3$  (2.29 mL, 23.9 mmol). The reaction mass was stirred for 1 h slowly raising to rt. Reaction mass was basified with saturated  $\text{NaHCO}_3$  solution, extracted with EtOAc. Organic layers washed with brine, dried over sodium sulfate and concentrated in *vacuo*. Purification by silica gel column chromatography (0 to 13% EtOAc in hexane) afforded **1g** (2.00 g, 56%) as off white solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  11.27 (s, 1H), 9.67 (s, 1H), 7.27 (s, 1H), 6.46 (s, 1H), 6.38 (s, 1H), 6.03–5.96 (m, 1H), 5.19 (dd,  $J = 16.0, 2.8$  Hz, 1H), 5.18 (dd,  $J = 10.0, 2.8$  Hz, 1H), 3.37 (d,  $J = 6.4$  Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  194.59, 163.00, 162.27, 135.76, 119.01, 117.02, 115.29, 103.32, 103.28, 33.70. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{10}\text{H}_{11}\text{O}_3$  [ $\text{M} + \text{H}]^+$  179.0708; found 179.0700

**Table 1. The screened reaction conditions for the Suzuki coupling**

Entry	Base (2.5 equiv)	Catalyst (5 mol%)	Solvent	Temp (°C)	Time (h)	Yield (%)
1	K <sub>3</sub> PO <sub>4</sub>	Pd(dppf)Cl <sub>2</sub> .DCM	dioxane:H <sub>2</sub> O (4:1)	80	1	30
2	K <sub>2</sub> CO <sub>3</sub>	Pd(PPh <sub>3</sub> ) <sub>4</sub>	THF:EtOH:H <sub>2</sub> O (2:2:1),	80	1	70
3	K <sub>3</sub> PO <sub>4</sub>	Pd(dppf)Cl <sub>2</sub> .DCM	DMSO:H <sub>2</sub> O (4:1)	80	1	80
4	K <sub>3</sub> PO <sub>4</sub>	Pd(dppf)Cl <sub>2</sub> .DCM	DMF:H <sub>2</sub> O (4:1)	80	1	83

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3a

new experiment

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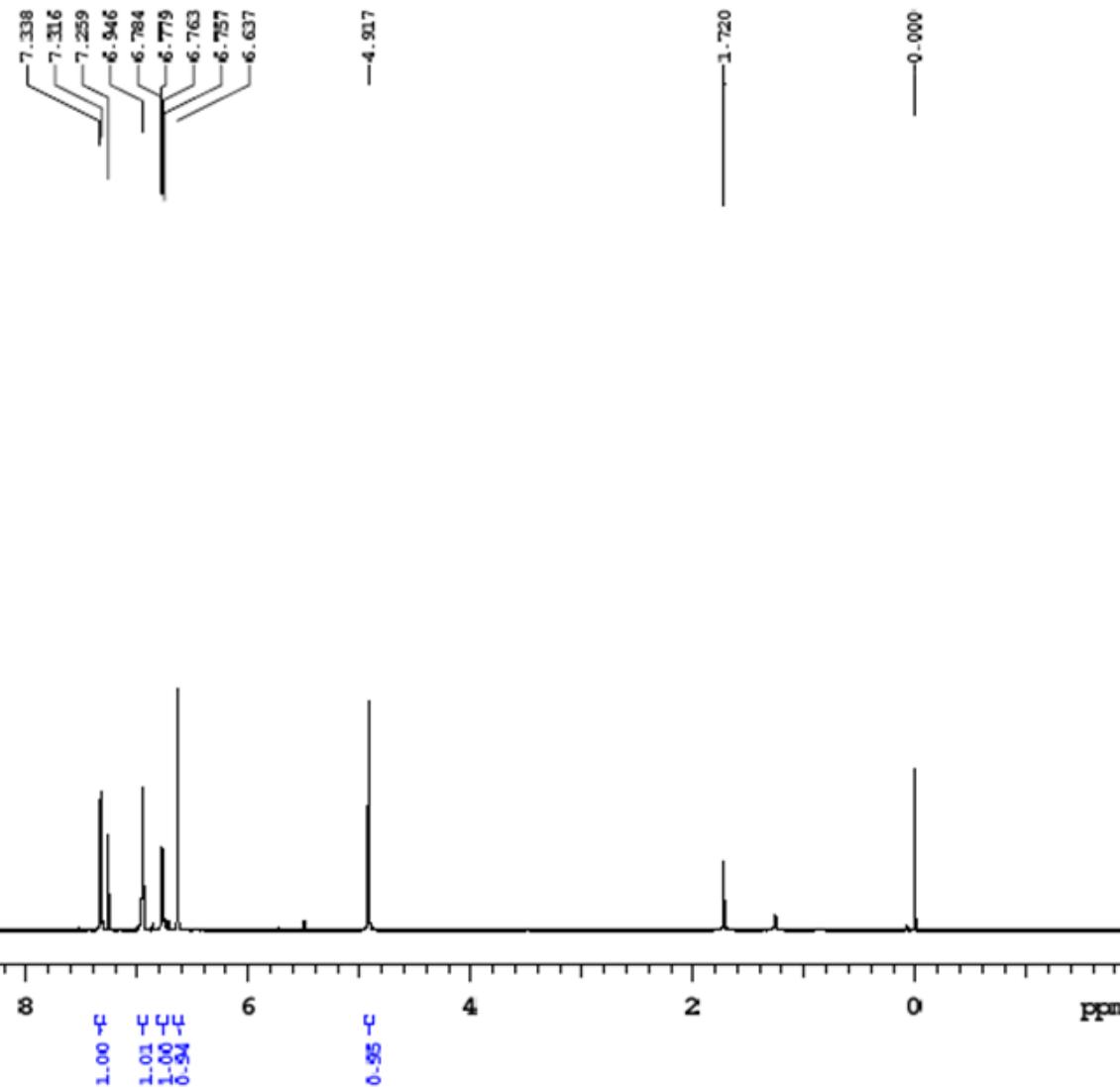
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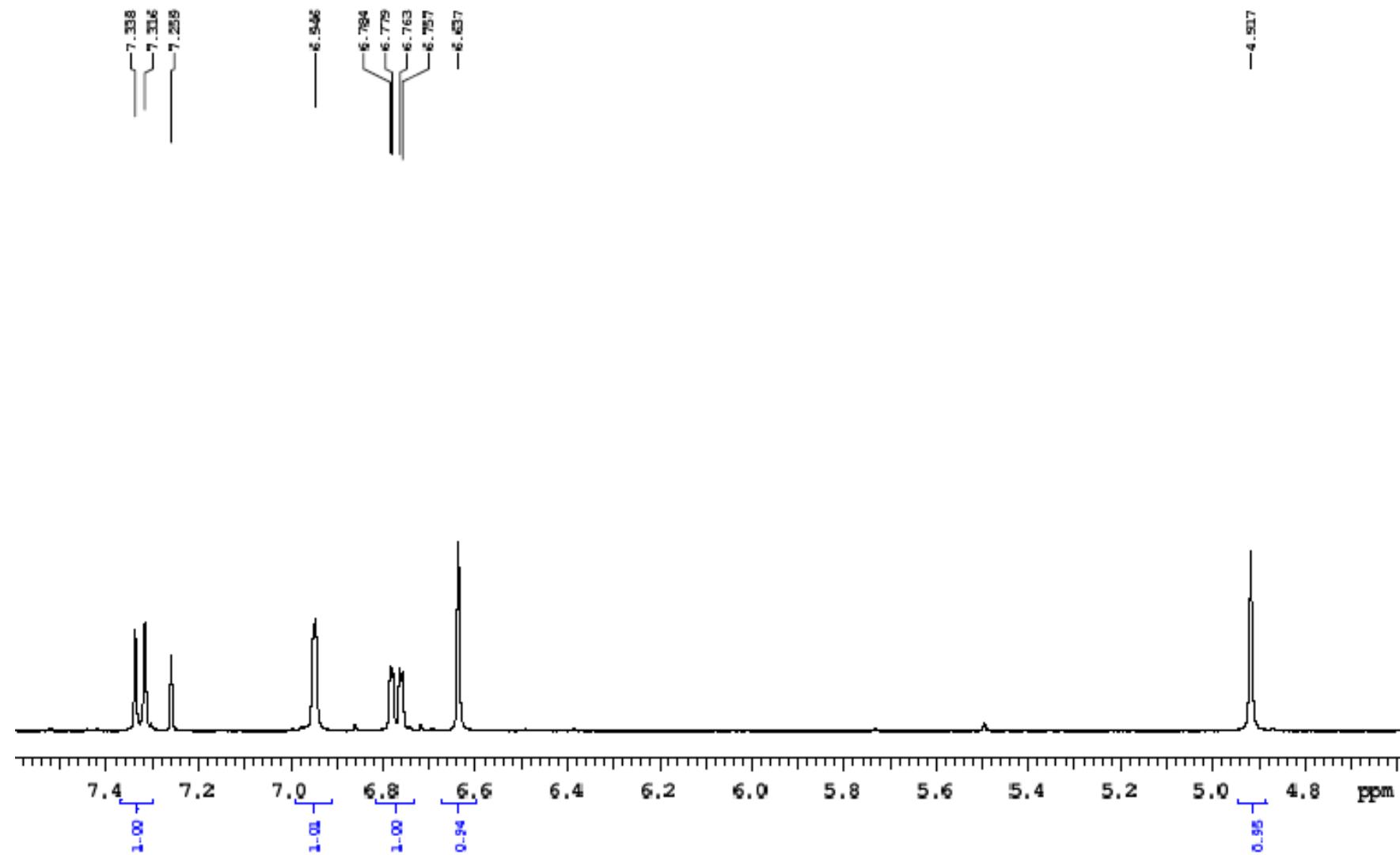
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Operator: klee

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Width 6410.3 Hz  
8 repetitions  
OBSERVE Hz, 399.8039100 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 28 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3a

new experiment

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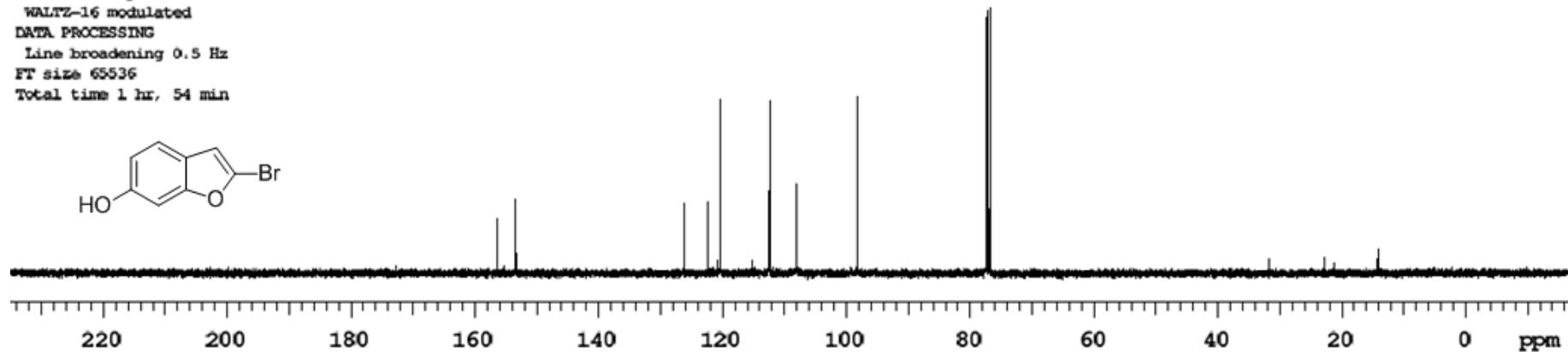
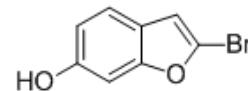
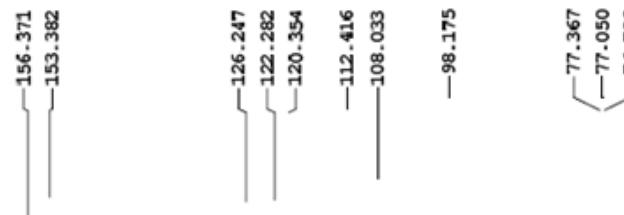
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Temp. 16.4 C / 289.6 K  
Operator: klee

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DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALFZ-16 modulated  
DATA PROCESSING  
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Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 3b

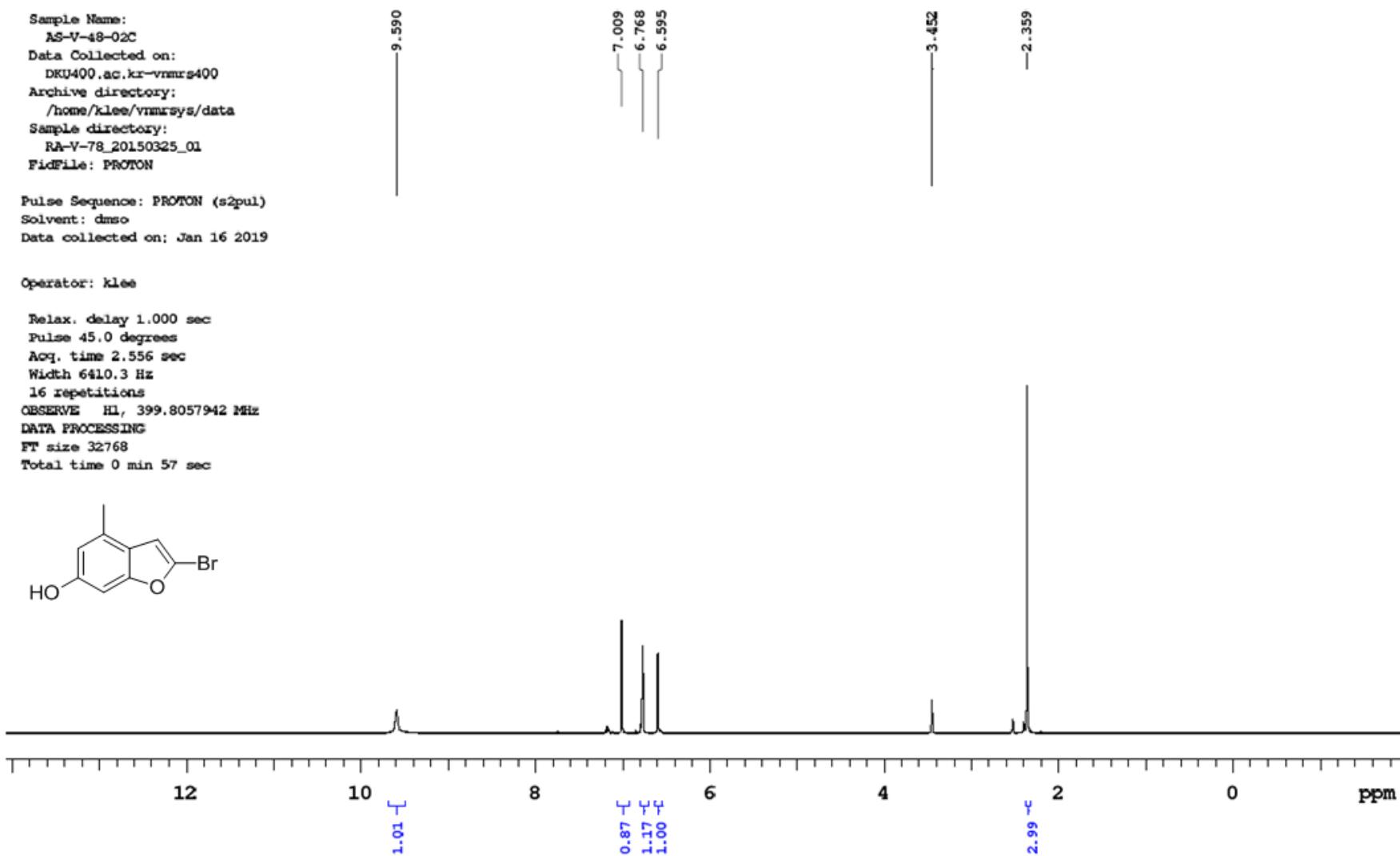
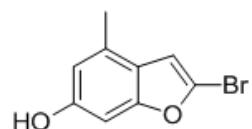
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Data collected on: Jan 16 2019

Operator: klee

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Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **3b**

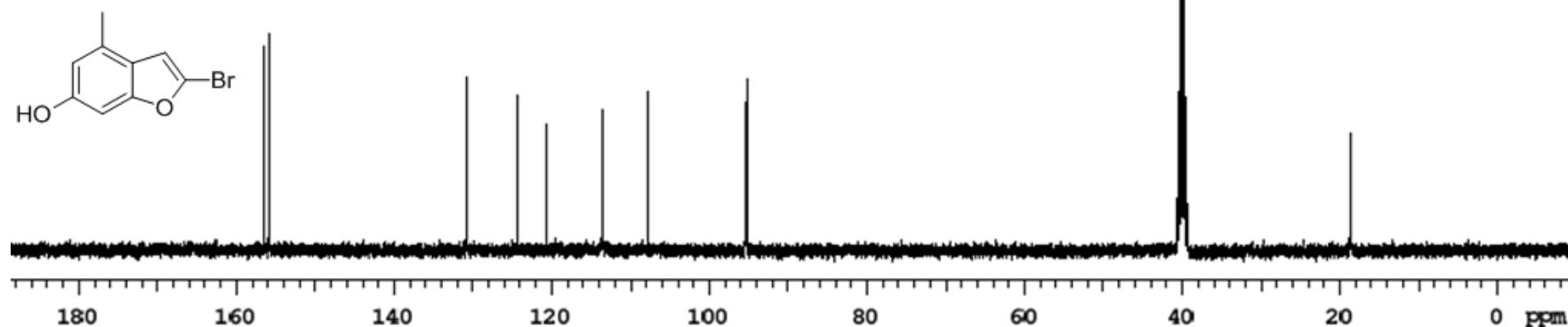
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Operator: klee

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 DECOUPLE H1, 399.8078135 MHz  
 Power 41 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
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 FT size 65536  
 Total time 3 hr, 10 min



<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3c

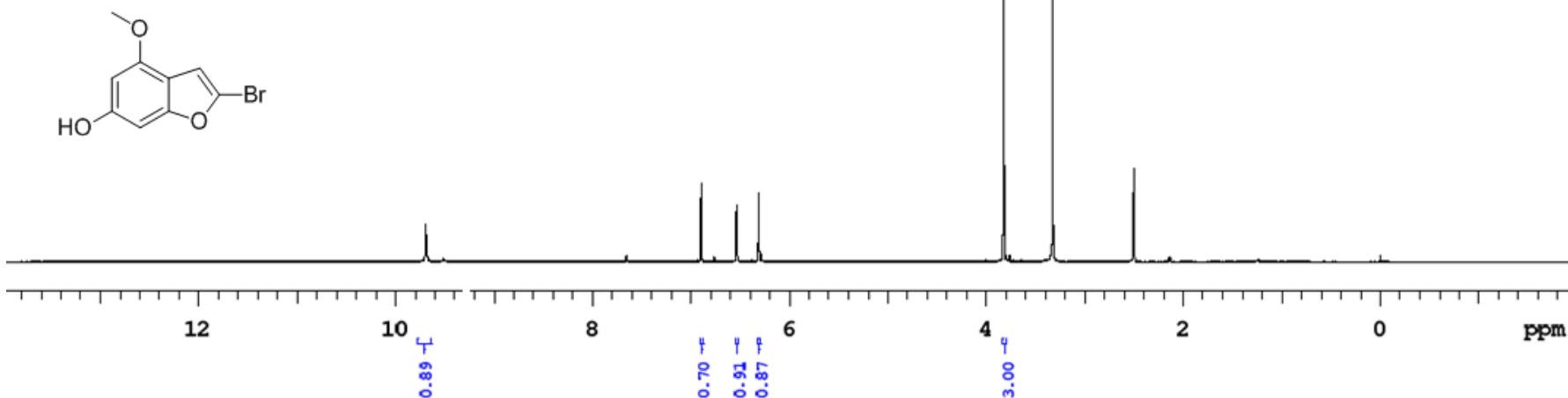
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Data collected on: Nov 7 2018

Operator: klee

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Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3c

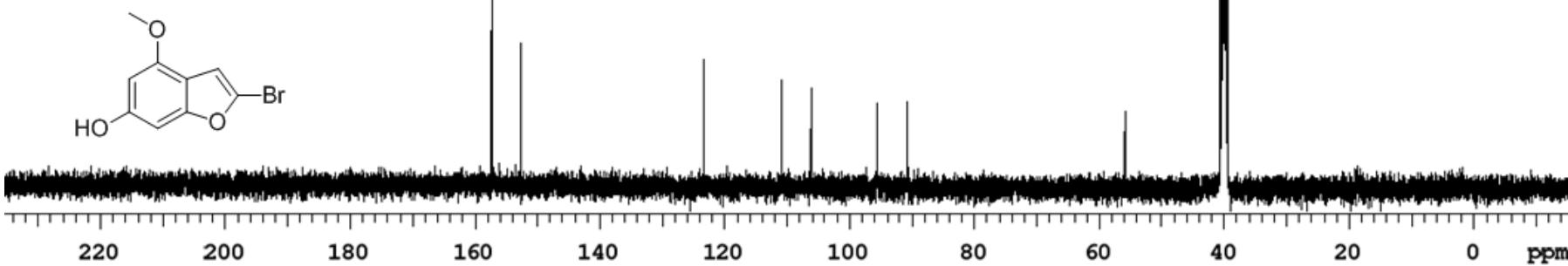
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Data collected on: Nov 7 2018

Operator: klee

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continuously on  
WALTZ-16 modulated  
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Total time 3 hr, 10 min



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 3d

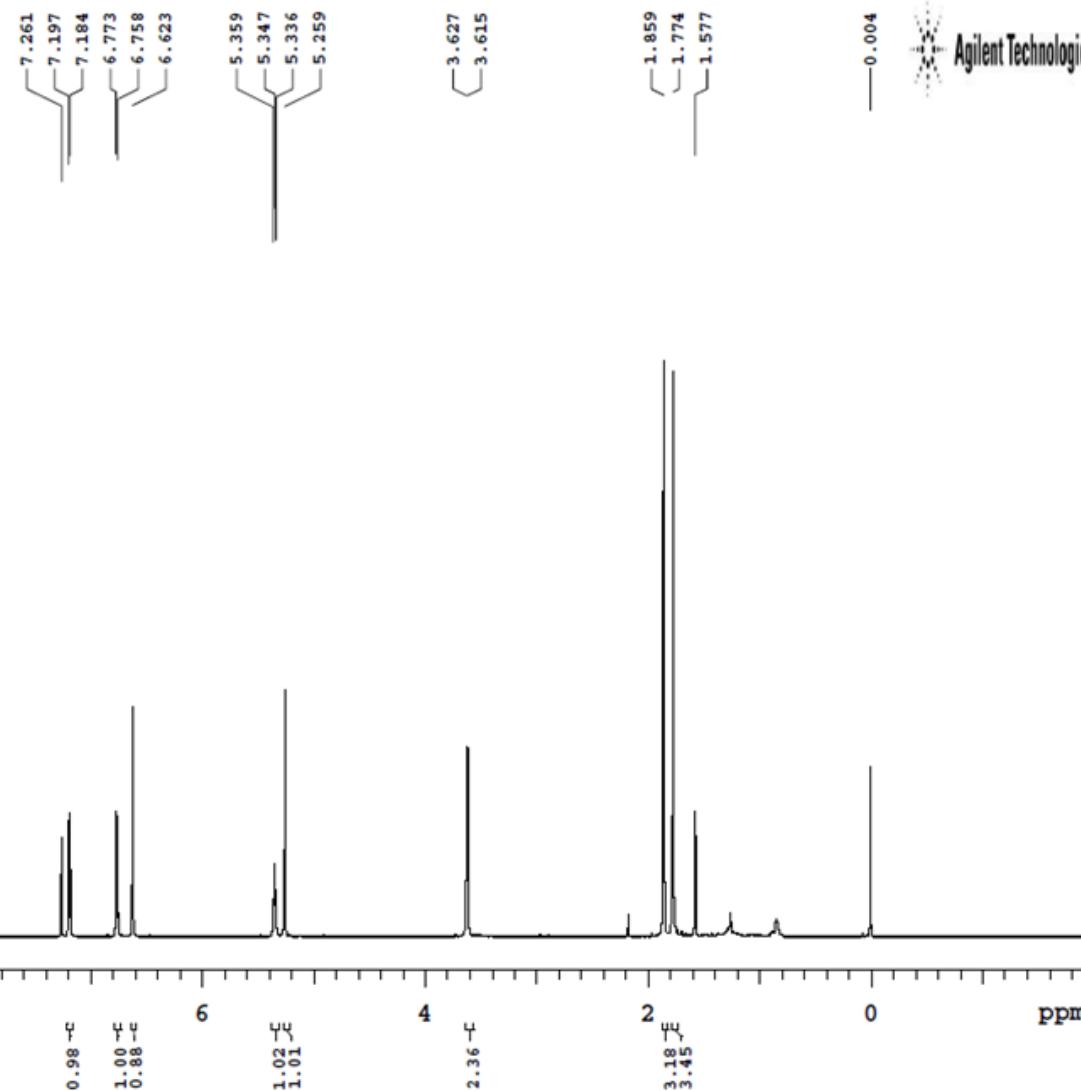
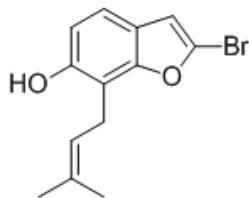
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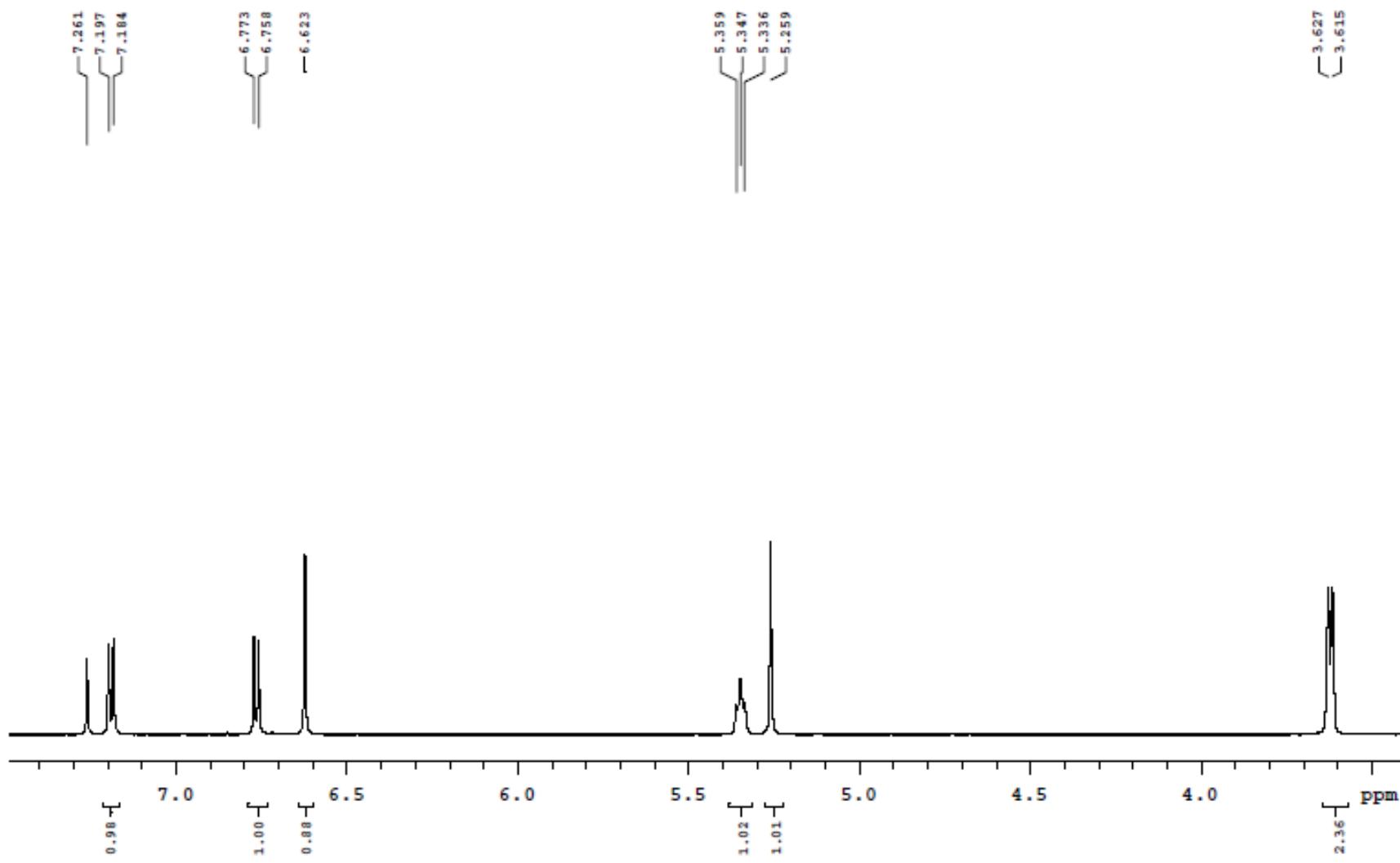
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Solvent: cdcl<sub>3</sub>  
Data collected on: Oct 27 2018

Operator: vnmr1

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<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) spectrum of compound 3d

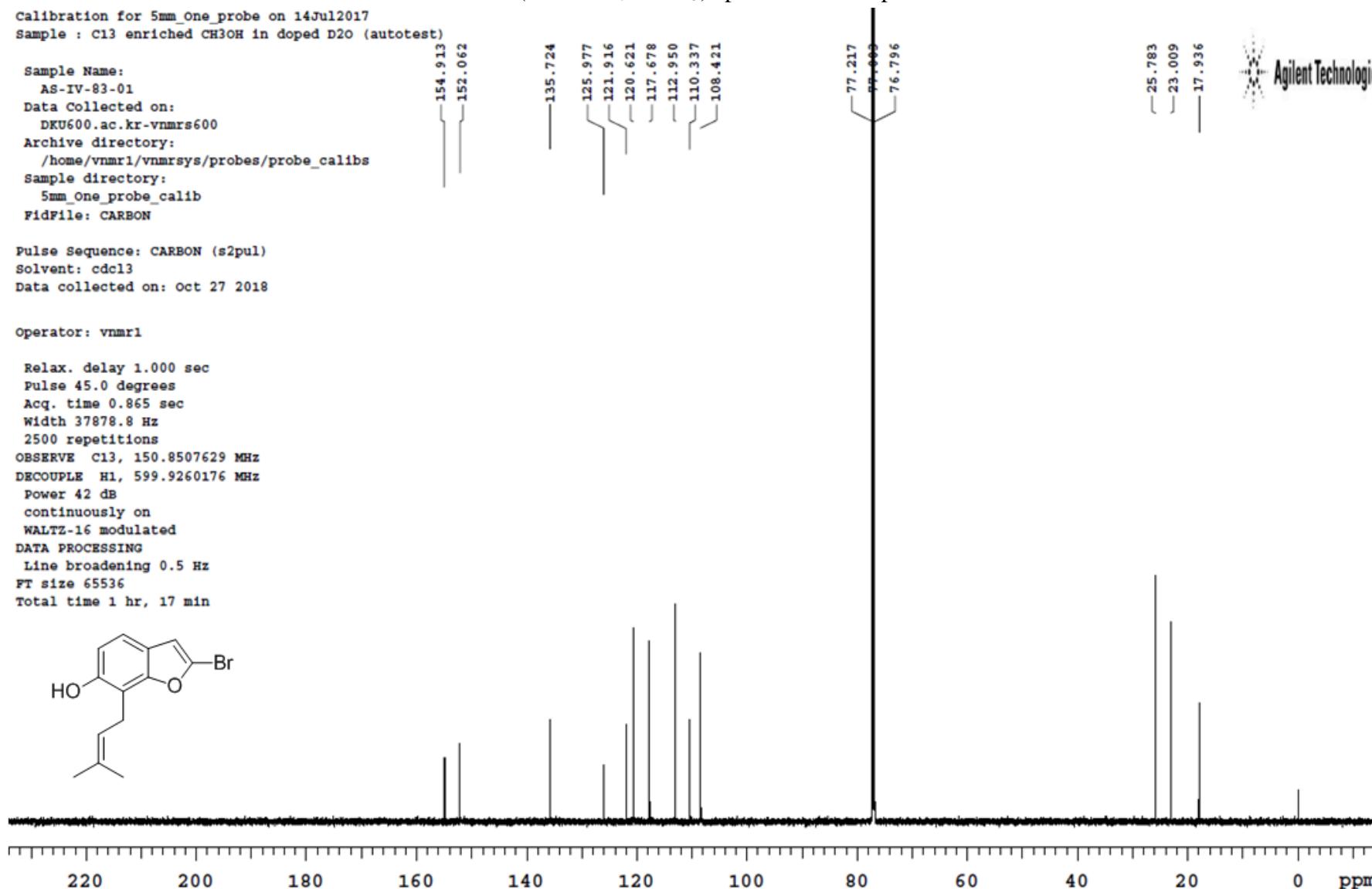
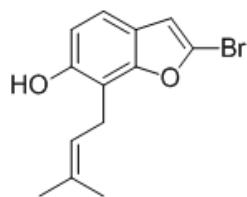
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FT size 65536  
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<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3e

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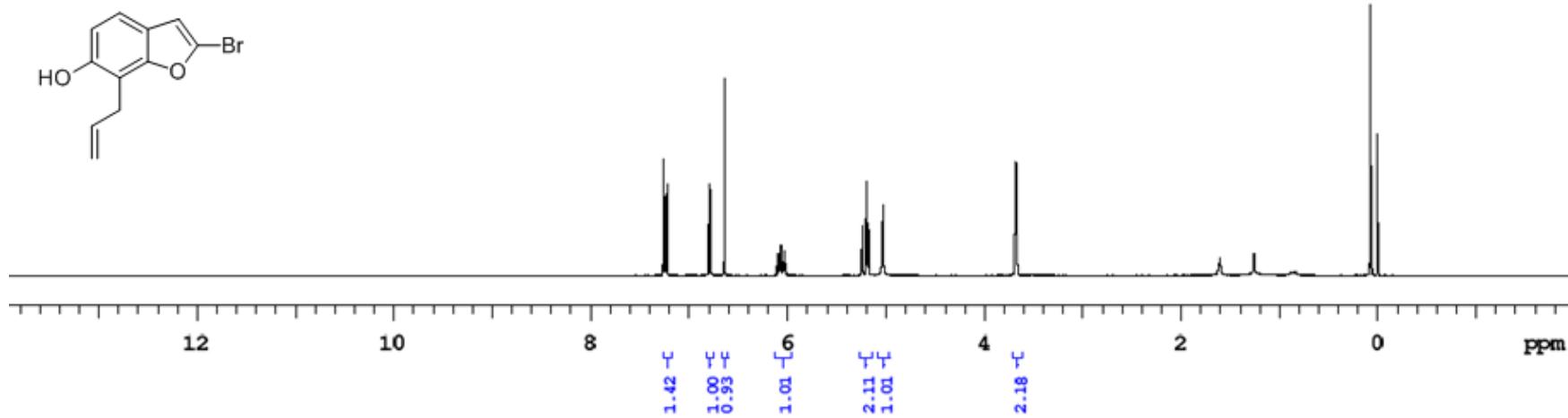
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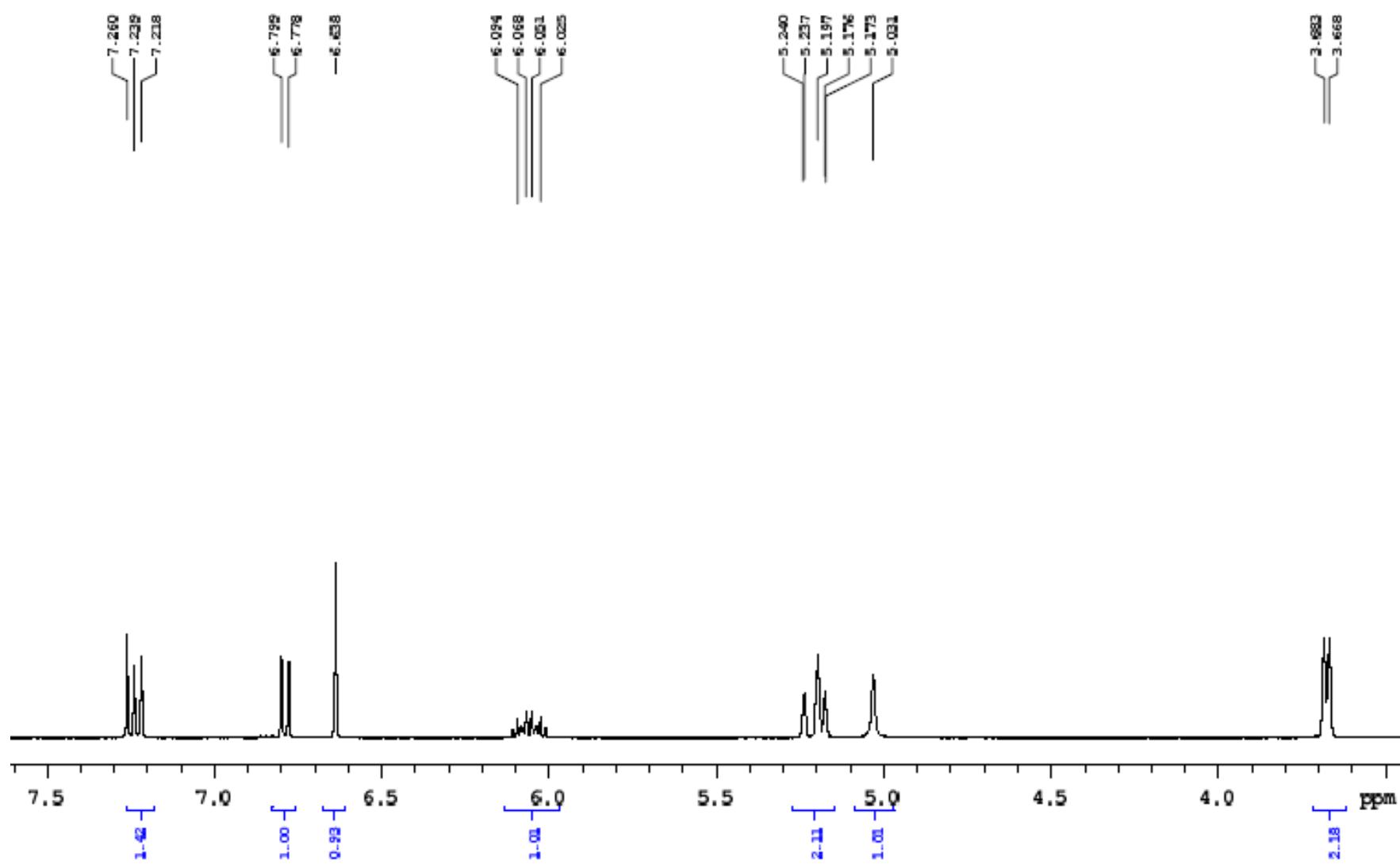
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Data collected on: Jan 14 2019

Operator: klee

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16 repetitions  
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DATA PROCESSING  
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Total time 9 min 57 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3e

STANDARD 1H OBSERVE - profile

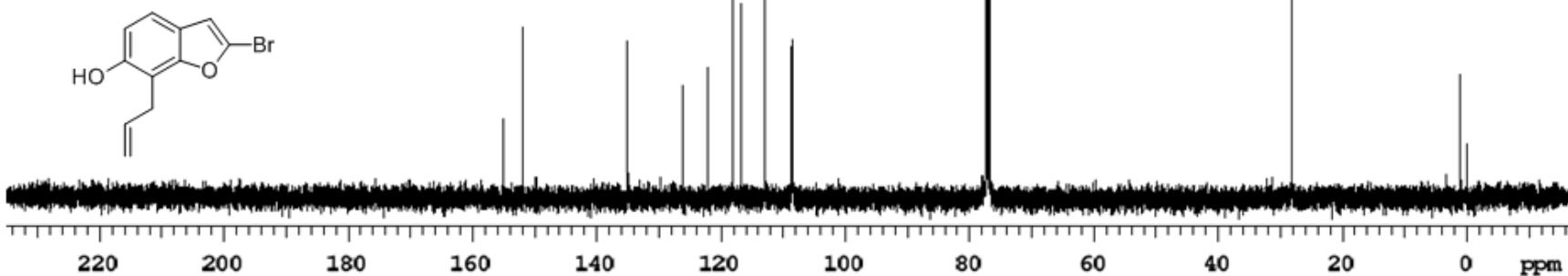
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Sample directory:  
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Operator: klee

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1344 repetitions  
OBSERVE C13, 100.5307749 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3f

STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-41-01  
Data Collected on:  
DKU400.ac.kr~vnmrs400  
Archive directory:

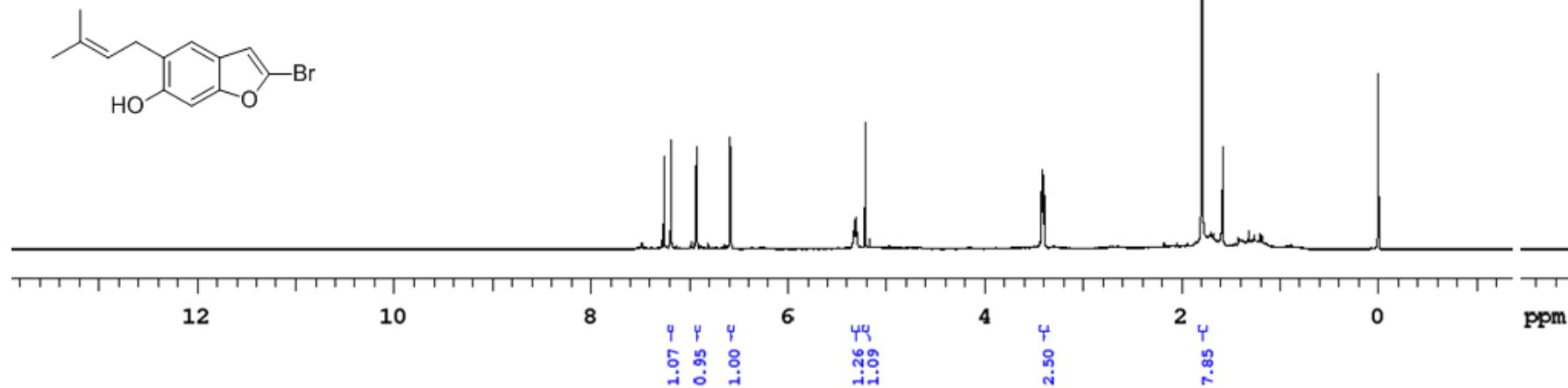
Sample directory:

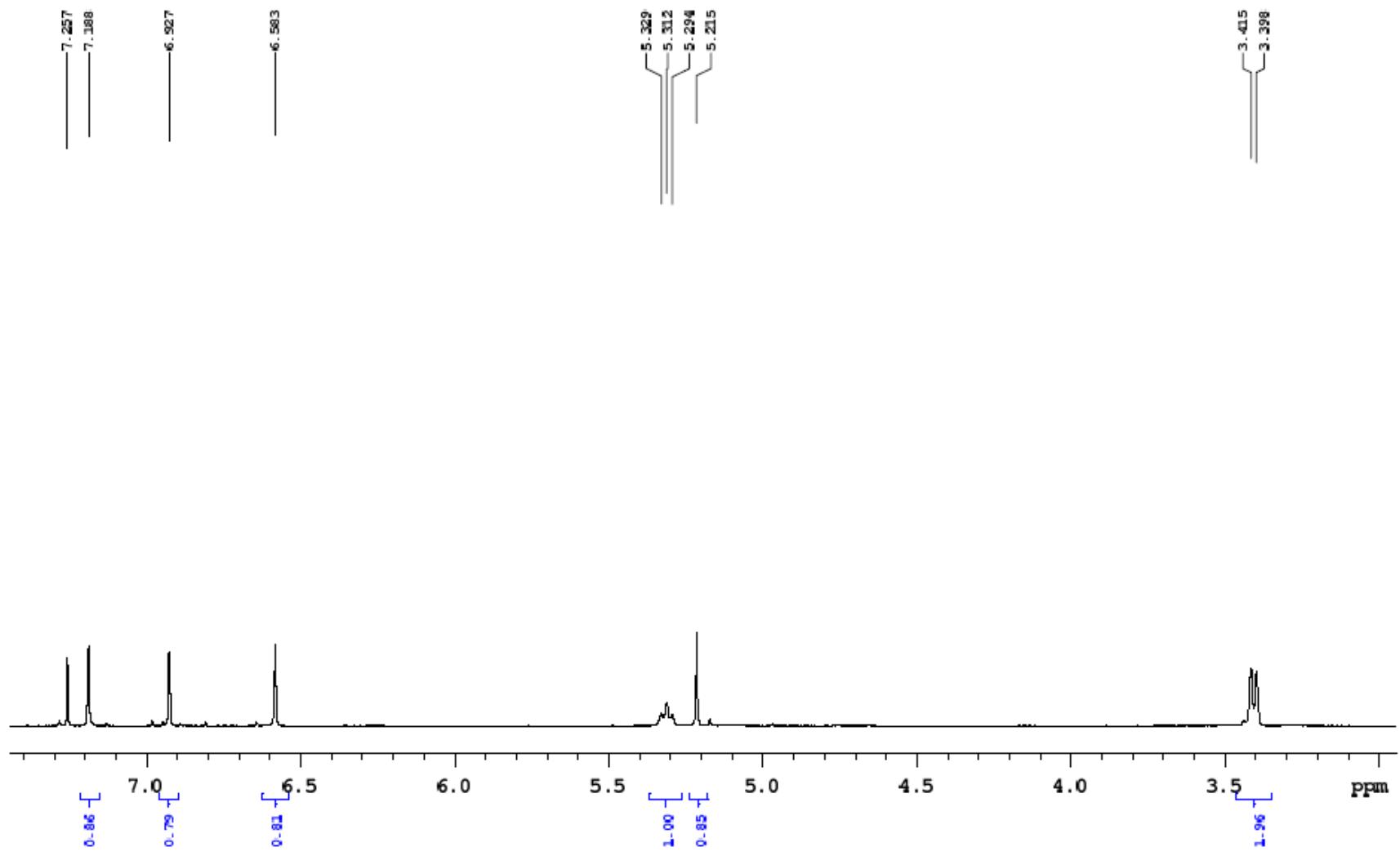
FidFile: AS-IV-41-01

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 19 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H1, 399.8039107 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3f

STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-41-01  
Data Collected on:  
DKU400.ac.kr-vmnrs400  
Archive directory:

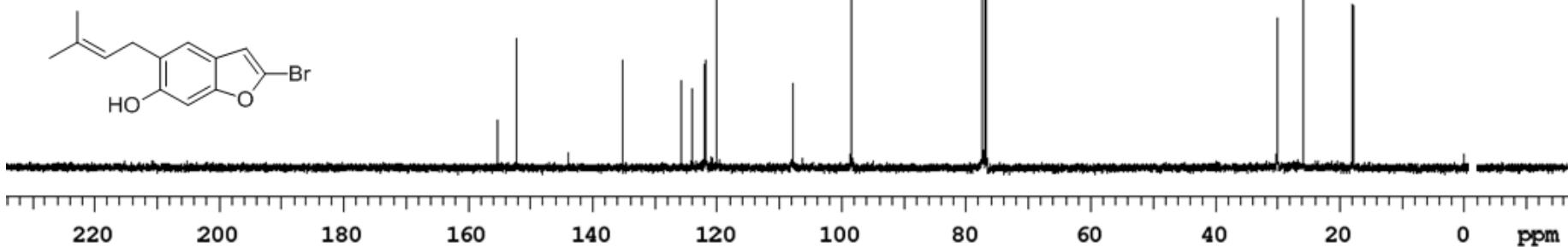
Sample directory:

FidFile: AS-IV-41-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl<sub>3</sub>  
Data collected on: Jul 19 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
960 repetitions  
OBSERVE C13, 100.5307726 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3g

new experiment

Sample Name:  
AS-TV-26-01  
Data Collected on:  
DKU400.ac.kr-vmrs400  
Archive directory:

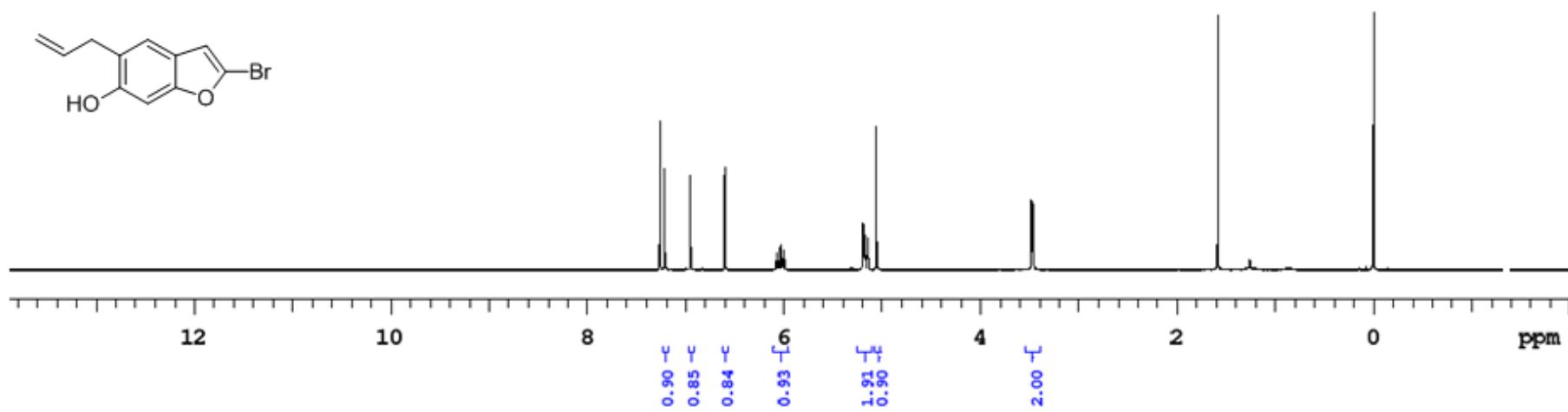
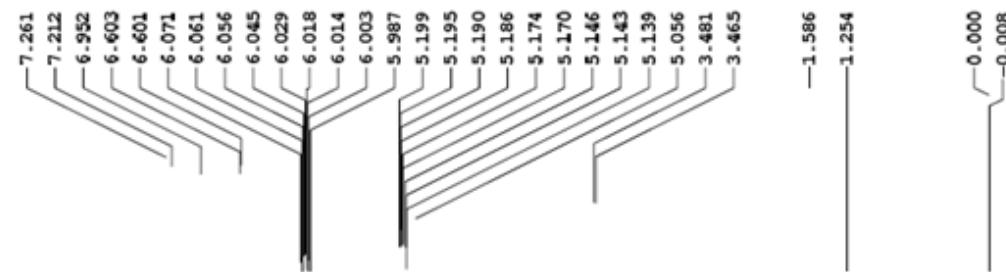
Sample directory:

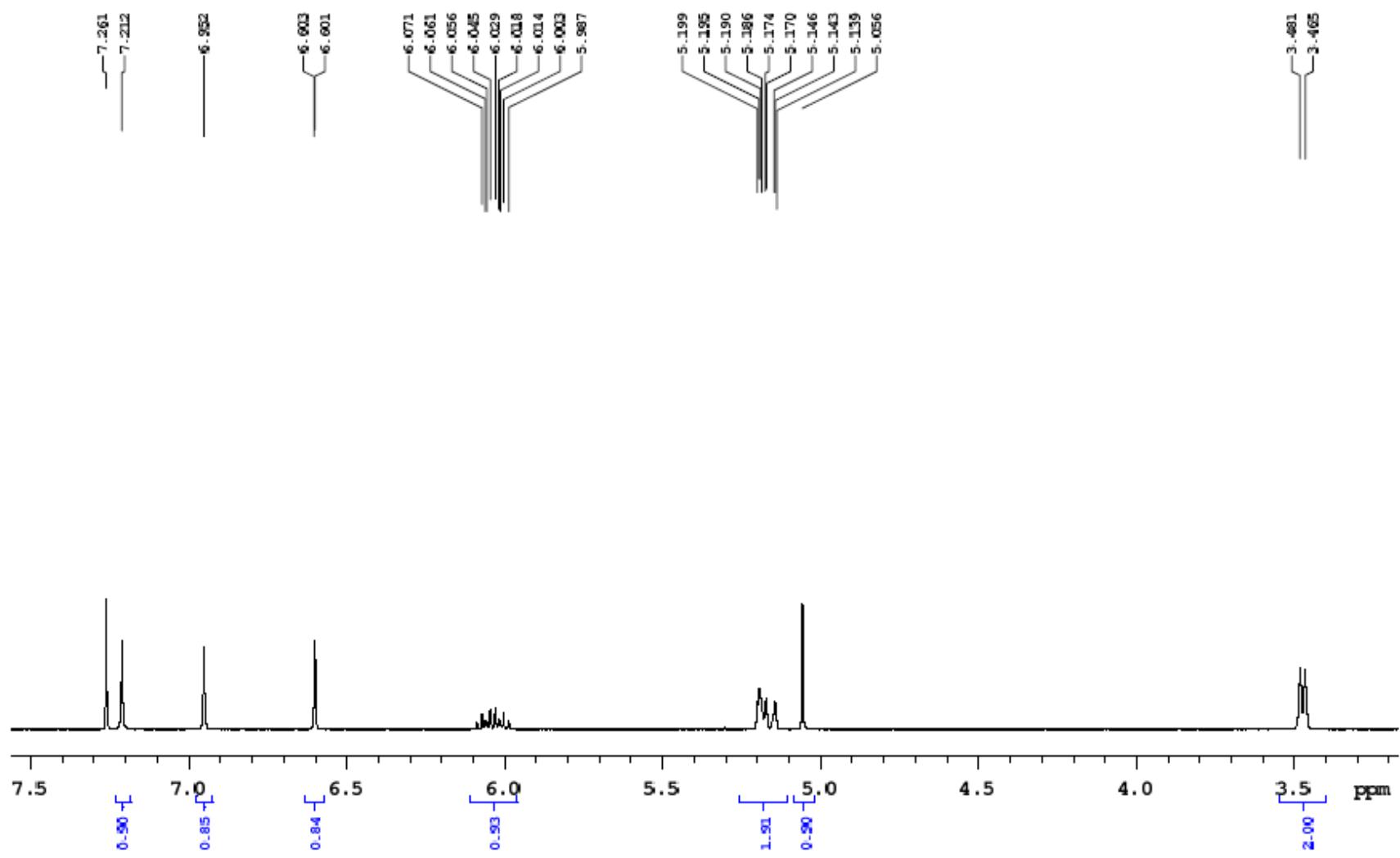
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 16 2018

Operator: klee

Relax, delay 1.000 sec  
Pulse 45.0 degrees  
Aq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H1, 399.8039092 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3g

new experiment

Sample Name:  
AS-IV-26-01  
Data Collected on:  
DRX400.ac:kr-vnmrs400  
Archive directory:

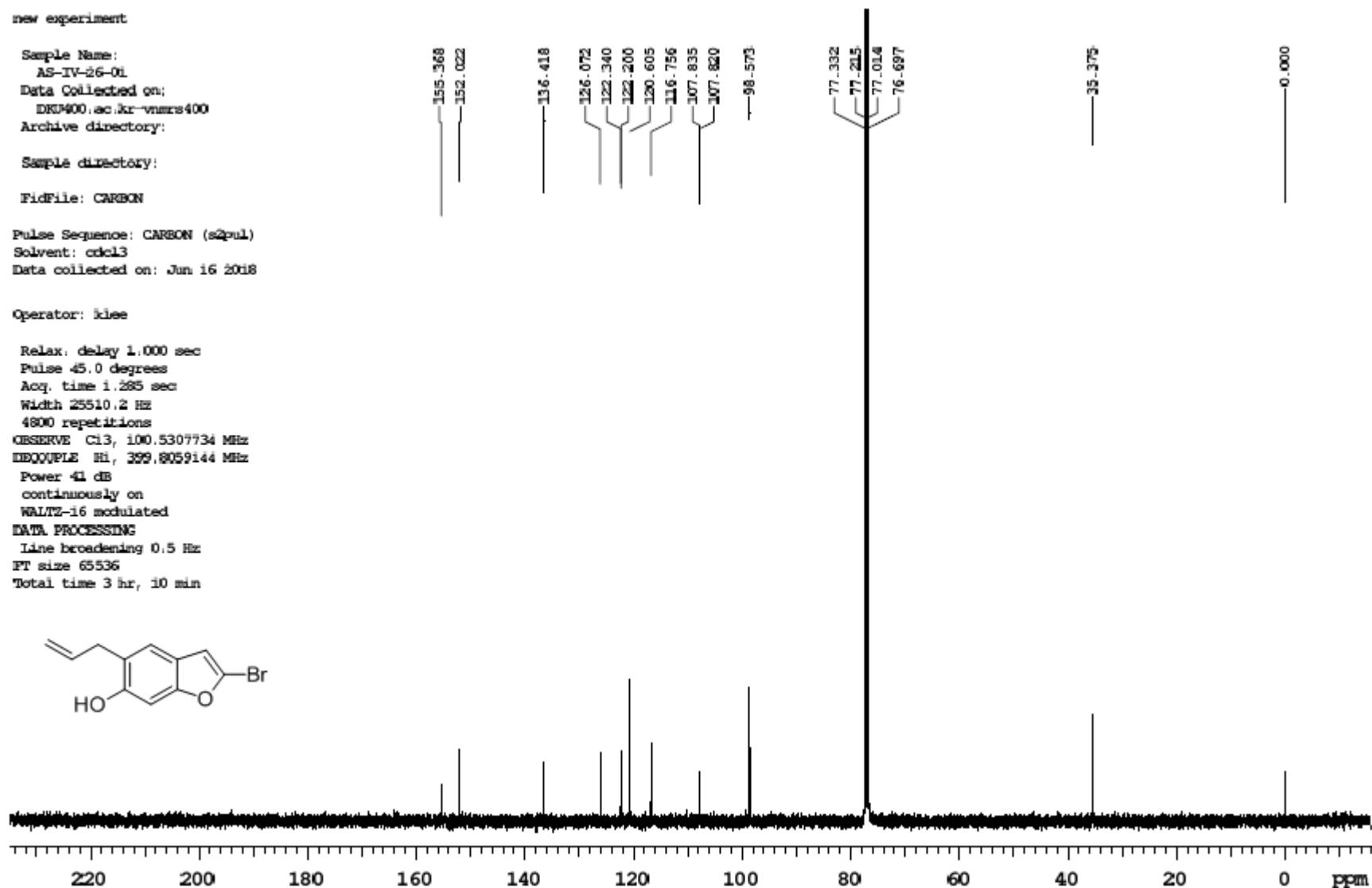
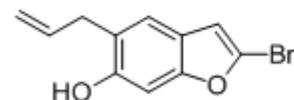
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 16 2018

Operator: klee

Relax: delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
4800 repetitions  
OBSERVE: C13, 100.5307734 MHz  
DEQCPMLE: HI, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 10 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3h

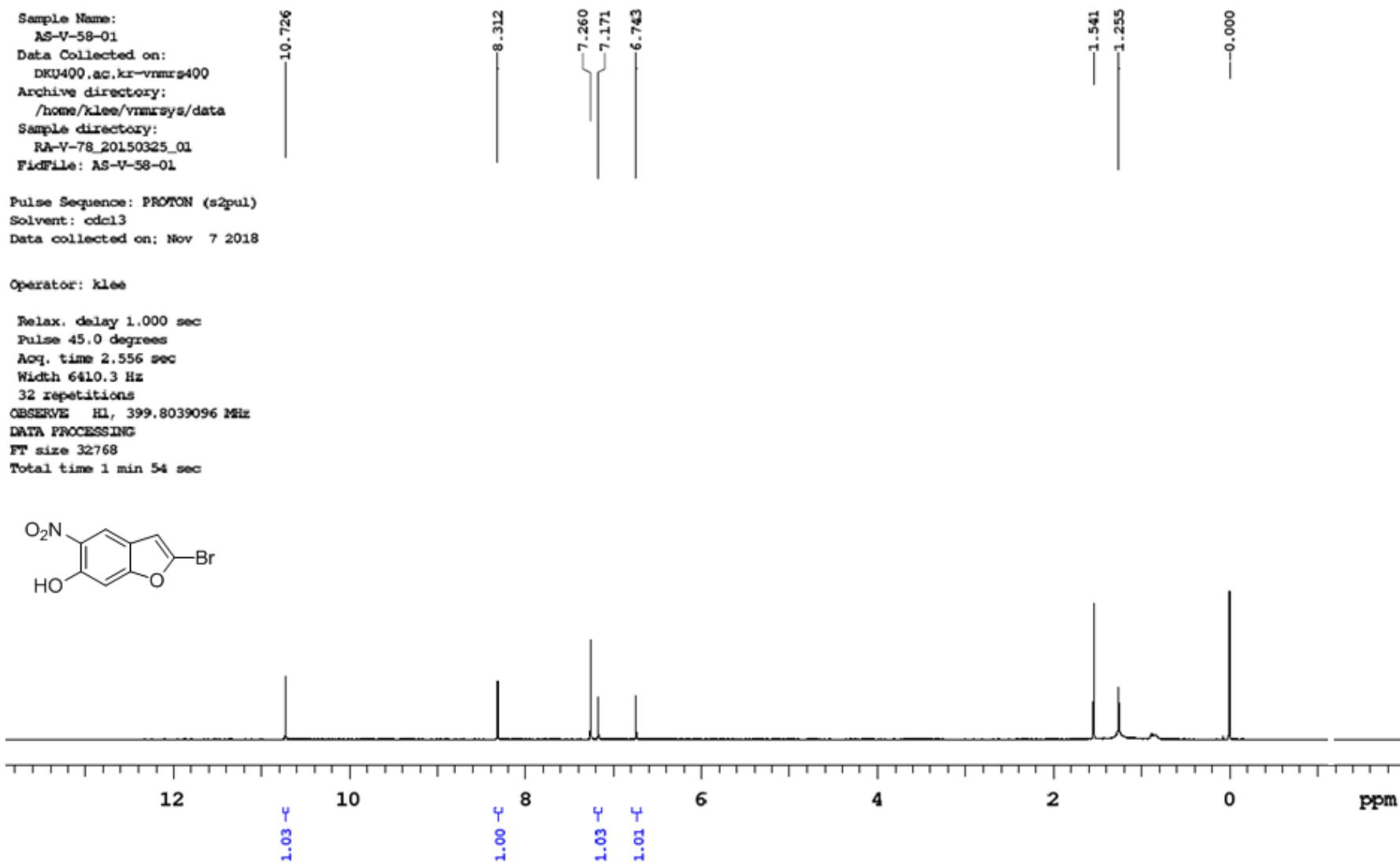
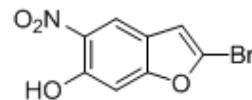
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-58-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-58-01

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Aq. time 2.556 sec  
Width 6410.3 Hz  
32 repetitions  
OBSERVE H1, 399.8039096 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min 54 sec



<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3h

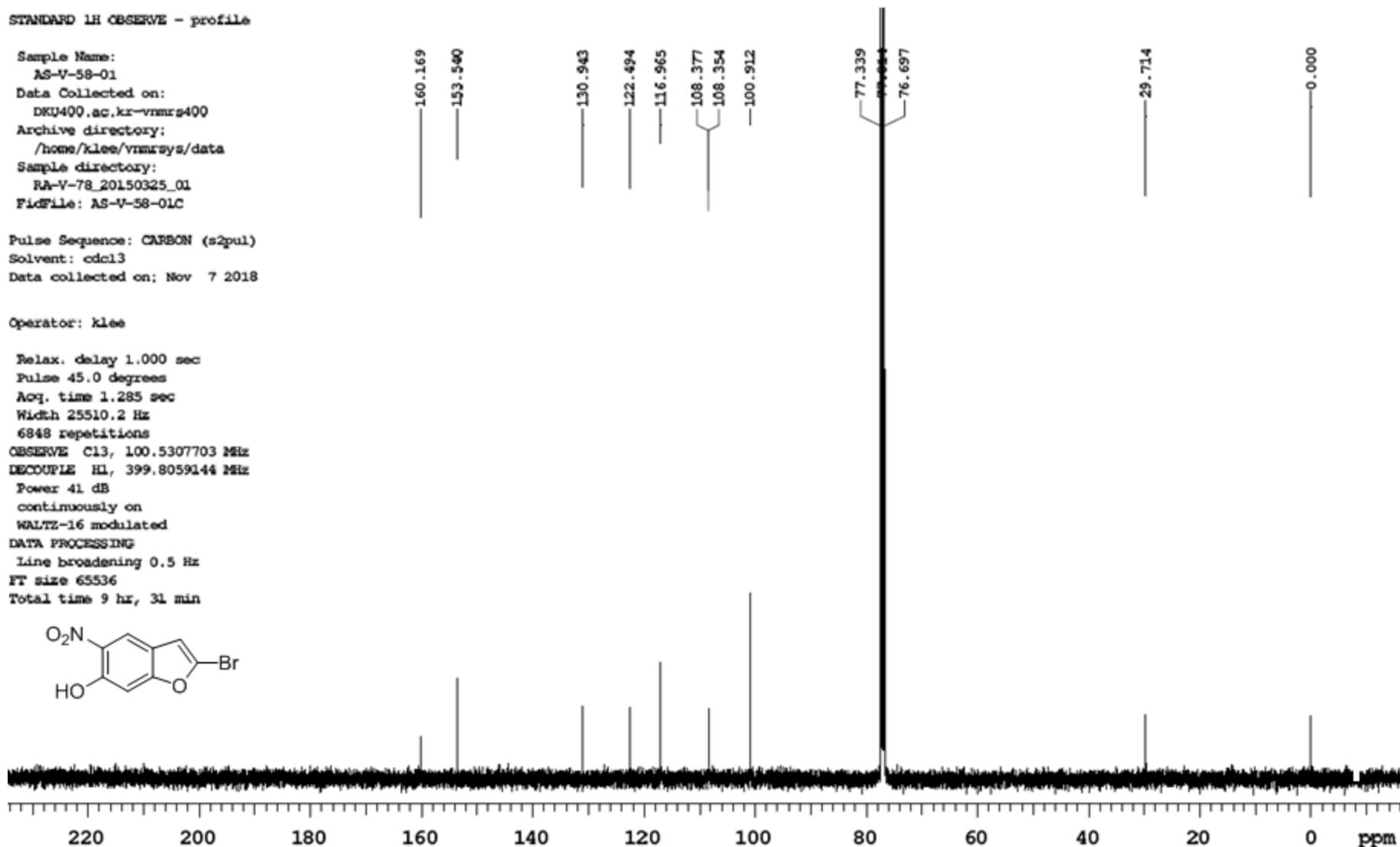
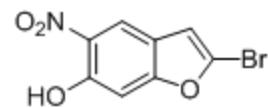
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-58-01  
Data Collected on:  
DRX400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-58-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Aq. time 1.285 sec  
Width 25510.2 Hz  
6848 repetitions  
OBSERVE C13, 100.5307703 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 hr, 31 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3i

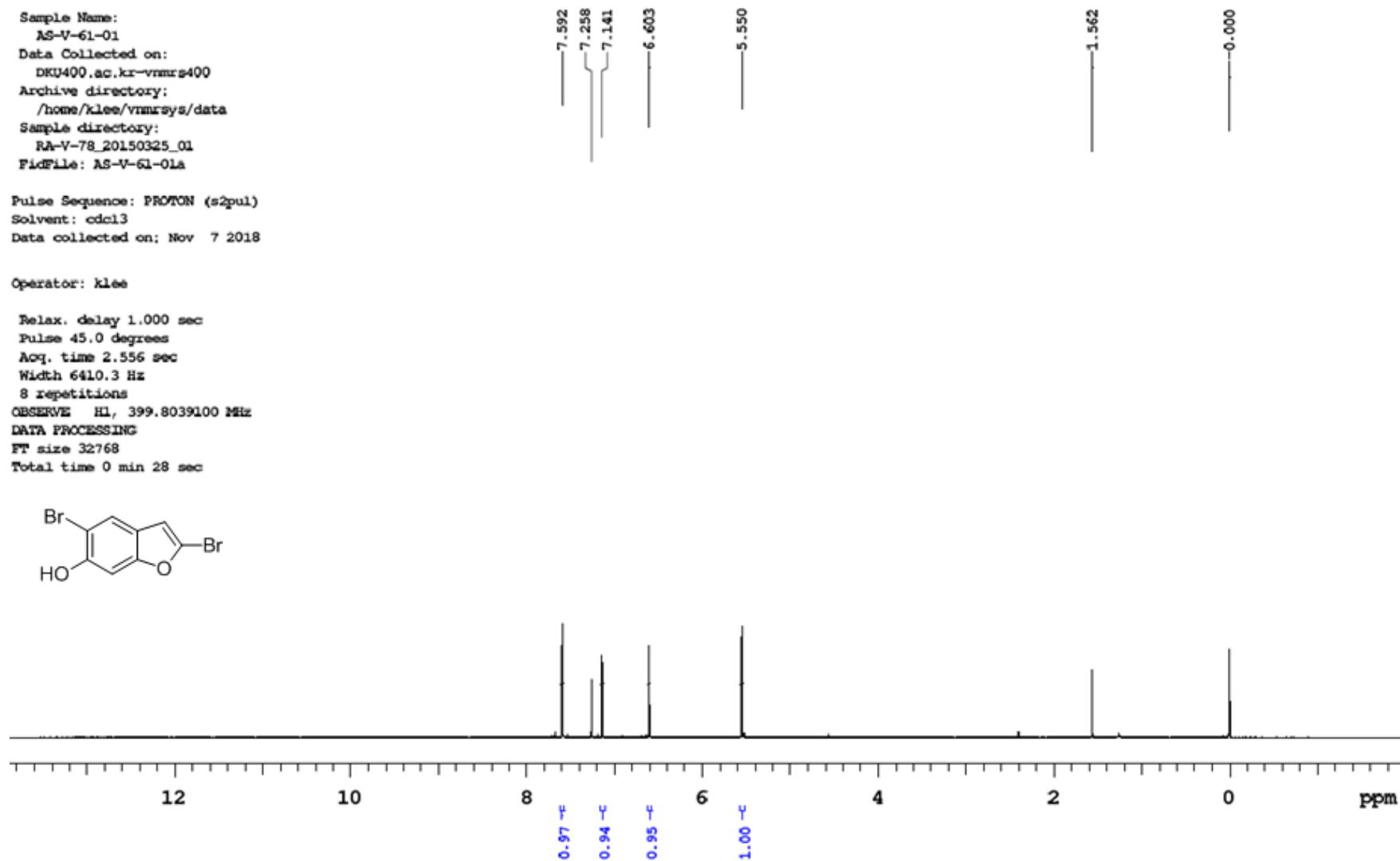
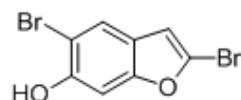
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-61-01  
Data Collected on:  
DKU400.ac.kx-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-61-01a

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl<sub>3</sub>  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Aqc. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE H1, 399.8039100 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 28 sec



<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3i

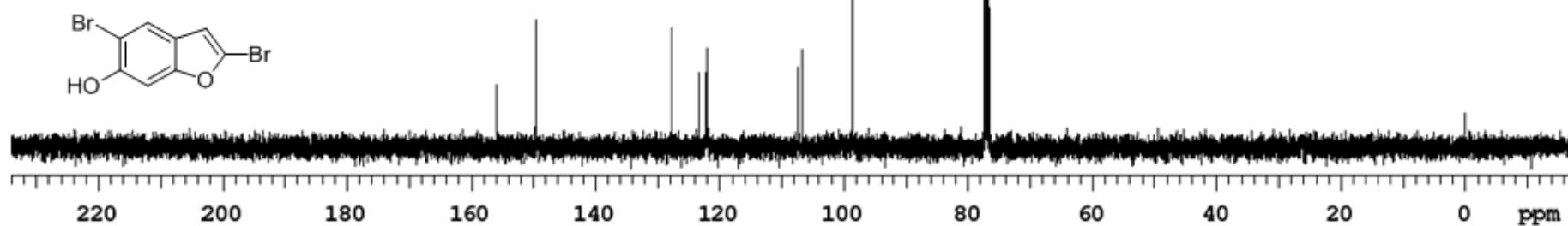
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-61-01  
Data Collected on:  
DKU400.ac,kr=vnmrss400  
Archive directory:  
/home/klee/vnmrssys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-61-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
960 repetitions  
OBSERVE C13, 100.5307745 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3j

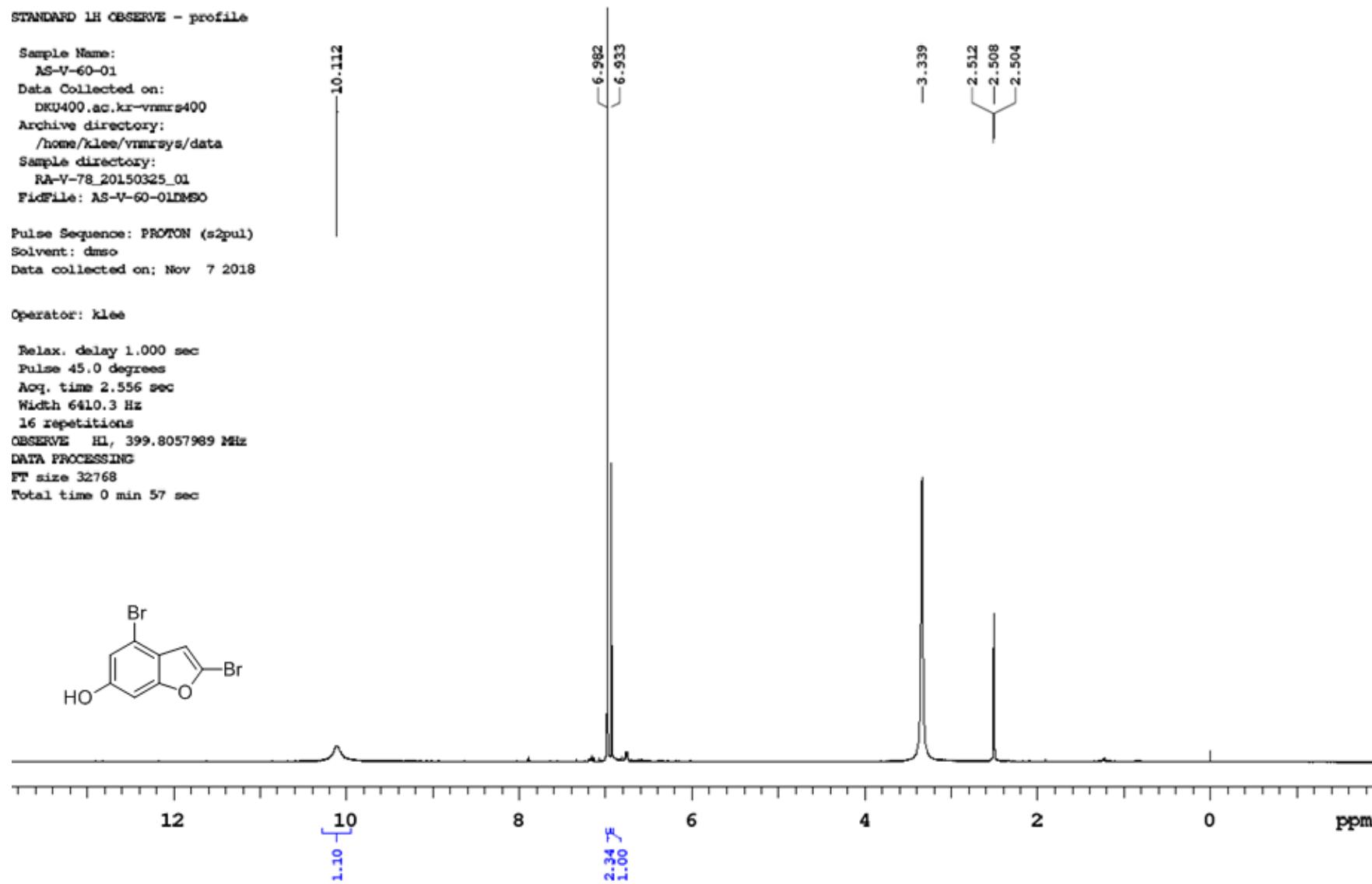
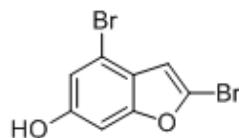
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-60-01  
Data Collected on:  
DKU400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-60-01DMSO

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Aq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H1, 399.8057989 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3j

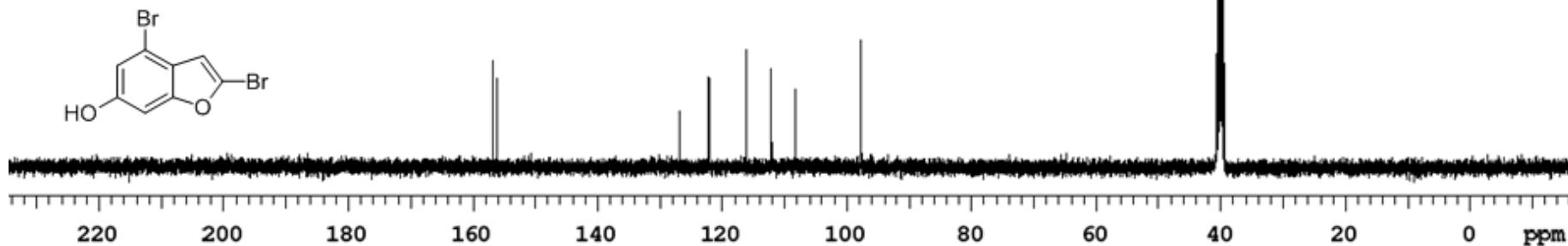
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-60-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-60-01DMSOC

Pulse Sequence: CARBON (s2pul)  
Solvent: dmso  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Aq. time 1.285 sec  
Width 25510.2 Hz  
384 repetitions  
OBSERVE C13, 100.5312520 MHz  
DECOUPLE H1, 399.8078135 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 10 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3k

STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-57-02  
Data Collected on:  
DKU400.ac.kr-vmars400  
Archive directory:

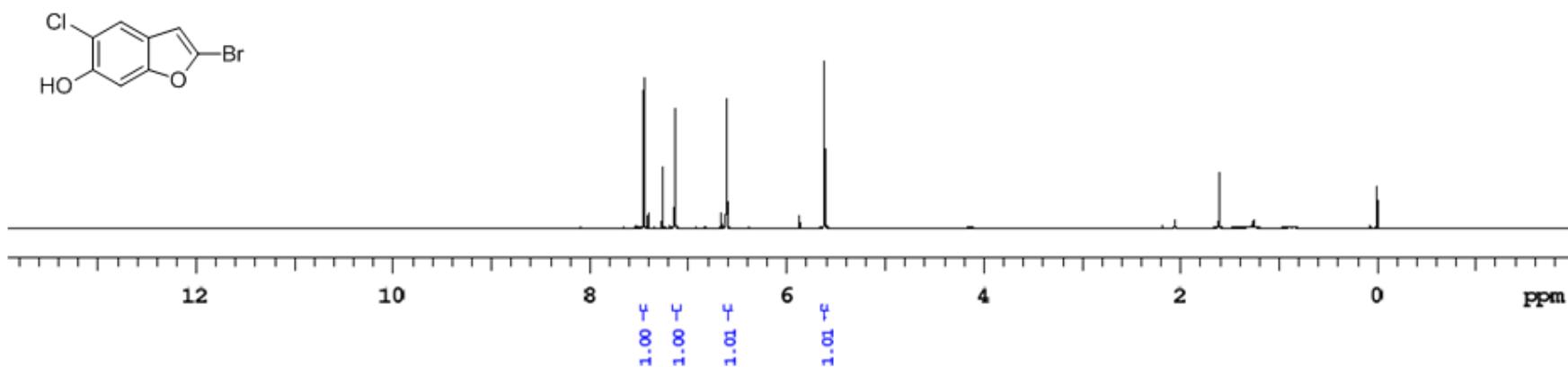
Sample directory:

FidFile: AS-V-57-02

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl<sub>3</sub>  
Data collected on: Jan 14 2019

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE HL, 399.8039100 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3k

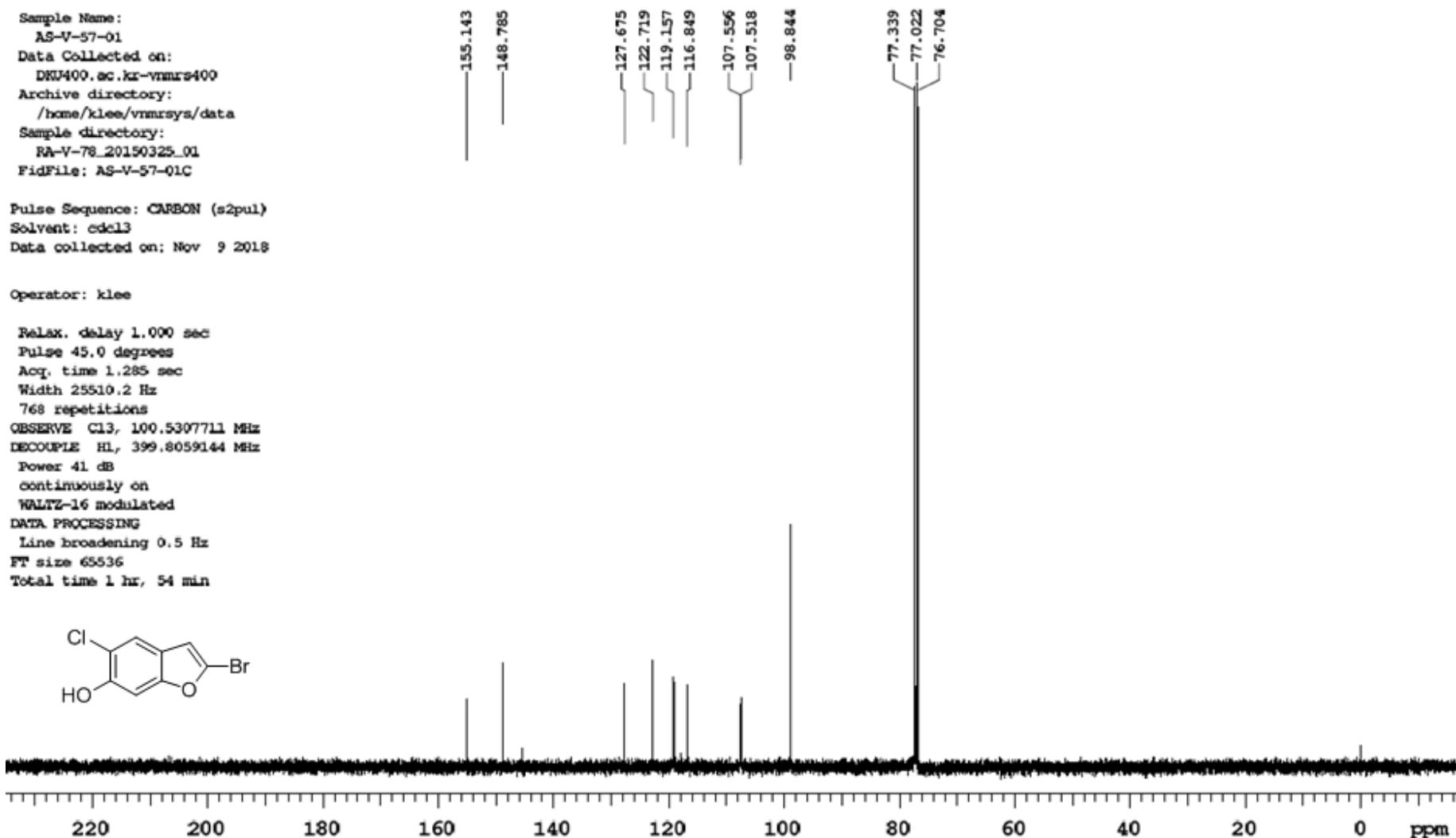
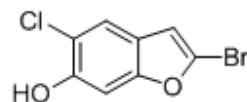
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-57-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-57-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 9 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
768 repetitions  
OBSERVE Cl3, 100.5307711 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3l

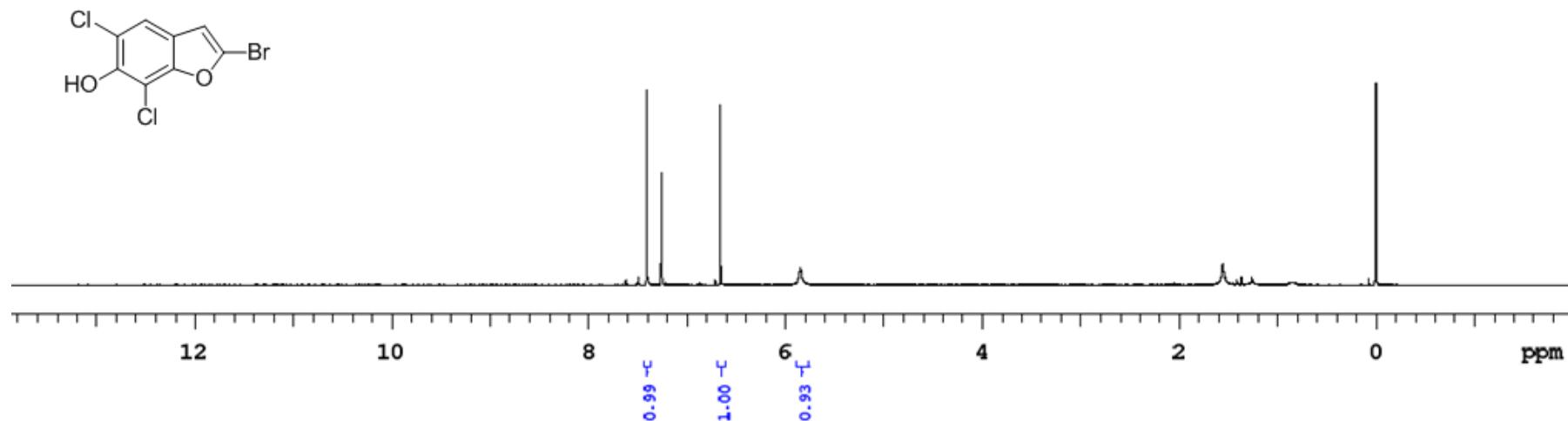
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-62-01  
Data Collected on:  
DKU400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-62-01a

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 8 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE HI, 399.8039096 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 3l

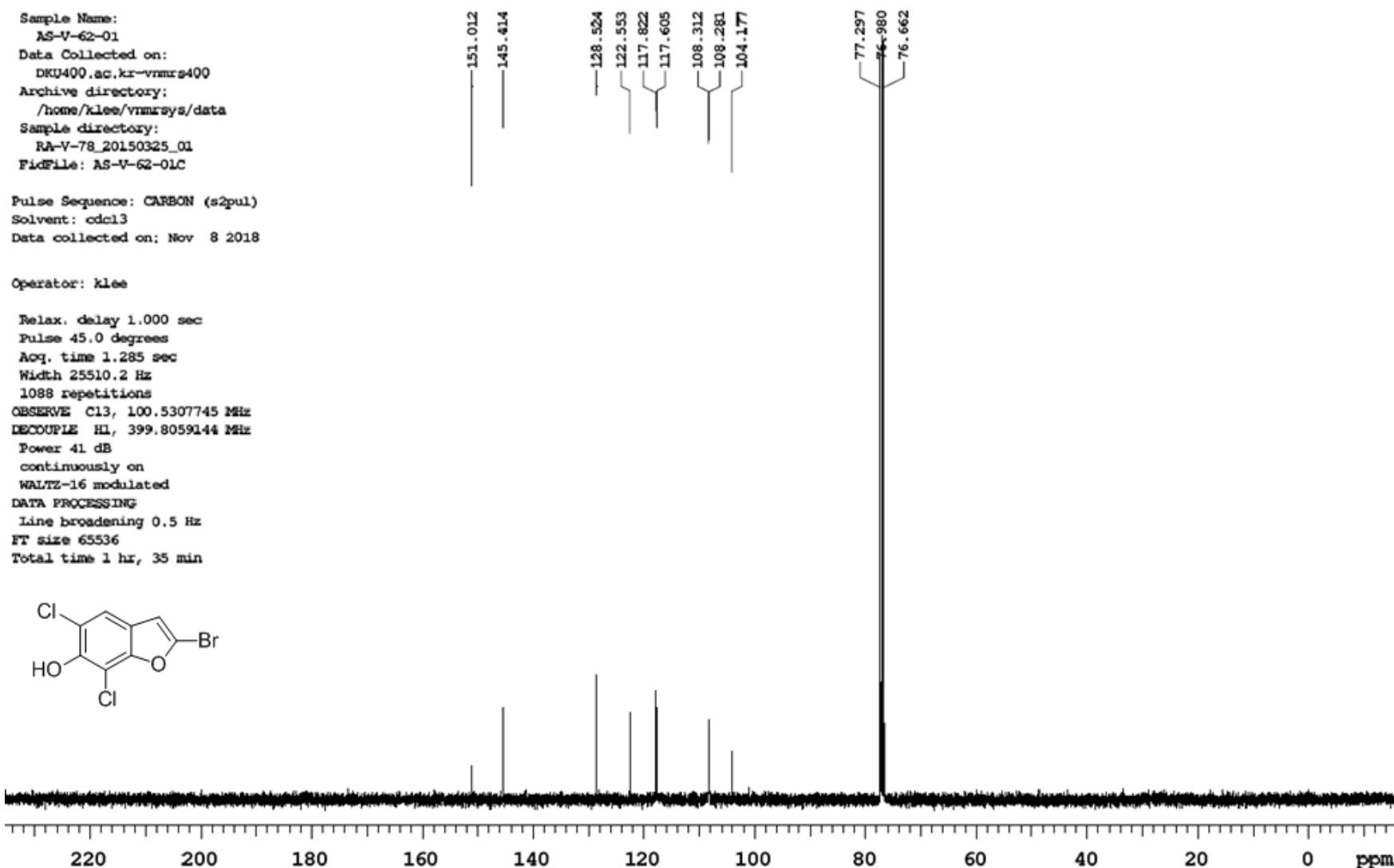
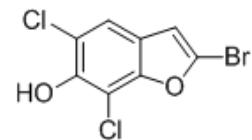
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-62-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-62-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 8 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1088 repetitions  
OBSERVE C13, 100.5307745 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 35 min



<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 3m

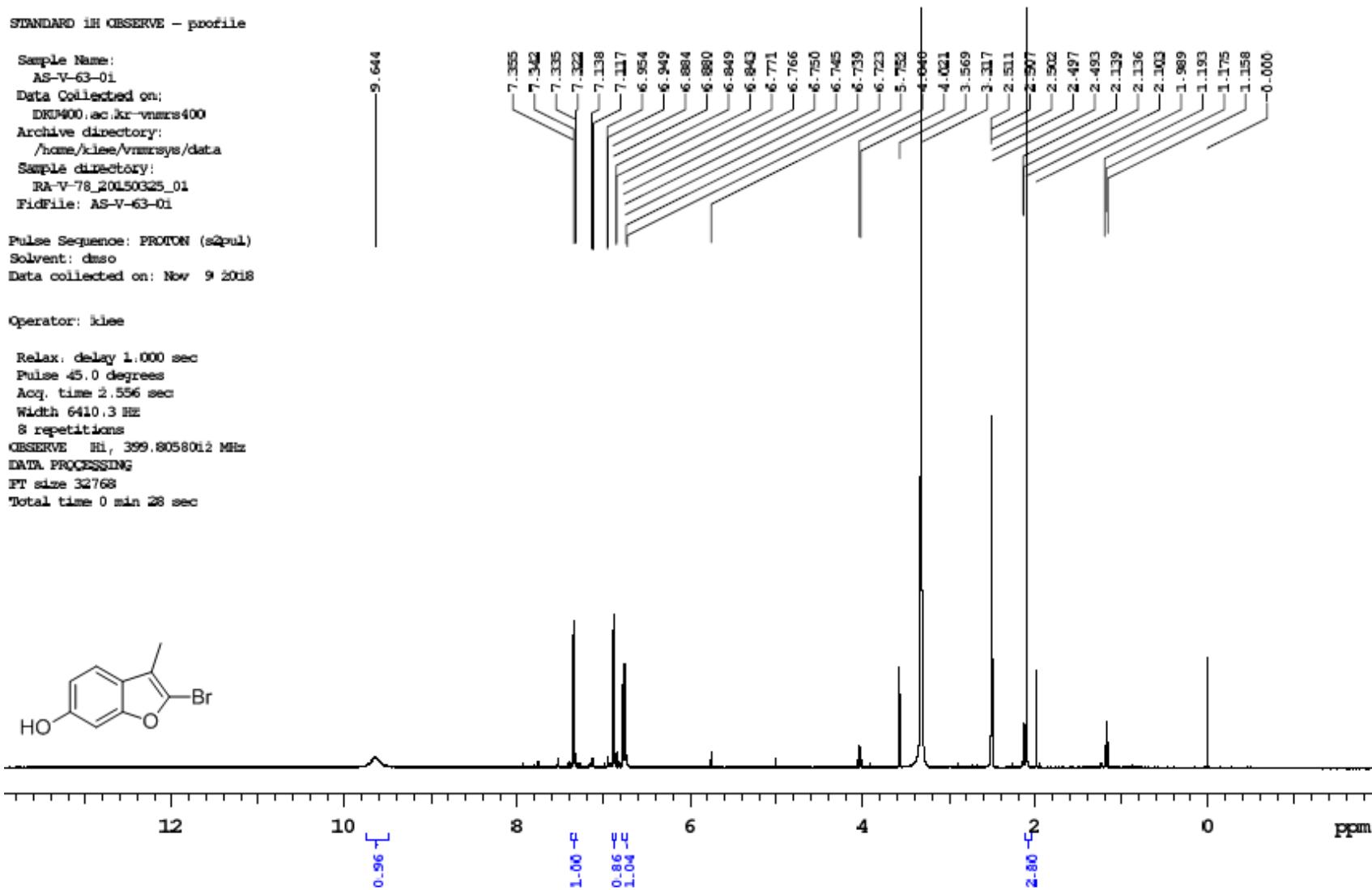
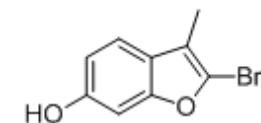
STANDARD 1H OBSERVE - profile

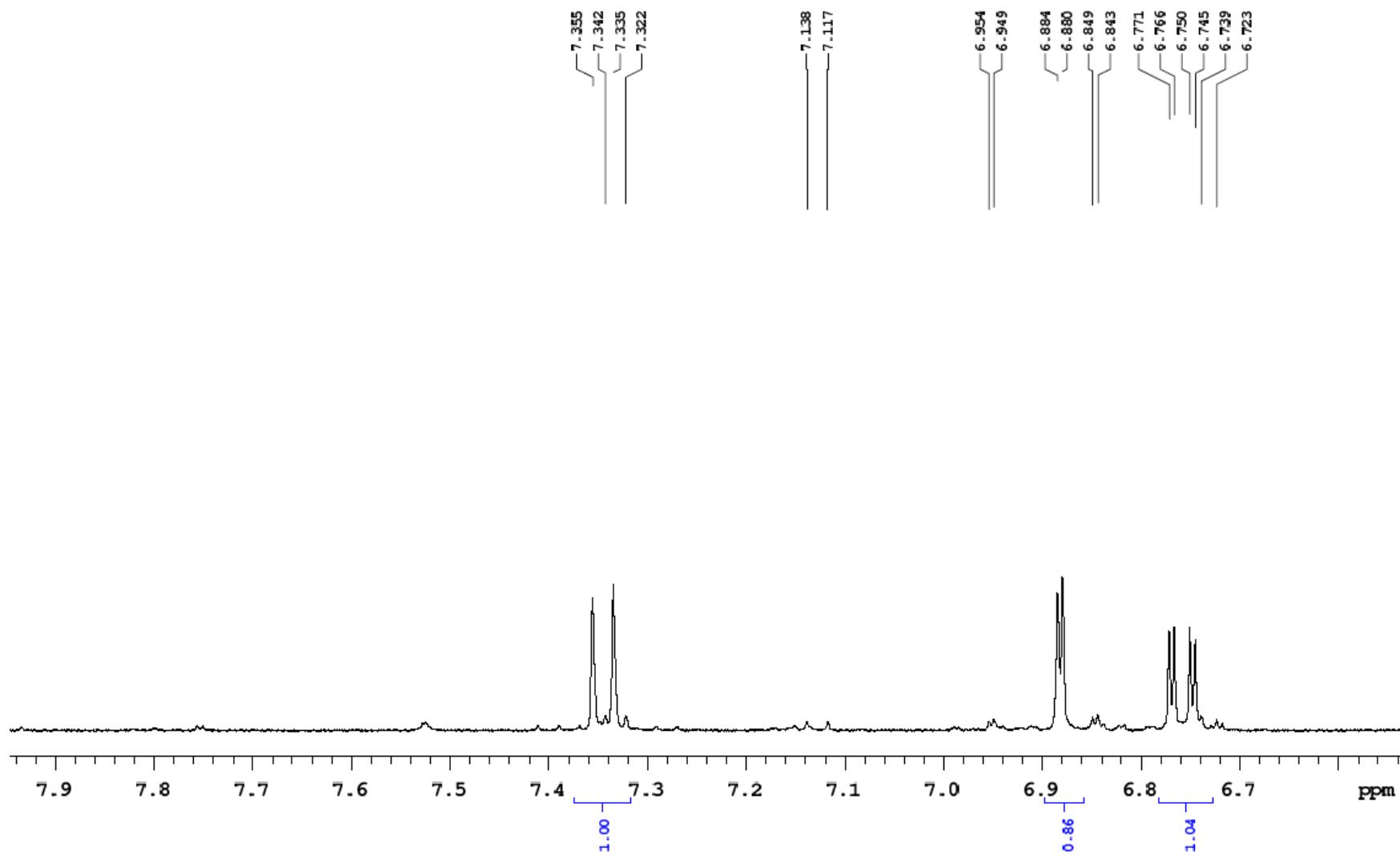
Sample Name:  
AS-V-63-01  
Data Collected on:  
DRX400.acq.Jar-vnmrsys400  
Archive directory:  
/home/kilee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-63-01

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: Nov 9 2018

Operator: kilee

Relax: delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE HI, 399.80580i2 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 28 sec





<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) spectrum of compound 3m

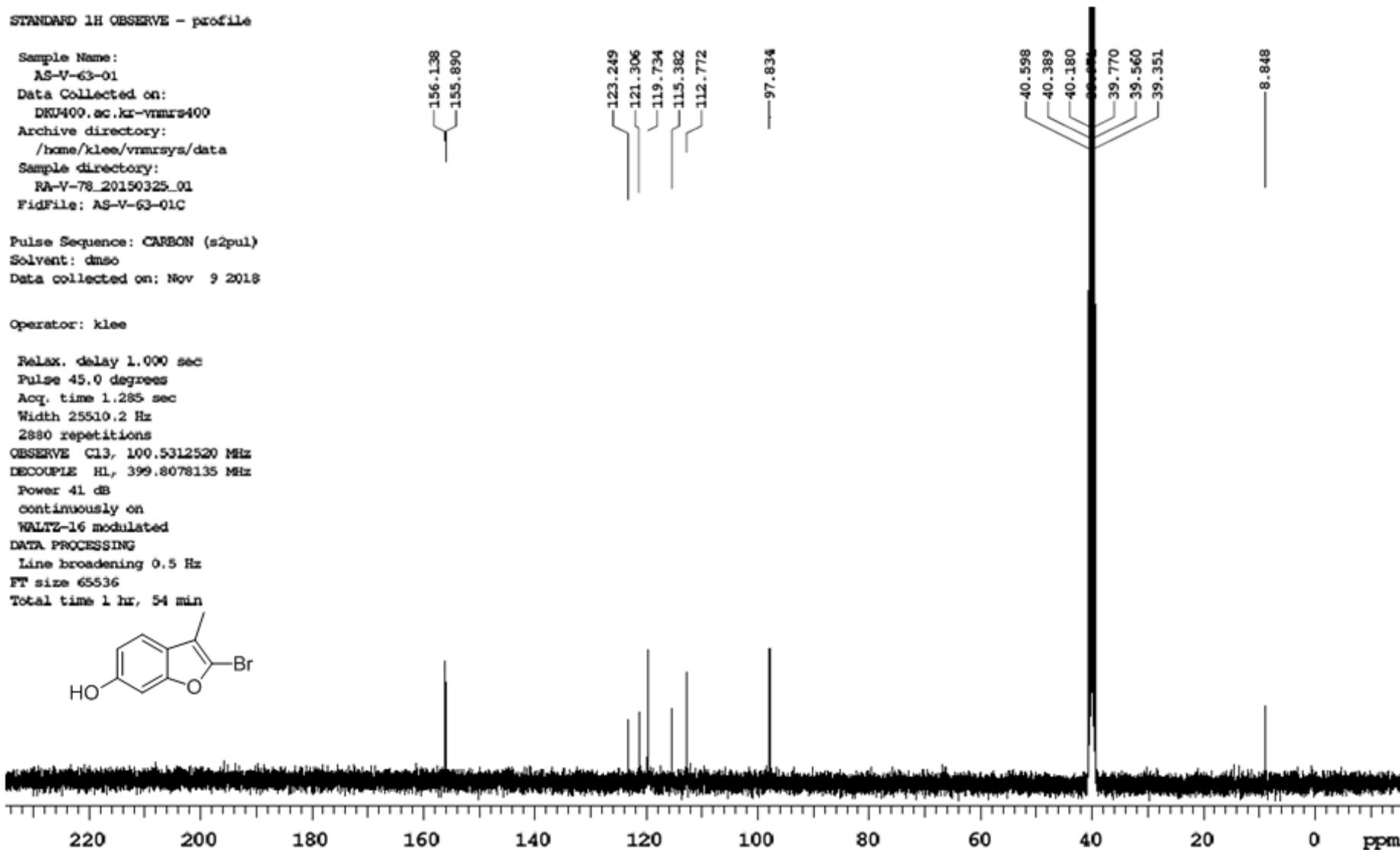
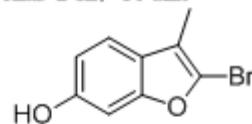
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-63-01  
Data Collected on:  
DKU400.sc.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-63-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: dmso  
Data collected on: Nov 9 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
2880 repetitions  
OBSERVE Cl3, 100.5312520 MHz  
DECOUPLE H1, 399.8078135 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) spectrum of compound 13

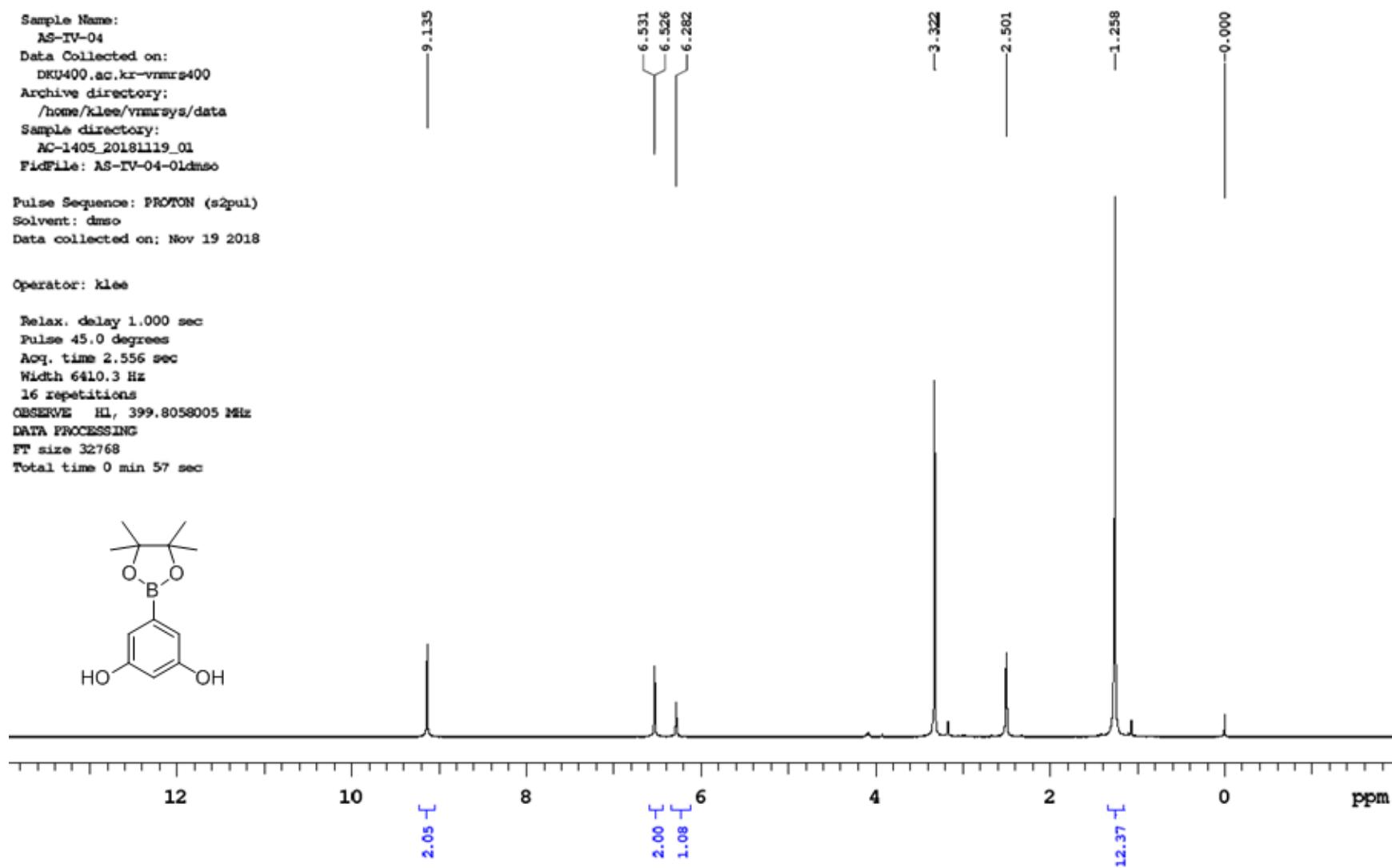
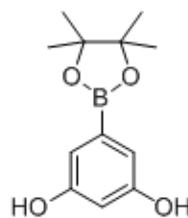
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-04  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
AC-1405\_20181119\_01  
FidFile: AS-IV-04-01dmso

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: Nov 19 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H1, 399.8058005 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) spectrum of compound 13

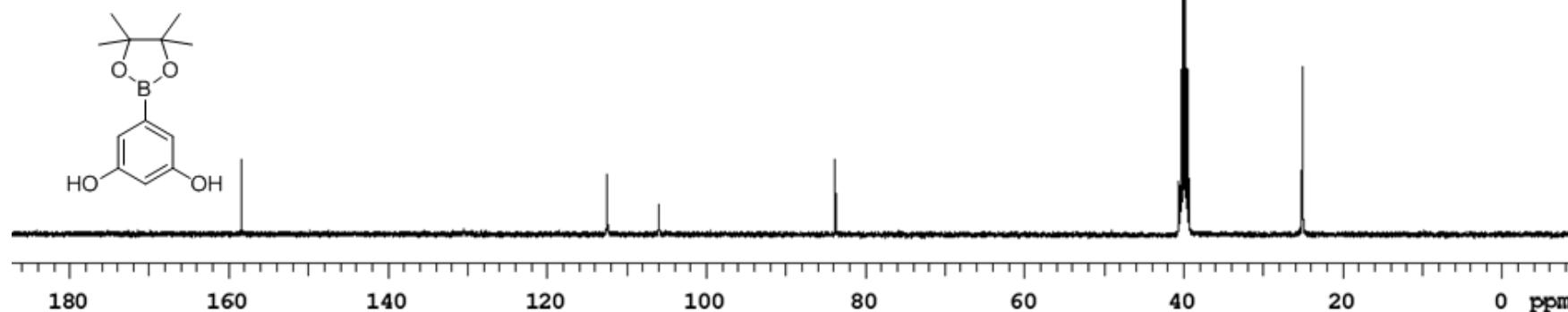
STANDARD 1H OBSERVE - profile

Sample Name: AS-IV-04  
 Data Collected on: DKU400.ac.kr-vnmrs400  
 Archive directory: /home/klee/vnmrsys/data  
 Sample directory: AC-1405\_20181119\_01  
 FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
 Solvent: dmso  
 Data collected on: Nov 19 2018

Temp. 25.5 C / 298.6 K  
 Operator: klee

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Aq. time 1.285 sec  
 Width 25510.2 Hz  
 1664 repetitions  
 OBSERVE C13, 100.5312520 MHz  
 DECOUPLE H1, 399.8078135 MHz  
 Power 41 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 3 hr, 10 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **14**

STANDARD 1H OBSERVE - profile

Sample Name:  
AS-TV-43-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:

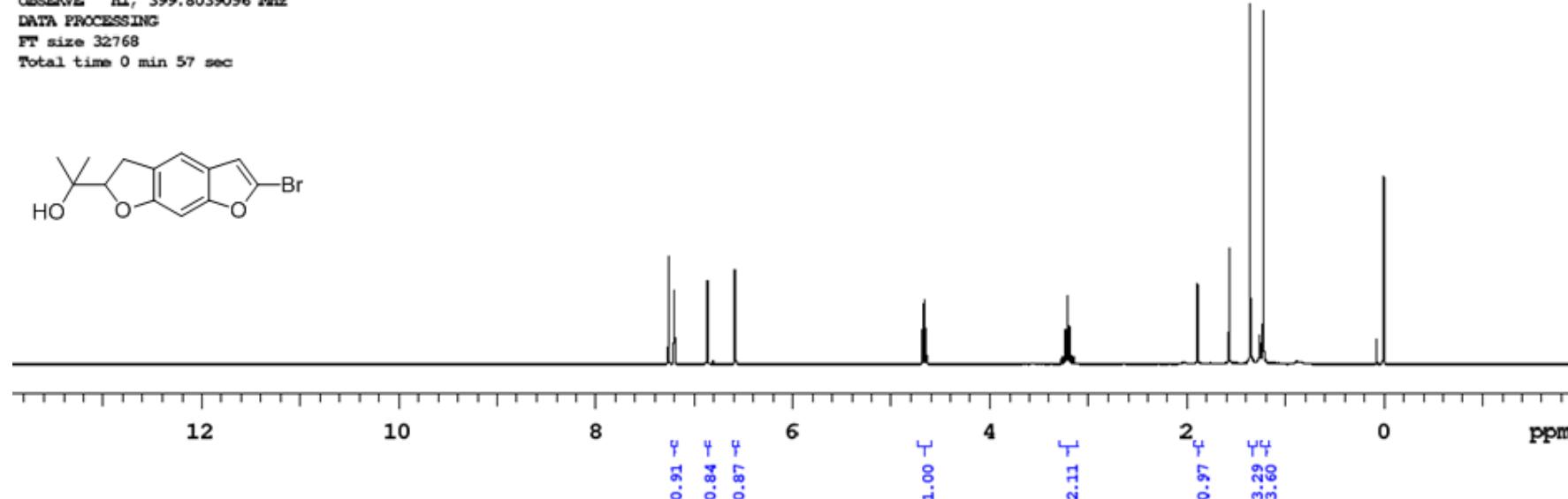
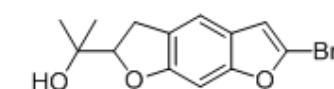
Sample directory:

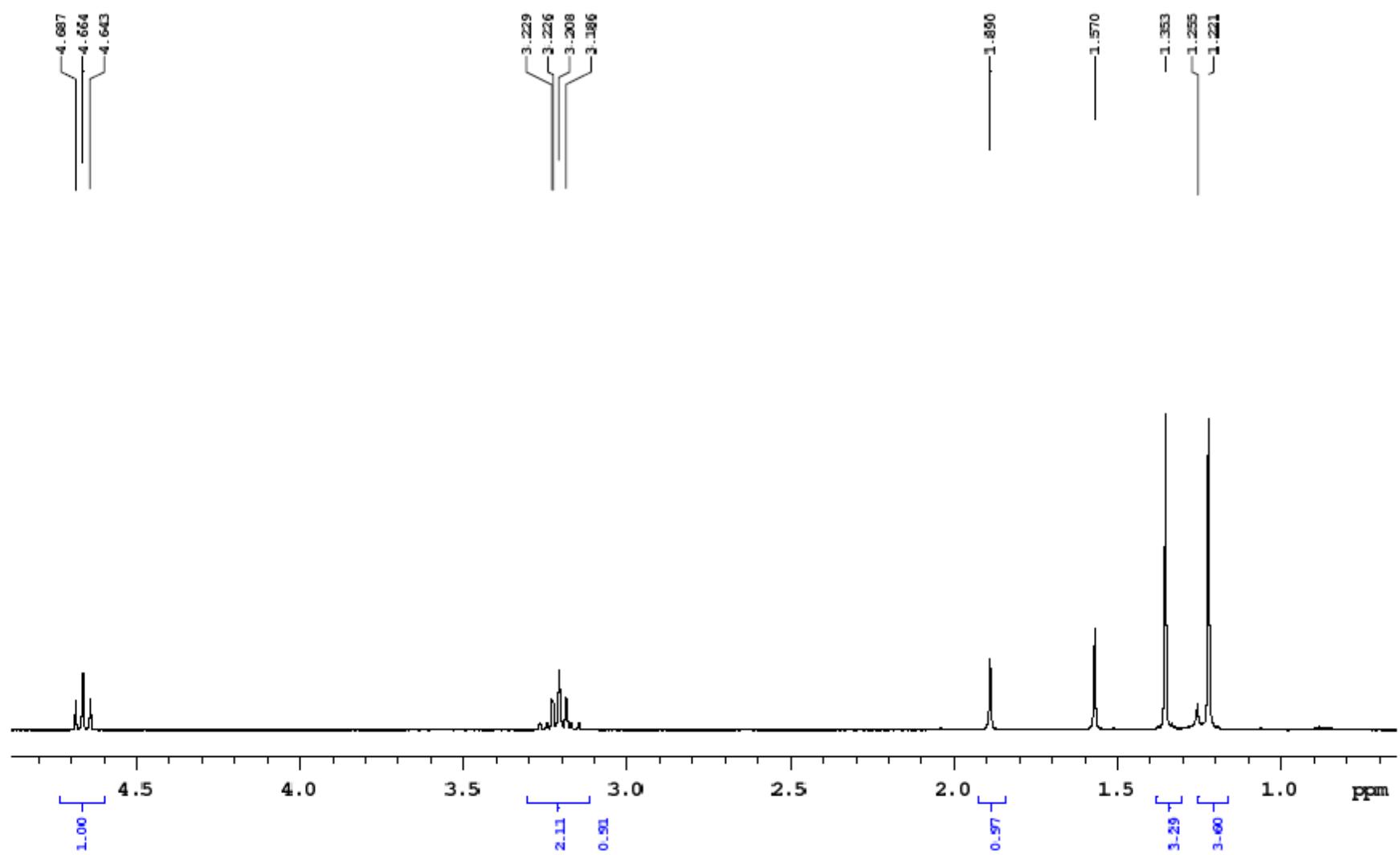
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl<sub>3</sub>  
Data collected on: Jul 20 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H1, 399.8039096 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound **14**

STANDARD 1H OBSERVE - profile

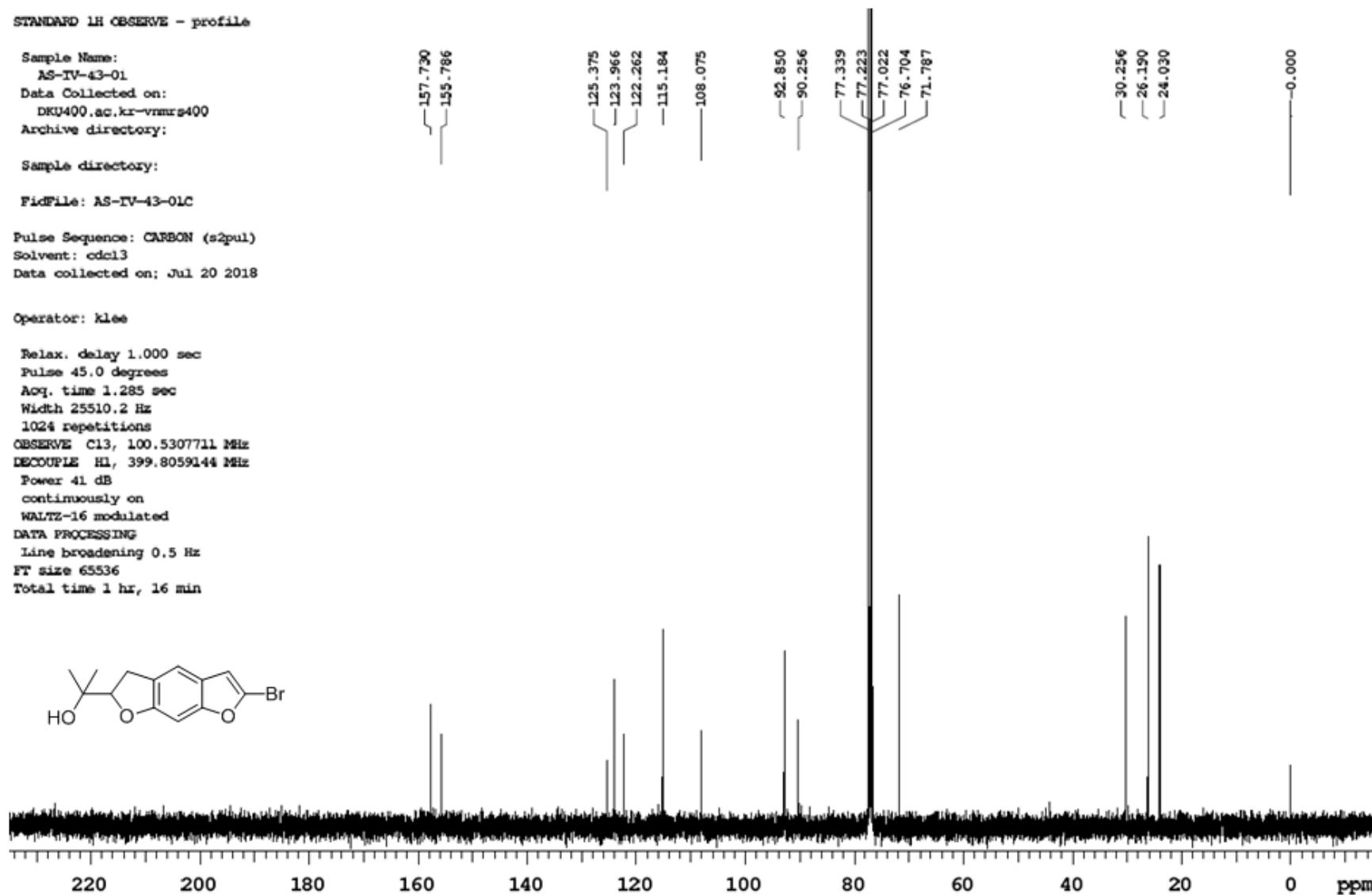
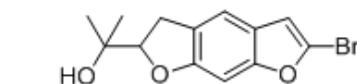
Sample Name:  
AS-IV-43-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:

Sample directory:  
FidFile: AS-IV-43-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 20 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1024 repetitions  
OBSERVE C13, 100.5307711 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 16 min



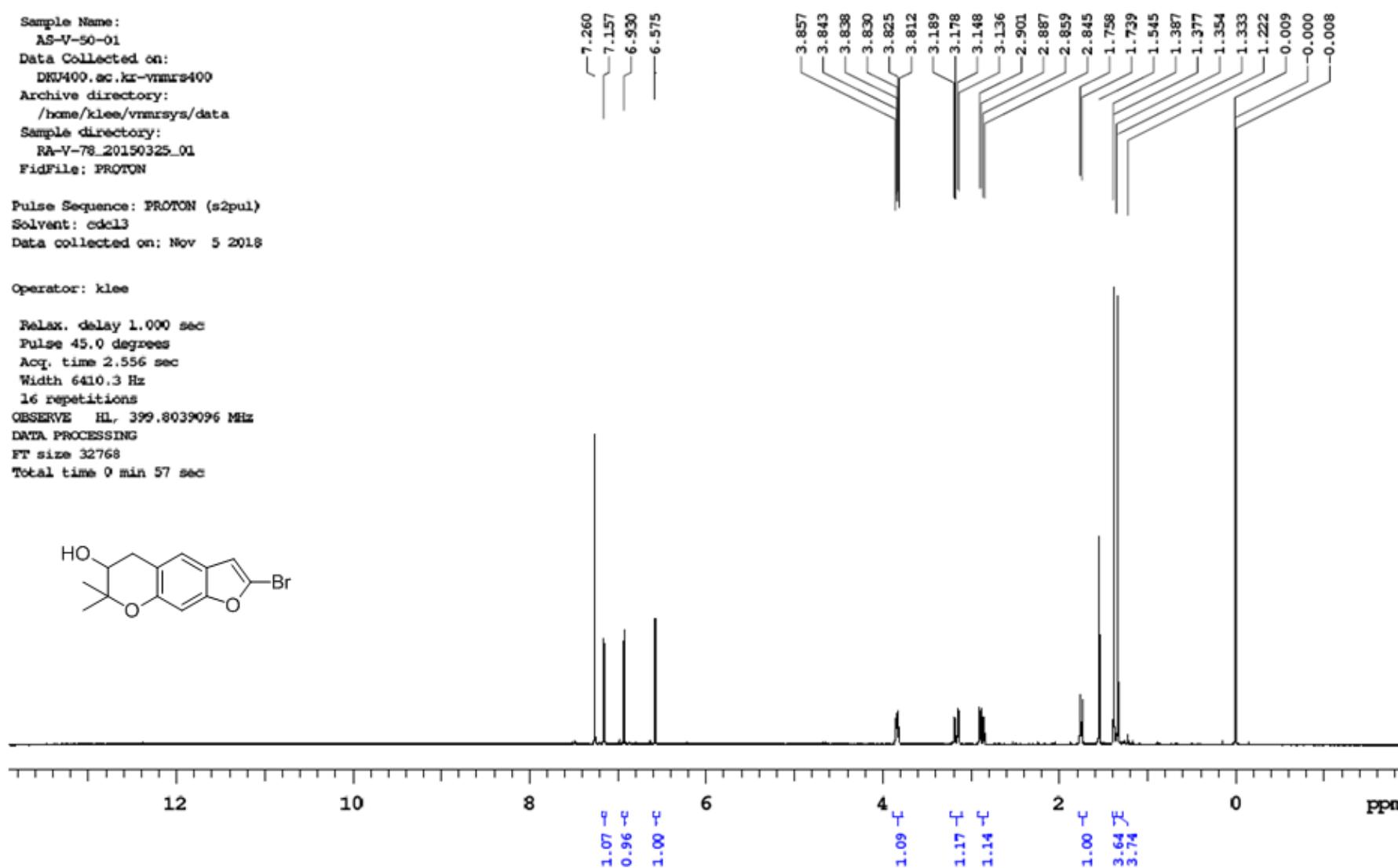
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **15**

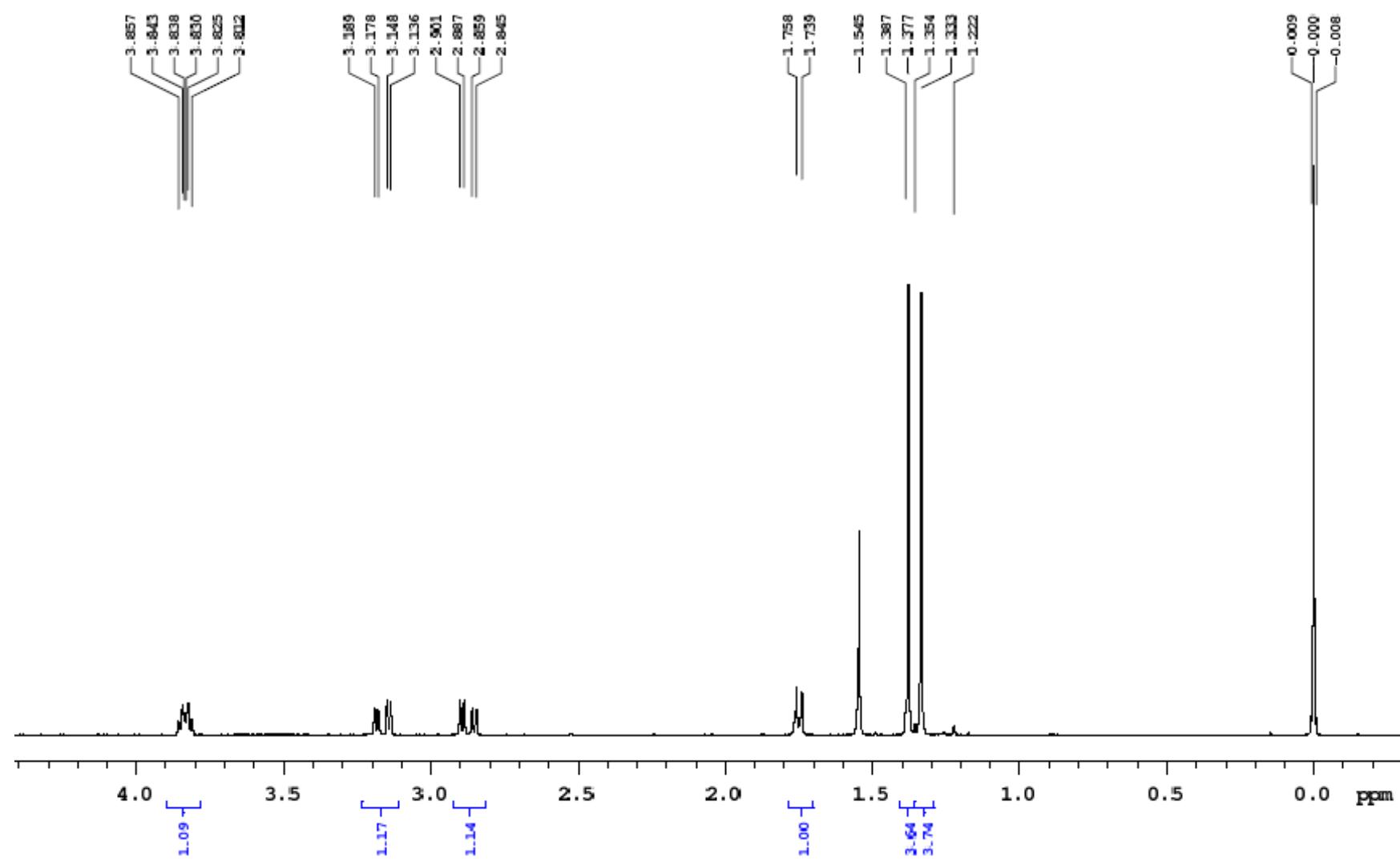
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-50-01  
Data Collected on:  
DRX400.sc.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: PROTON  
  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl<sub>3</sub>  
Data collected on: Nov 5 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H, 399.8039096 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 15

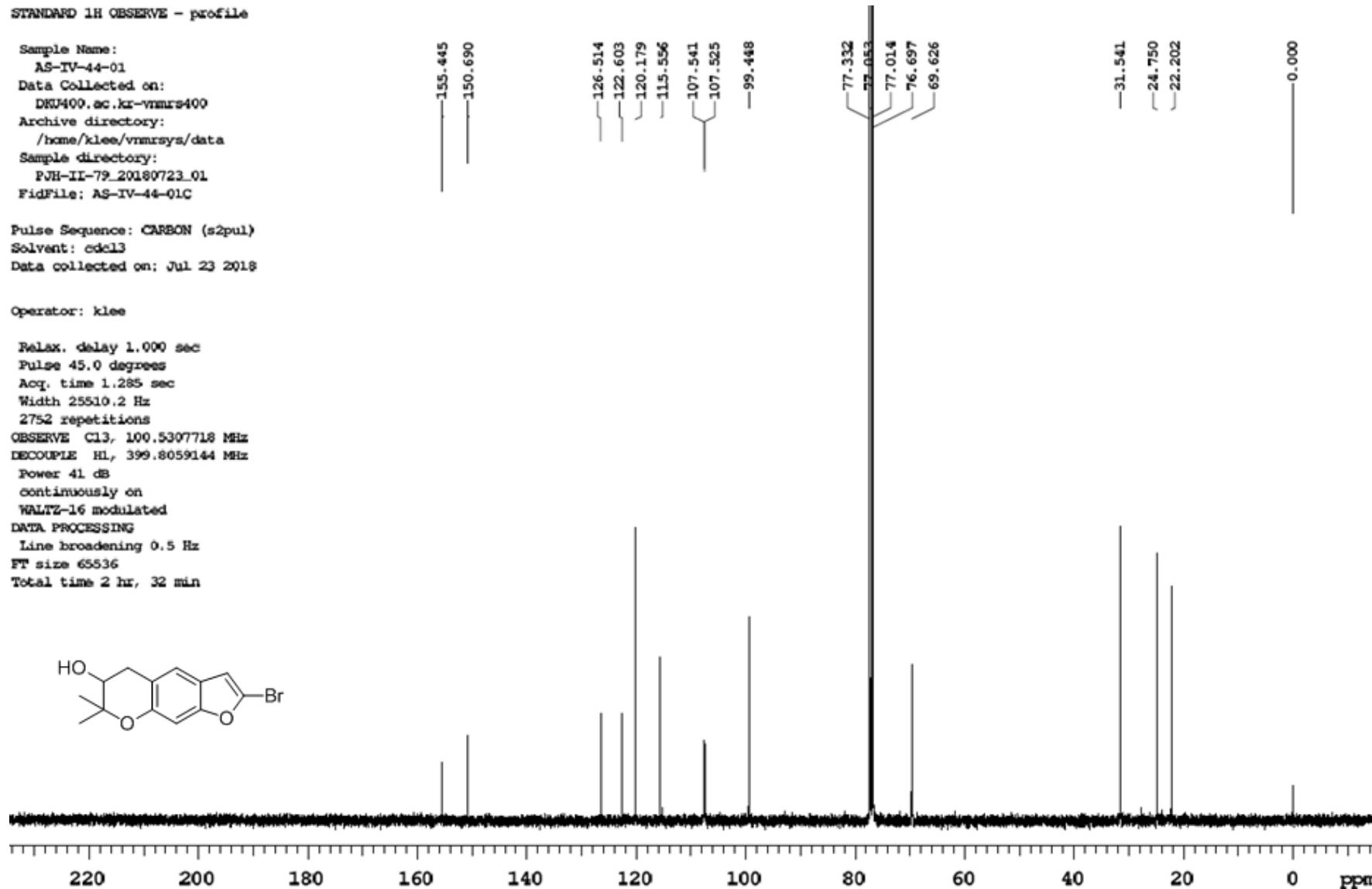
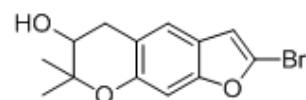
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-44-01  
Data Collected on:  
DKU400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
PJH-II-79\_20180723\_01  
FidFile: AS-IV-44-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 23 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
2752 repetitions  
OBSERVE Cl3, 100.5307718 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 2 hr, 32 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **16**

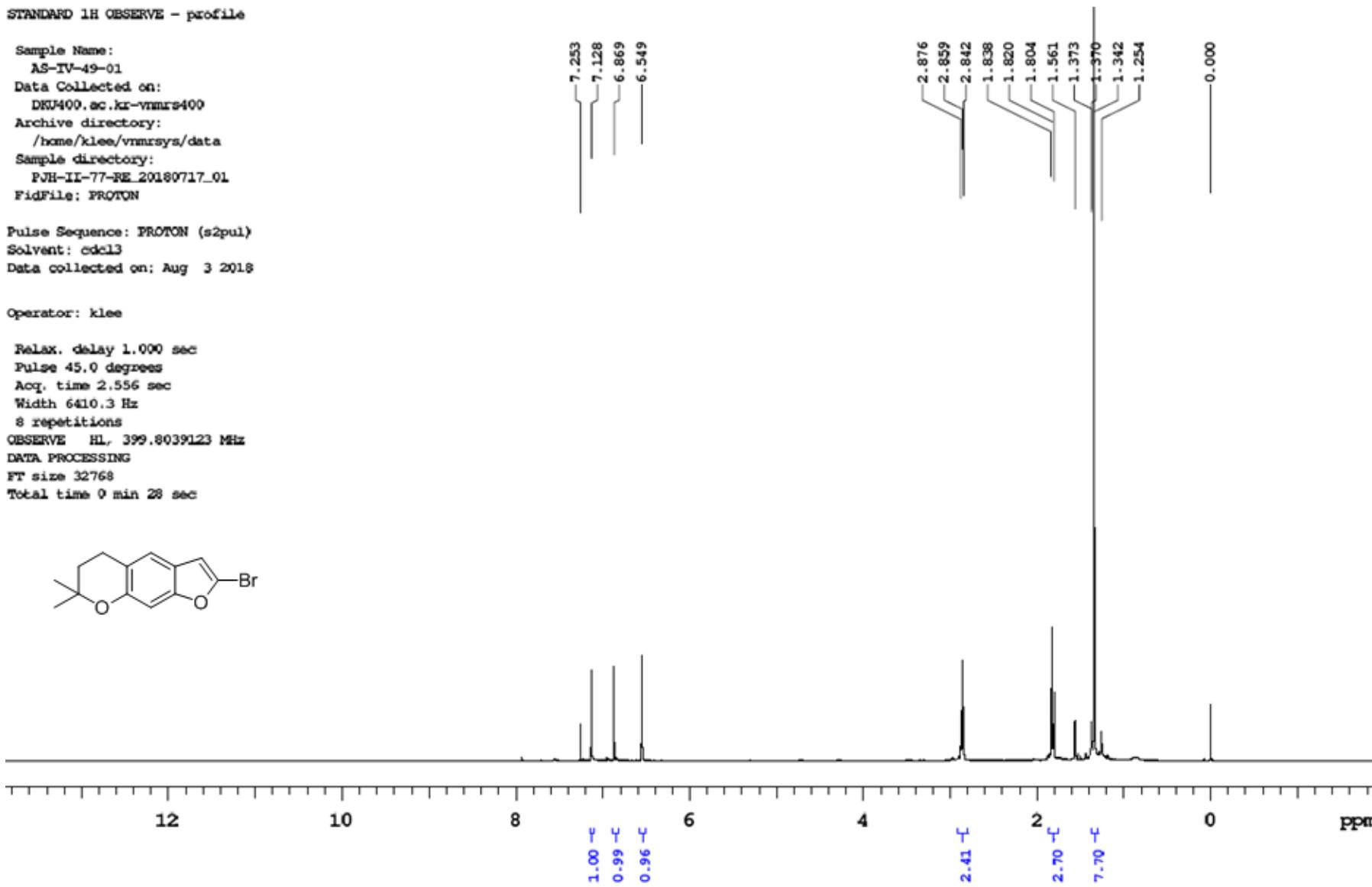
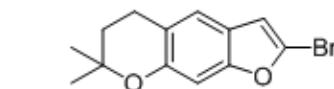
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-49-01  
Data Collected on:  
DKJ400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
PJH-II-77-RE\_20180717\_01  
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl<sub>3</sub>  
Data collected on: Aug 3 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE HL 399.8039123 MHz  
DATA PROCESSING  
FT size 32768  
Total time 9 min 28 sec



<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound **16**

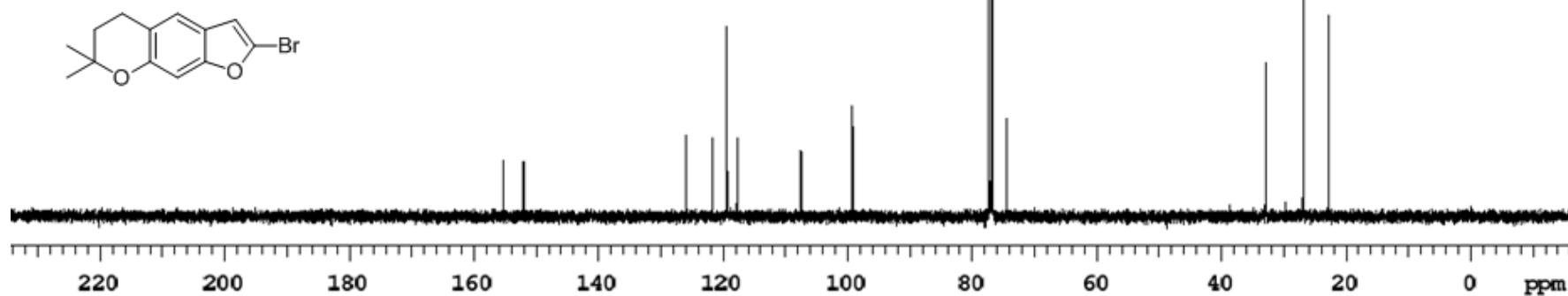
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-49-01  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
PJH-II-77-RE\_20180717\_01  
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Aug 3 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Aqc. time 1.285 sec  
Width 25510.2 Hz  
384 repetitions  
OBSERVE CL3, 100.5307745 MHz  
DECOUPLE HL, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **17**

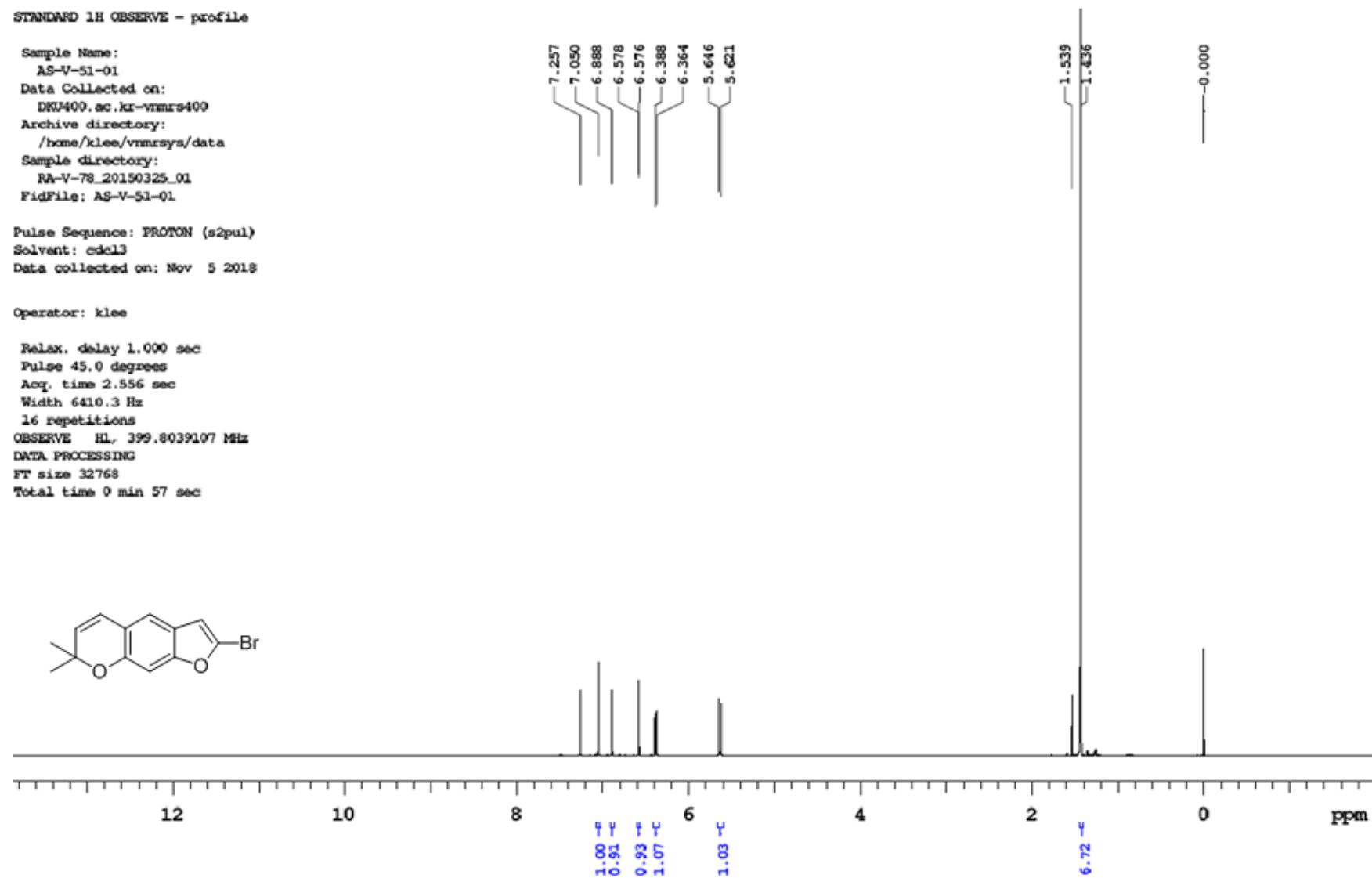
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-51-01  
Data Collected on:  
DKU400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-51-01

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 5 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H,L 399.8039107 MHz  
DATA PROCESSING  
FT size 32768  
Total time 9 min 57 sec



<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 17

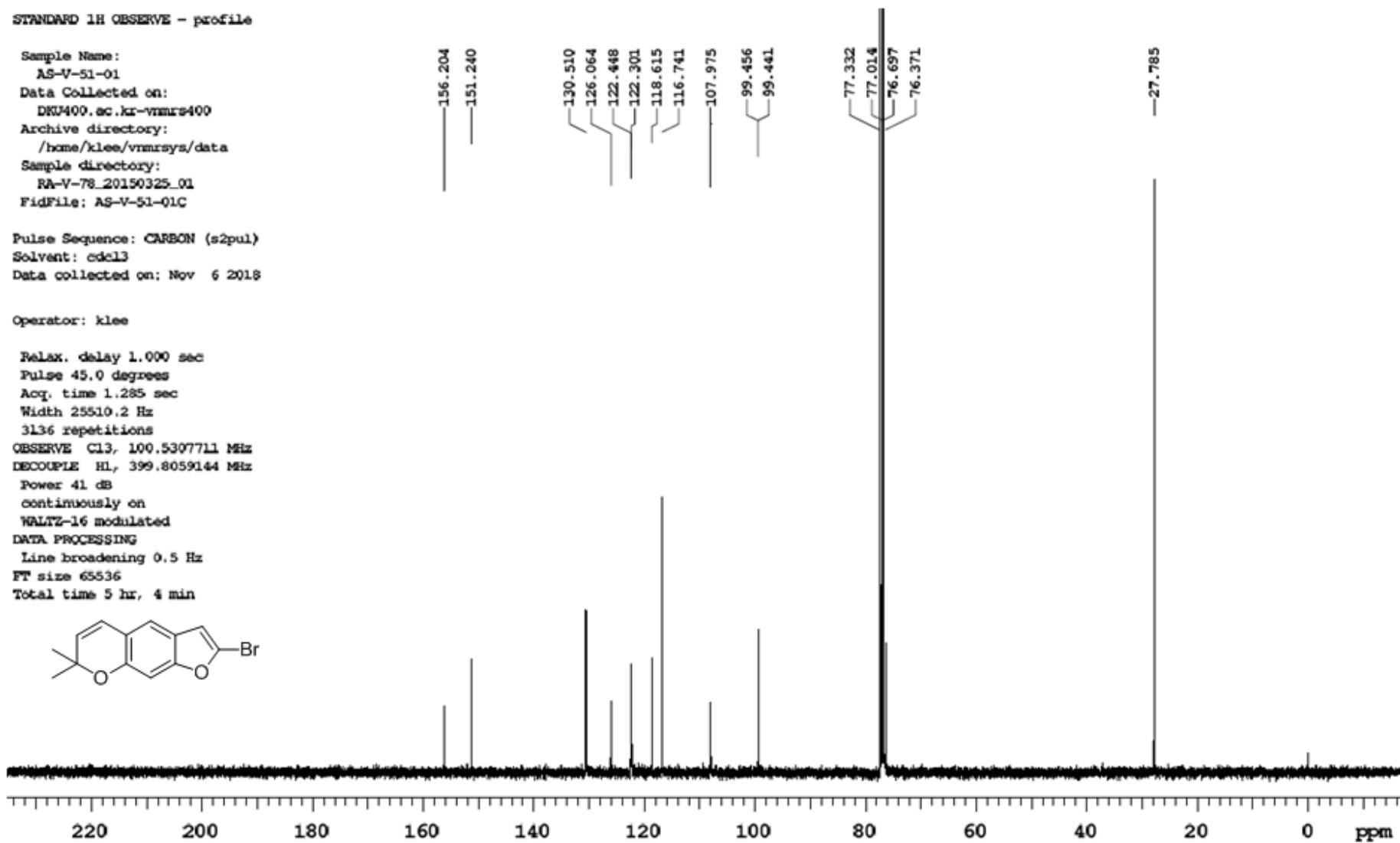
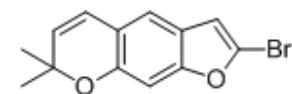
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-51-01  
Data Collected on:  
DKU400.ac.kr-vmnars400  
Archive directory:  
/home/klee/vmnarsys/data  
Sample directory:  
RA-V-78\_20190325\_01  
FidFile: AS-V-51-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 6 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
3136 repetitions  
OBSERVE CL3, 100.5307711 MHz  
DECOUPLE HL, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 5 hr, 4 min



<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) spectrum of moracin M (**4**)

new experiment

Sample Name:  
AS-IV-34-01  
Data Collected on:  
DKU400.ac.kr-vmnrs400  
Archive directory:

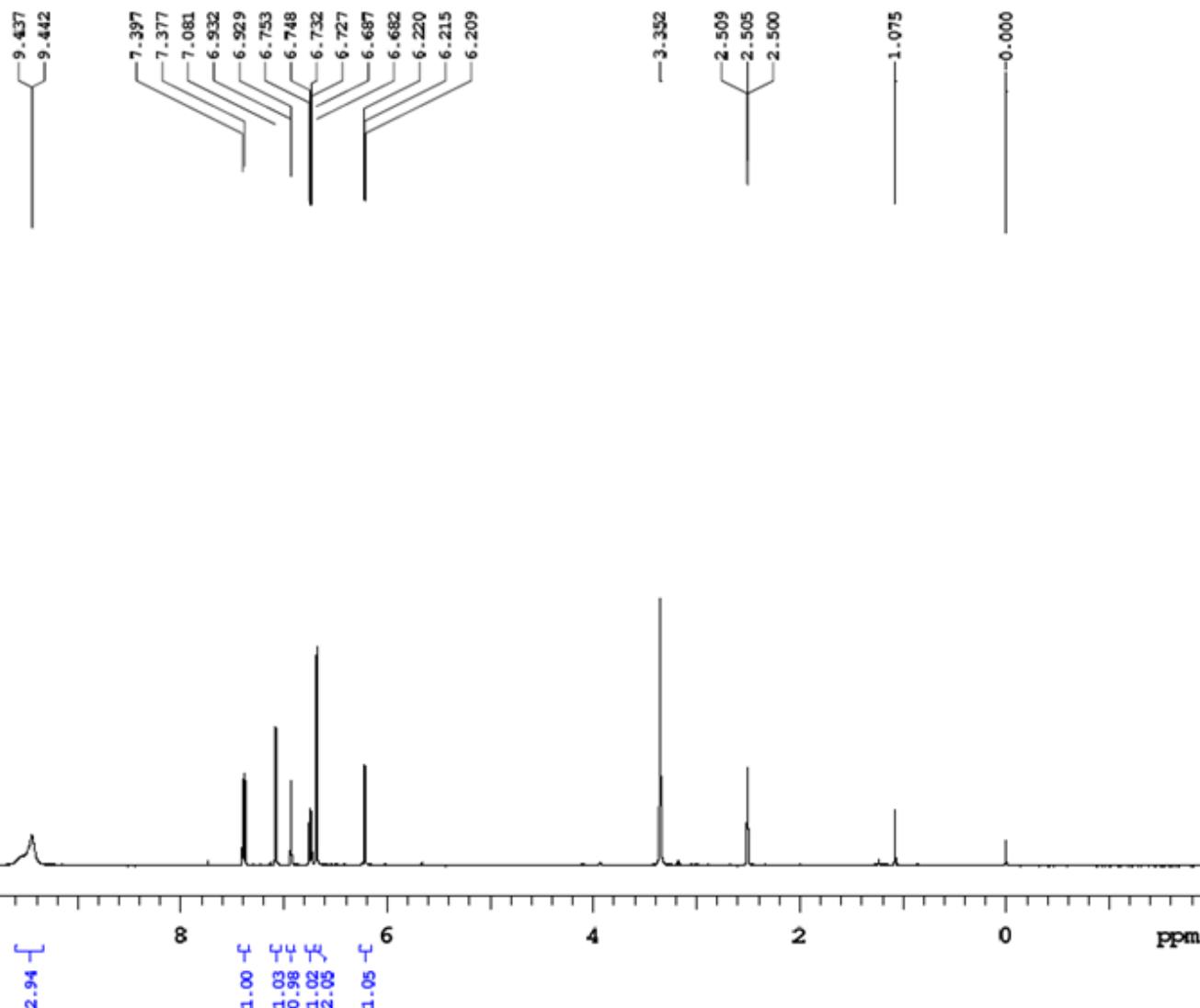
Sample directory:

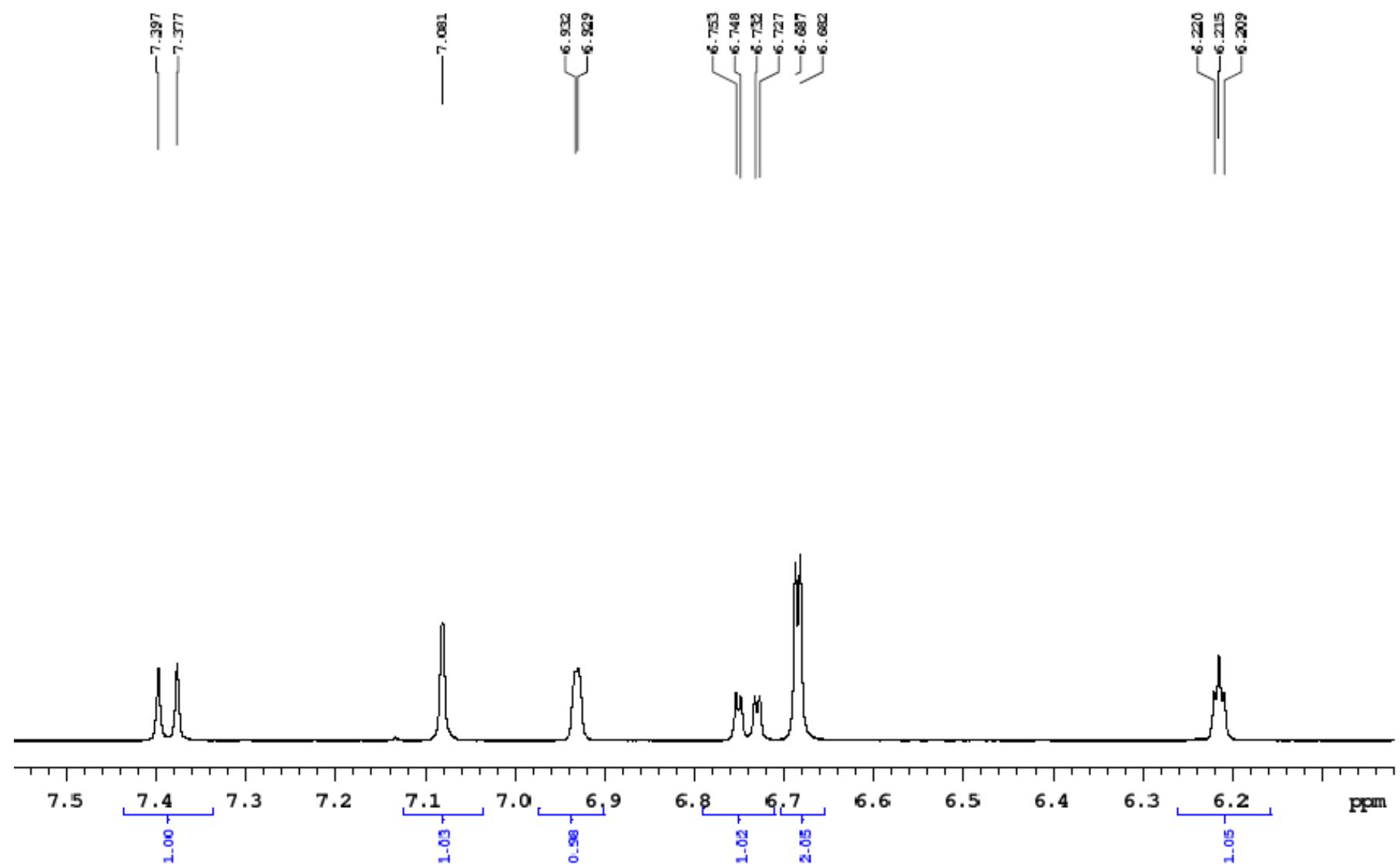
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: Jul 2 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE HL, 399.8058001 MHz  
DATA PROCESSING  
FT size 32768  
Total time 9 min 26 sec





new experiment

Sample Name:  
AS-IV-34-01  
Data Collected on:  
DKU400.ac.kr-vmrs400  
Archive directory:

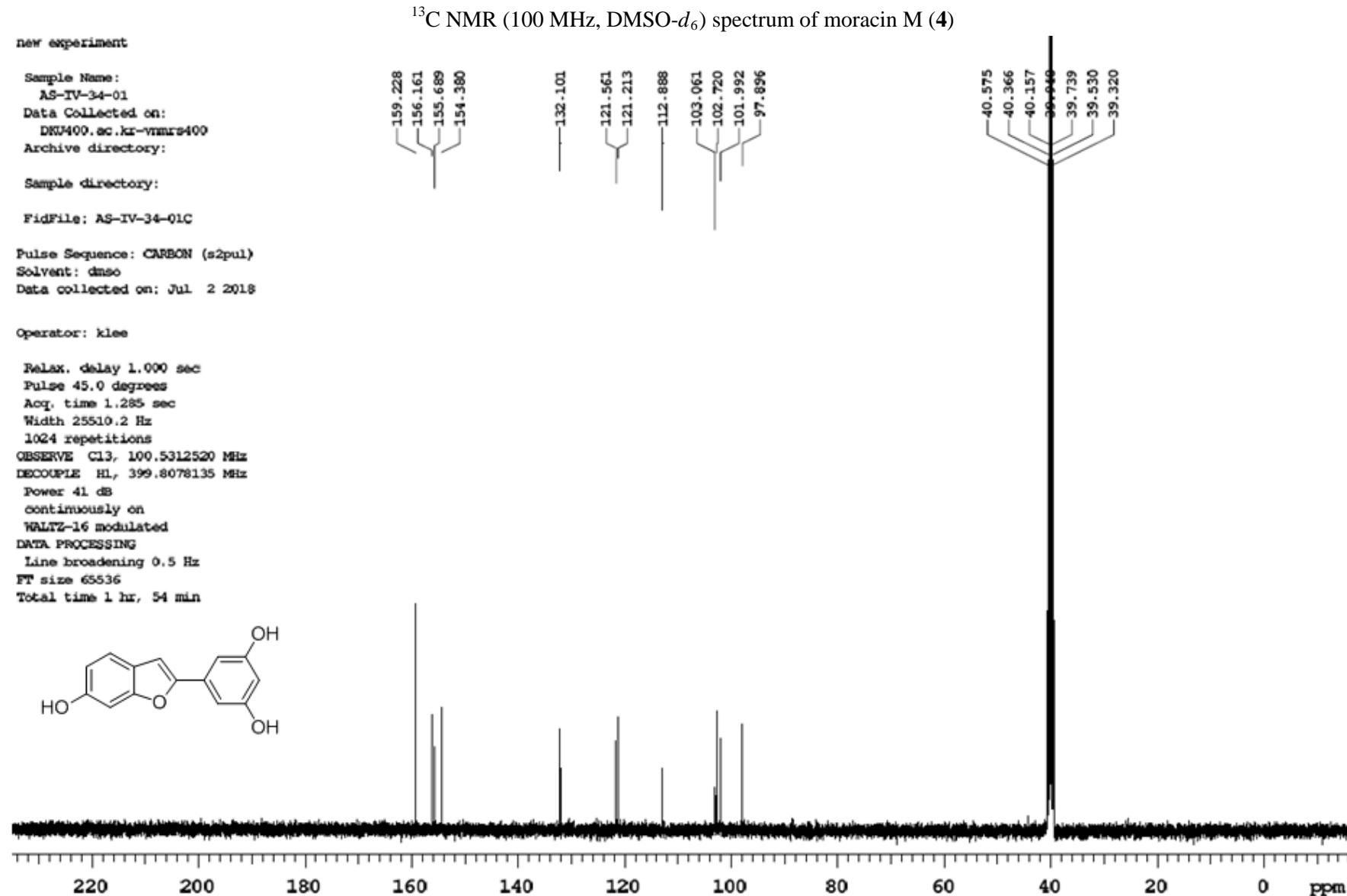
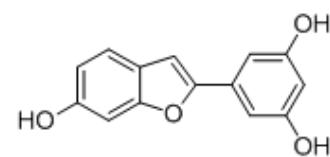
Sample directory:

FidFile: AS-IV-34-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: dmso  
Data collected on: Jul 2 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1024 repetitions  
OBSERVE Cl3, 100.5312520 MHz  
DECOUPLE H1, 399.8078135 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (600 MHz, methanol-*d*4) spectrum of moracin N (**5**)

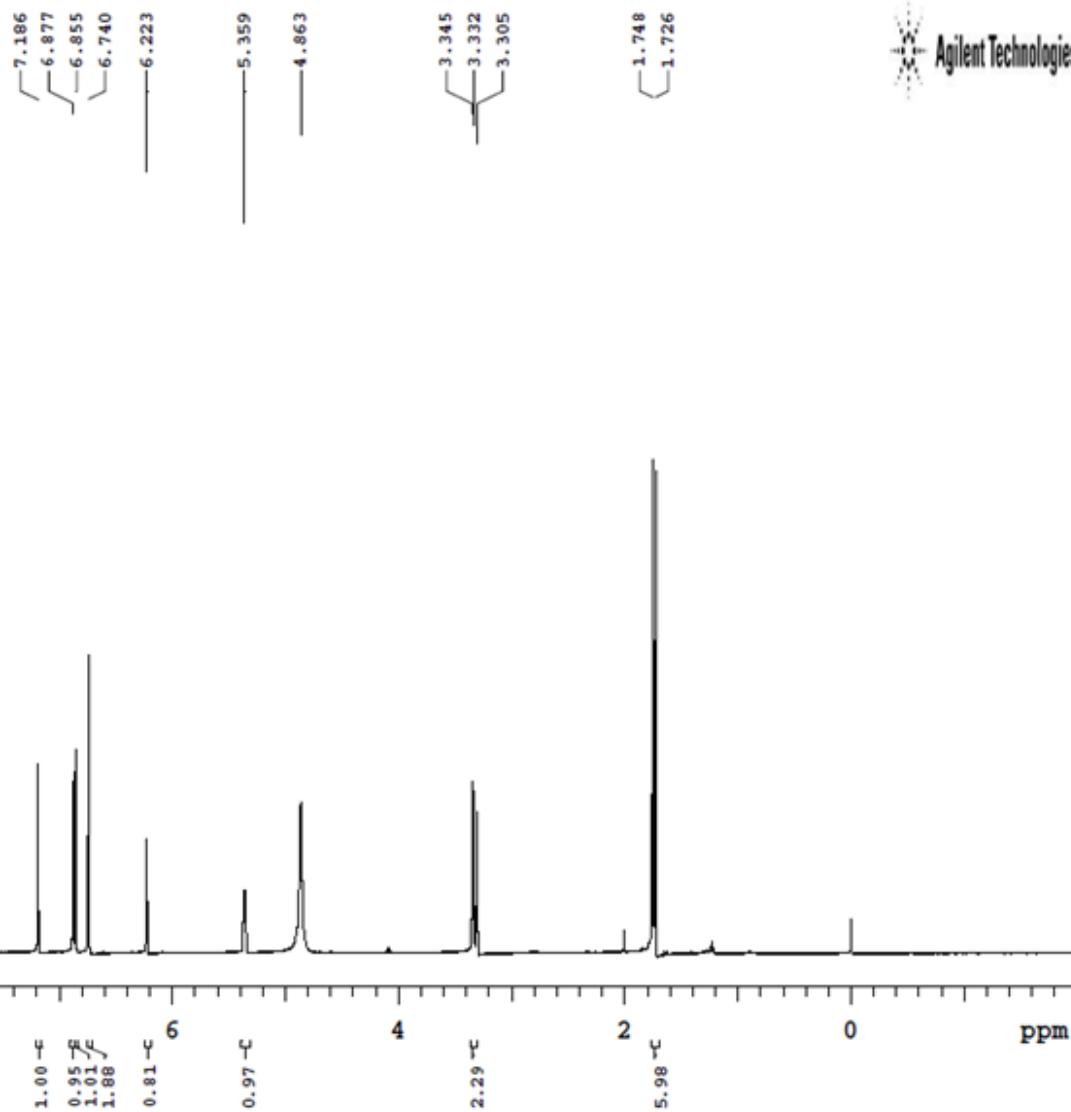
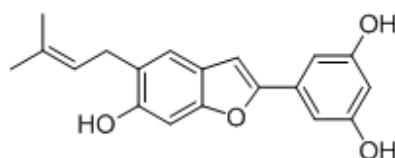
Calibration for 5mm\_One\_probe on 14Jul2017  
Sample : C13 enriched CH3OH in doped D2O (autotest)

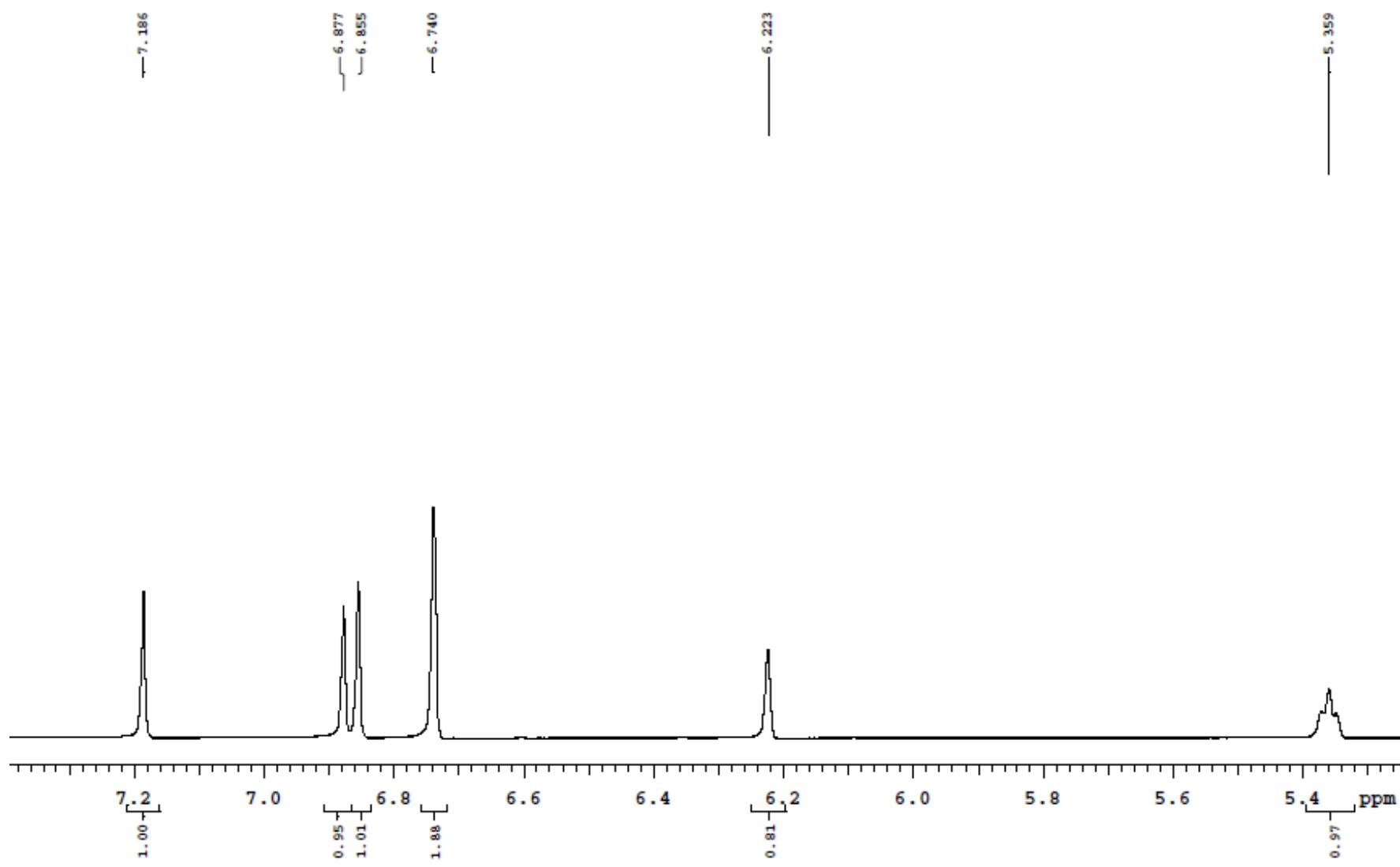
Sample Name:  
AS-IV-80-01  
Data Collected on:  
DKU600.ac.kr-vnmrsys600  
Archive directory:  
/home/vnmr1/vnmrsys/probes/probe\_calibs  
Sample directory:  
5mm\_One\_probe\_calib  
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Oct 16 2018

Operator: vnmr1

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.704 sec  
Width 9615.4 Hz  
16 repetitions  
OBSERVE H1, 599.9253817 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 43 sec





<sup>13</sup>C NMR (150 MHz, methanol-*d*4) spectrum of moracin N (**5**)

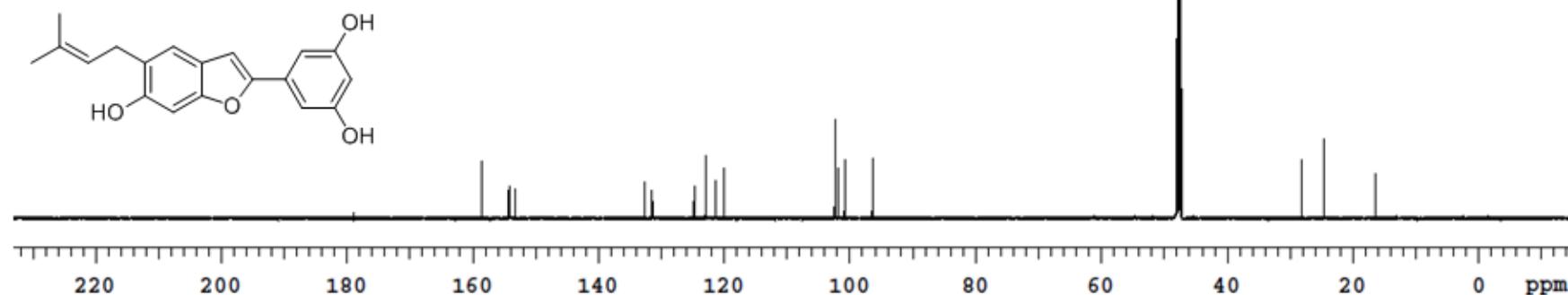
Calibration for 5mm\_One\_probe on 14Jul2017  
Sample : C13 enriched CH3OH in doped D2O (autotest)

Sample Name:  
AS-IV-80-01  
Data Collected on:  
DKU600.ac.kr-vnmrs600  
Archive directory:  
/home/vnmr1/vnmrsys/probes/probe\_calibs  
Sample directory:  
5mm\_One\_probe\_calib  
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3od  
Data collected on: Oct 16 2018

Operator: vnmr1

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.865 sec  
Width 37870.8 Hz  
2752 repetitions  
OBSERVE C13, 150.8513572 MHz  
DECOUPLE H1, 599.9283813 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 2 hr, 35 min



<sup>1</sup>H NMR (400 MHz, methanol-*d*<sub>4</sub>) spectrum of moracin O (**6**).

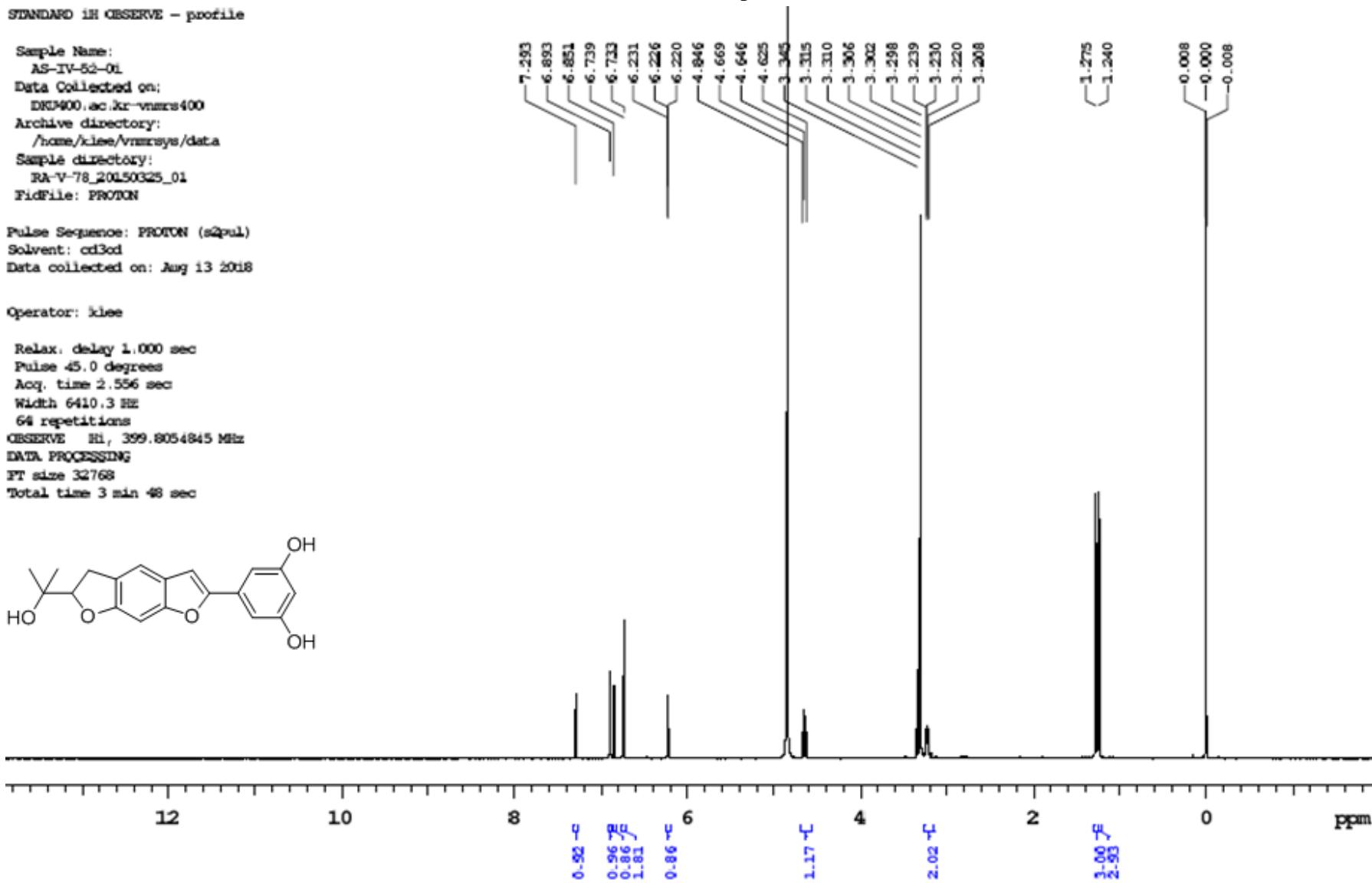
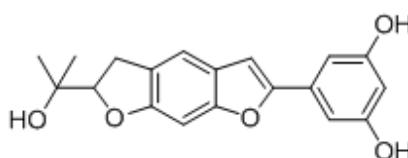
STANDARD 1H OBSERVE - profile

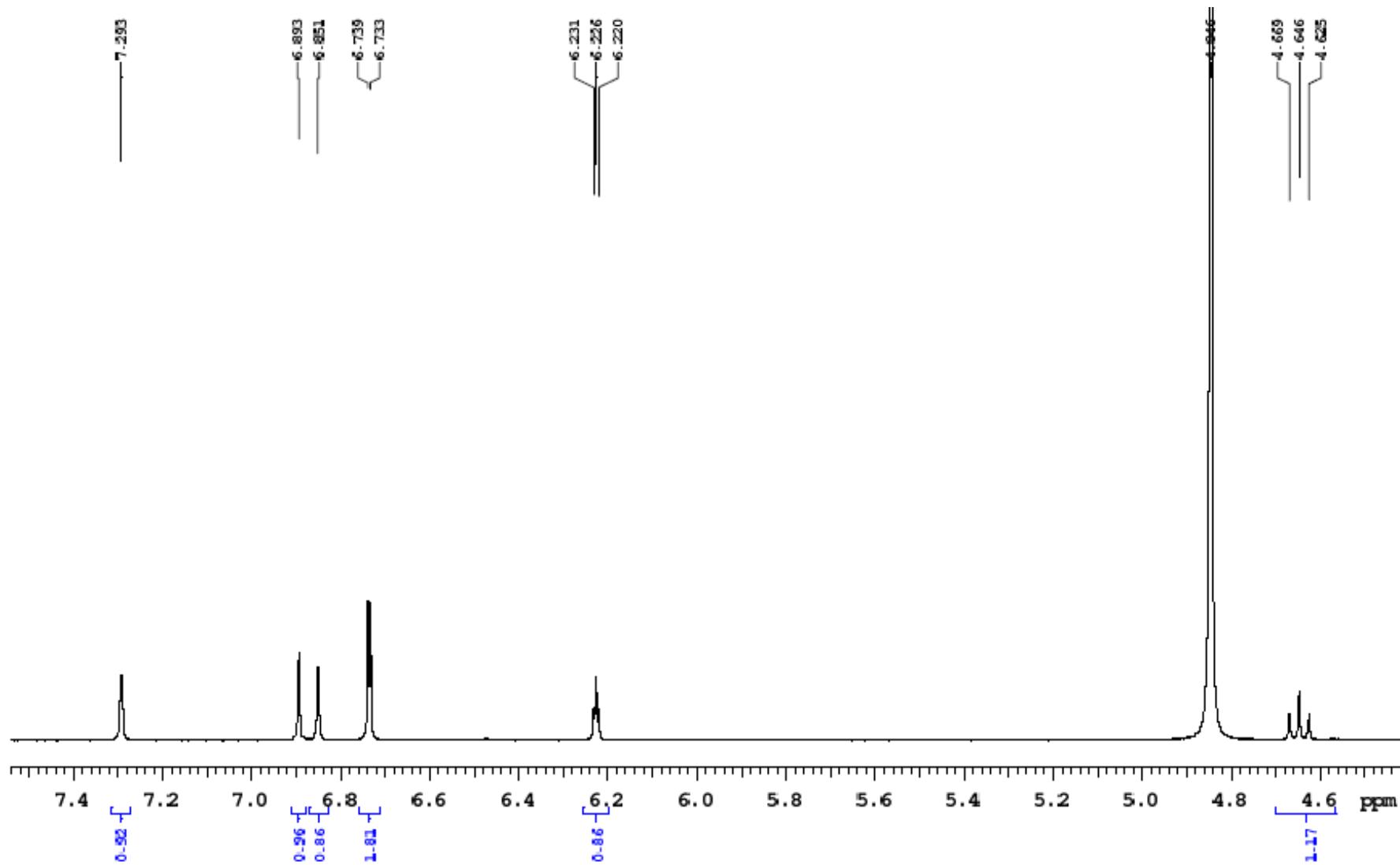
Sample Name:  
AS-IV-52-01  
Data Collected on:  
DK400.ac.kr-vnmrsys400  
Archive directory:  
/home/kilee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Aug 13 2018

Operator: kilee

Relax: delay 1.000 sec  
Pulse 45.0 degrees  
Aq. time 2.556 sec  
Width 6410.3 Hz  
64 repetitions  
OBSERVE HI, 399.8054845 MHz  
DATA PROCESSING  
FT size 32768  
Total time 3 min 48 sec





<sup>13</sup>C NMR (100 MHz, methanol-*d*<sub>4</sub>) spectrum of moracin O (**6**).

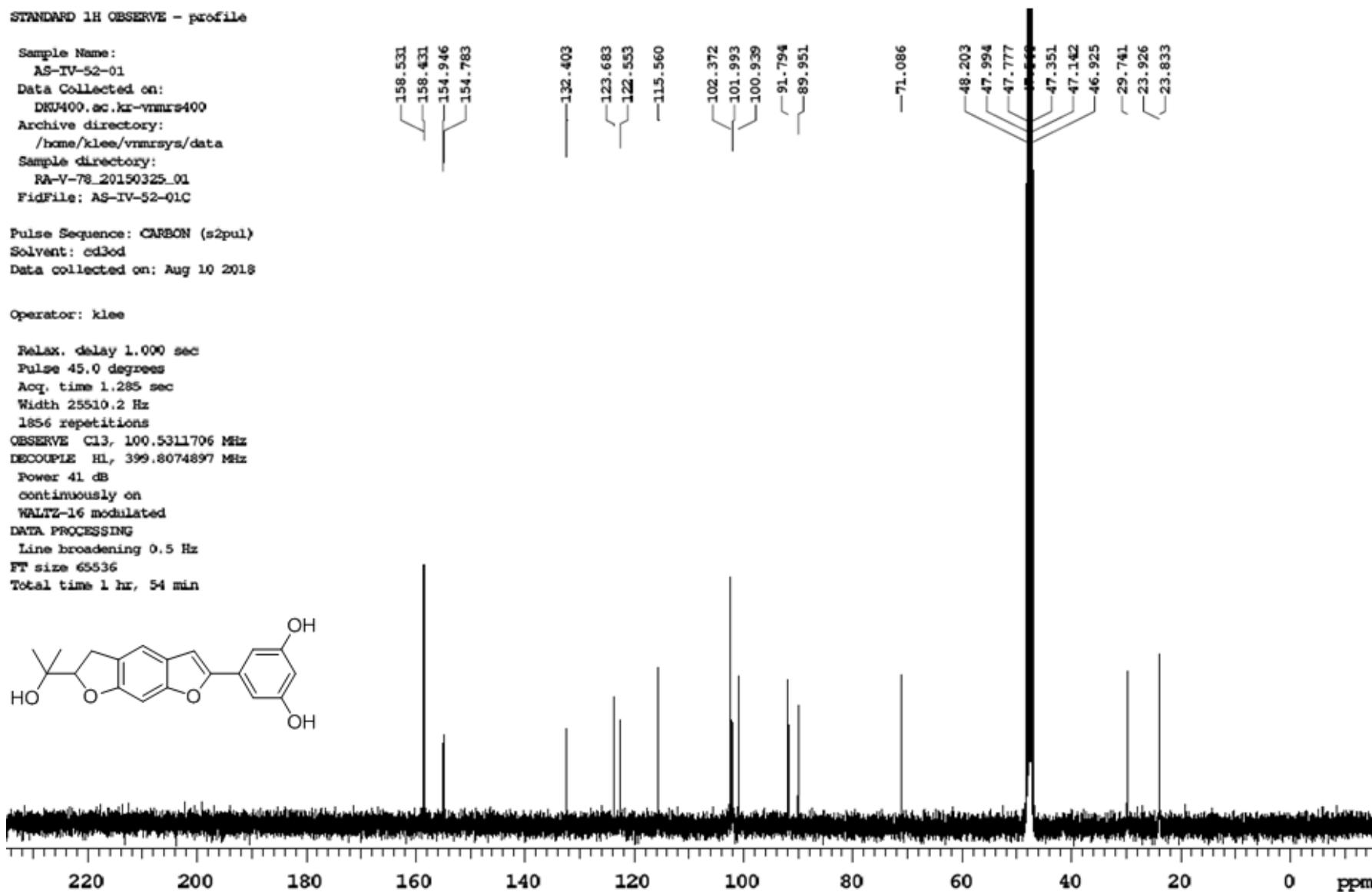
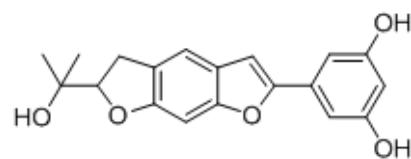
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-52-01  
Data Collected on:  
DKU400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-IV-52-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3od  
Data collected on: Aug 10 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1856 repetitions  
OBSERVE CL3, 100.5311706 MHz  
DECOUPLE HL, 399.8074897 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>H NMR (400 MHz, methanol-*d*<sub>4</sub>) spectrum of moracin P (**7**).

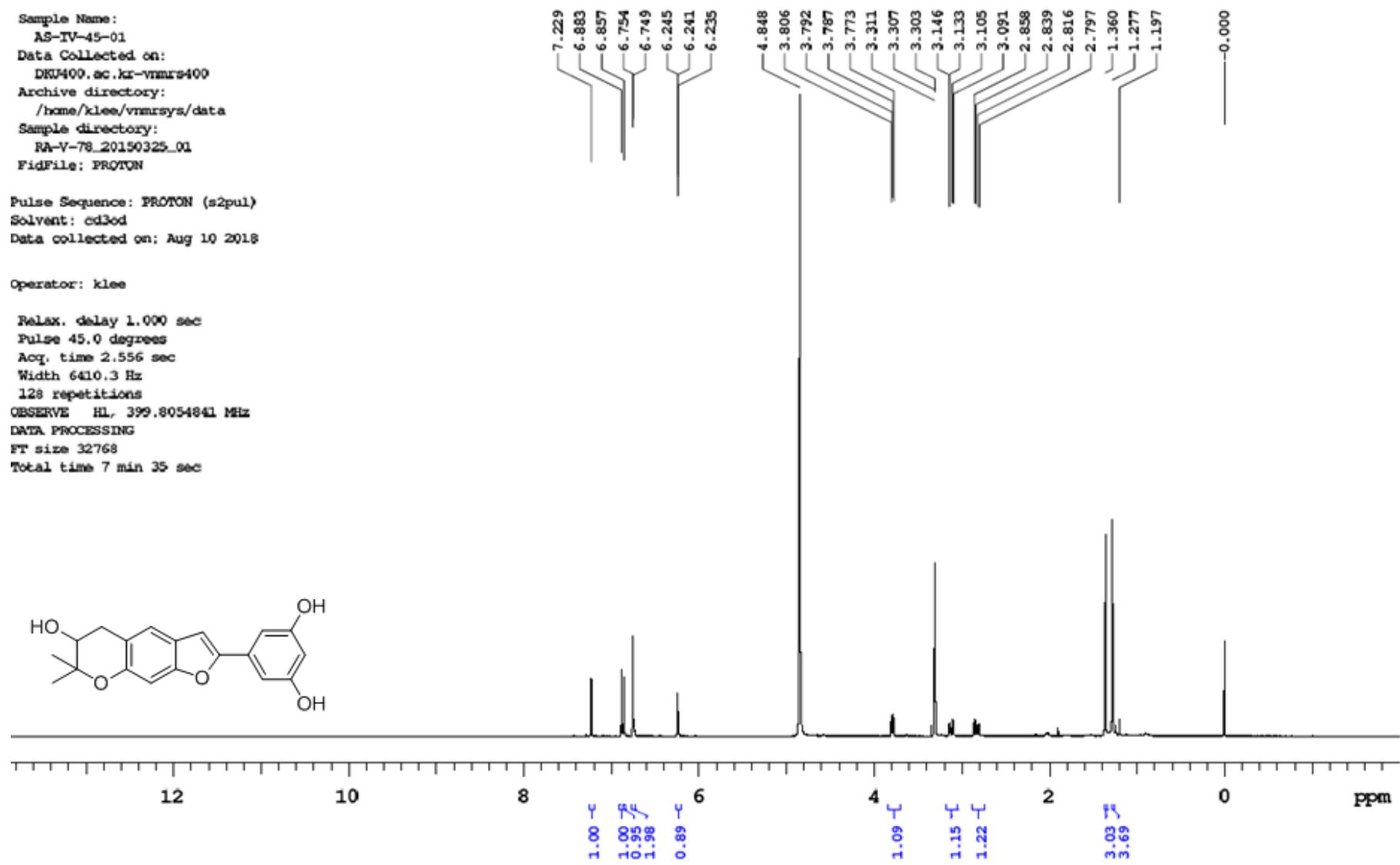
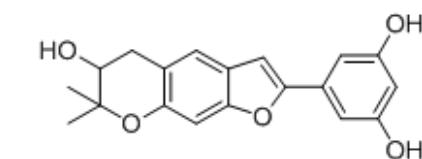
STANDARD 1H OBSERVE - profile

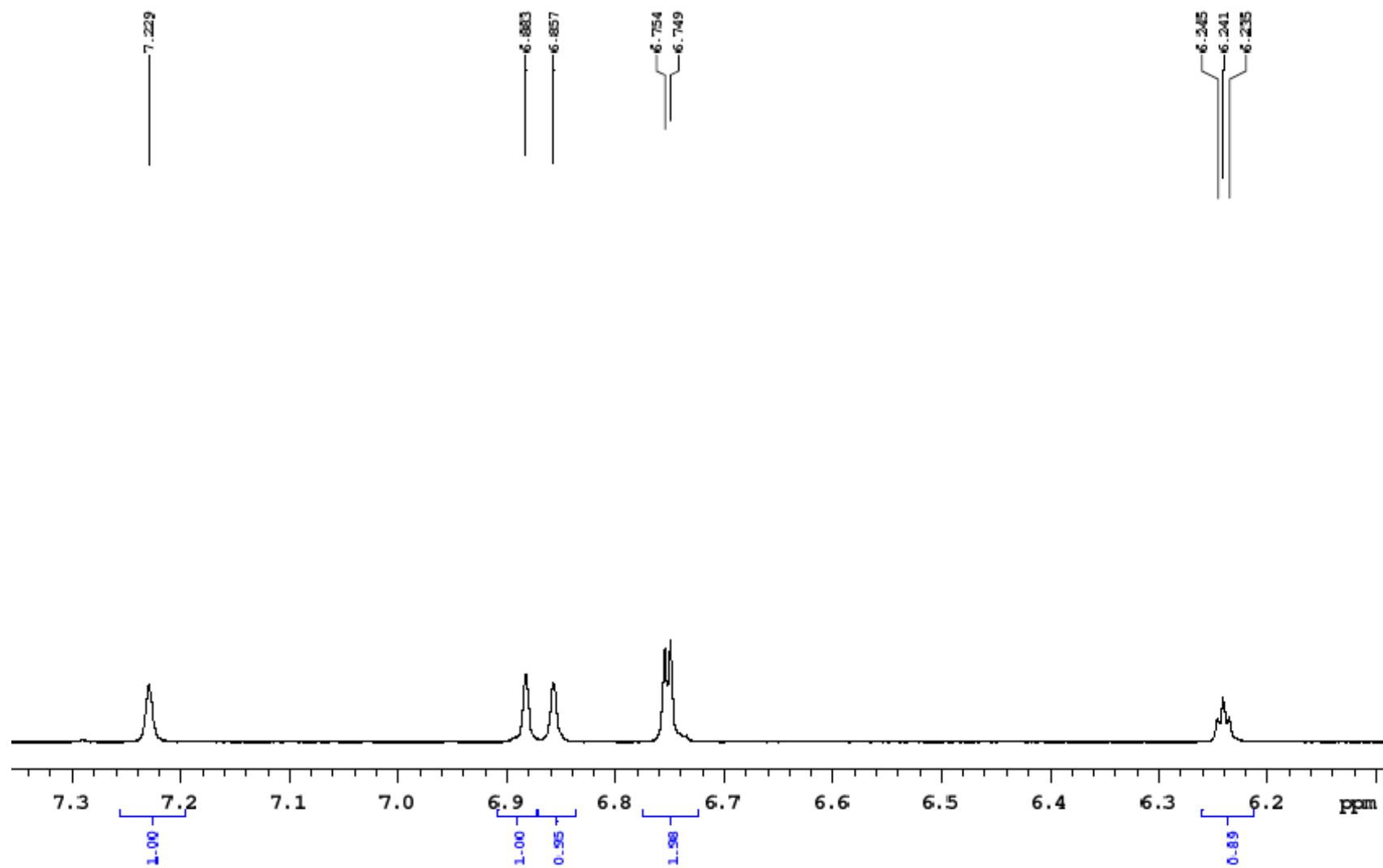
Sample Name:  
AS-IV-45-01  
Data Collected on:  
DKU400.ac.kr-vmnrsys400  
Archive directory:  
/home/klee/vmnrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdod  
Data collected on: Aug 10 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
128 repetitions  
OBSERVE HL 399.8054841 MHz  
DATA PROCESSING  
FT size 32768  
Total time 7 min 35 sec





<sup>13</sup>C NMR (100 MHz, methanol-*d*4) spectrum of moracin P (**7**).

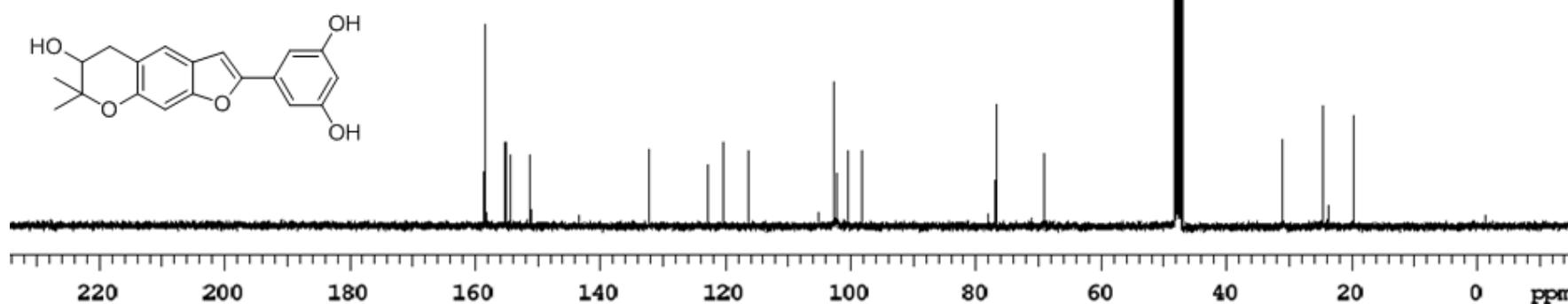
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-IV-45-01  
Data Collected on:  
DKU400.sc.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
PJH-II-79\_20180723\_01  
FidFile: AS-IV-45-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3od  
Data collected on: Jul 25 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
2304 repetitions  
OBSERVE CL3, 100.5311706 MHz  
DECOUPLE HL, 399.8074897 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 10 min



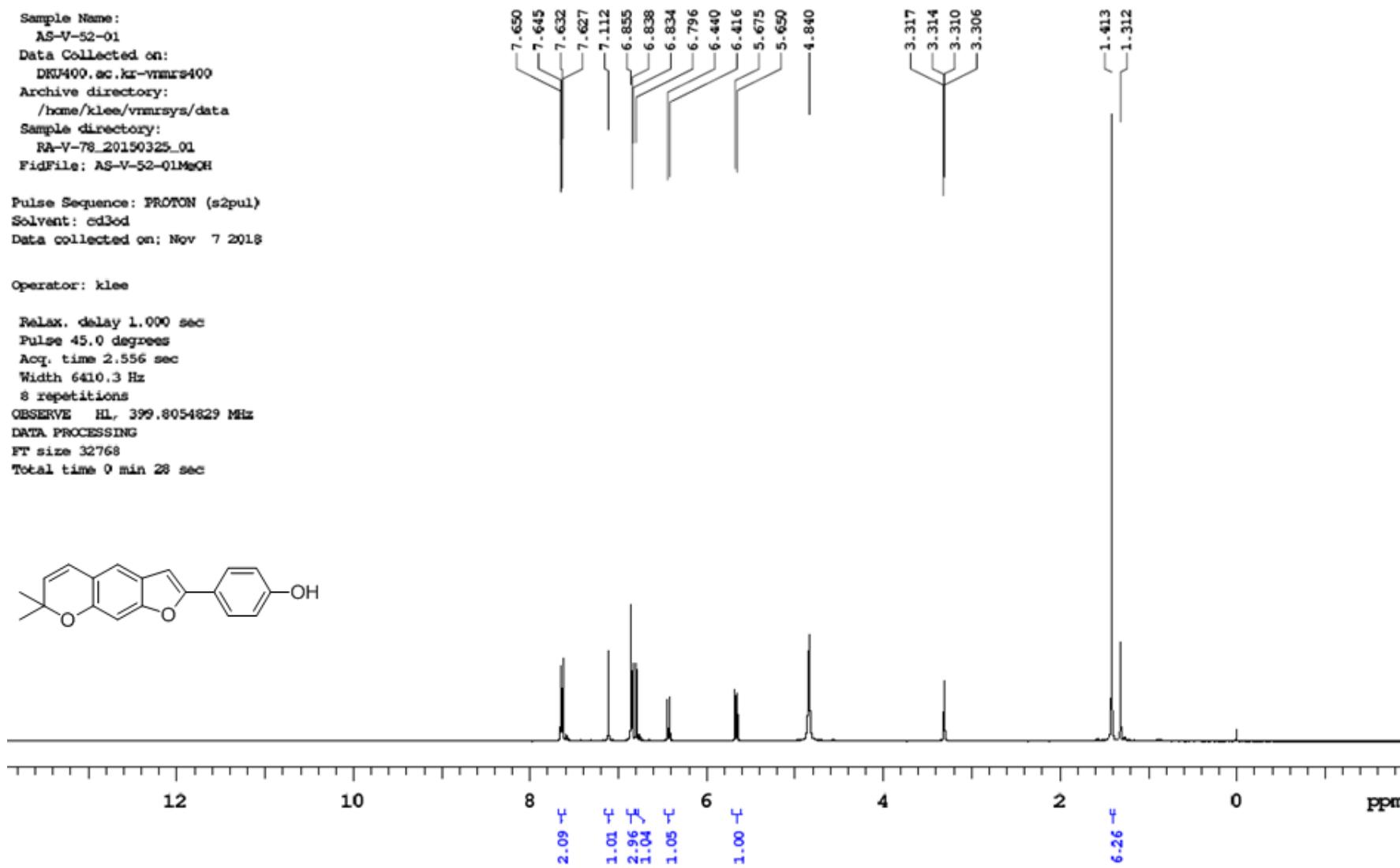
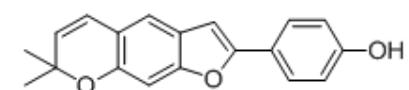
<sup>1</sup>H NMR (400 MHz, methanol-*d*4) spectrum of grammiphenoF (8).

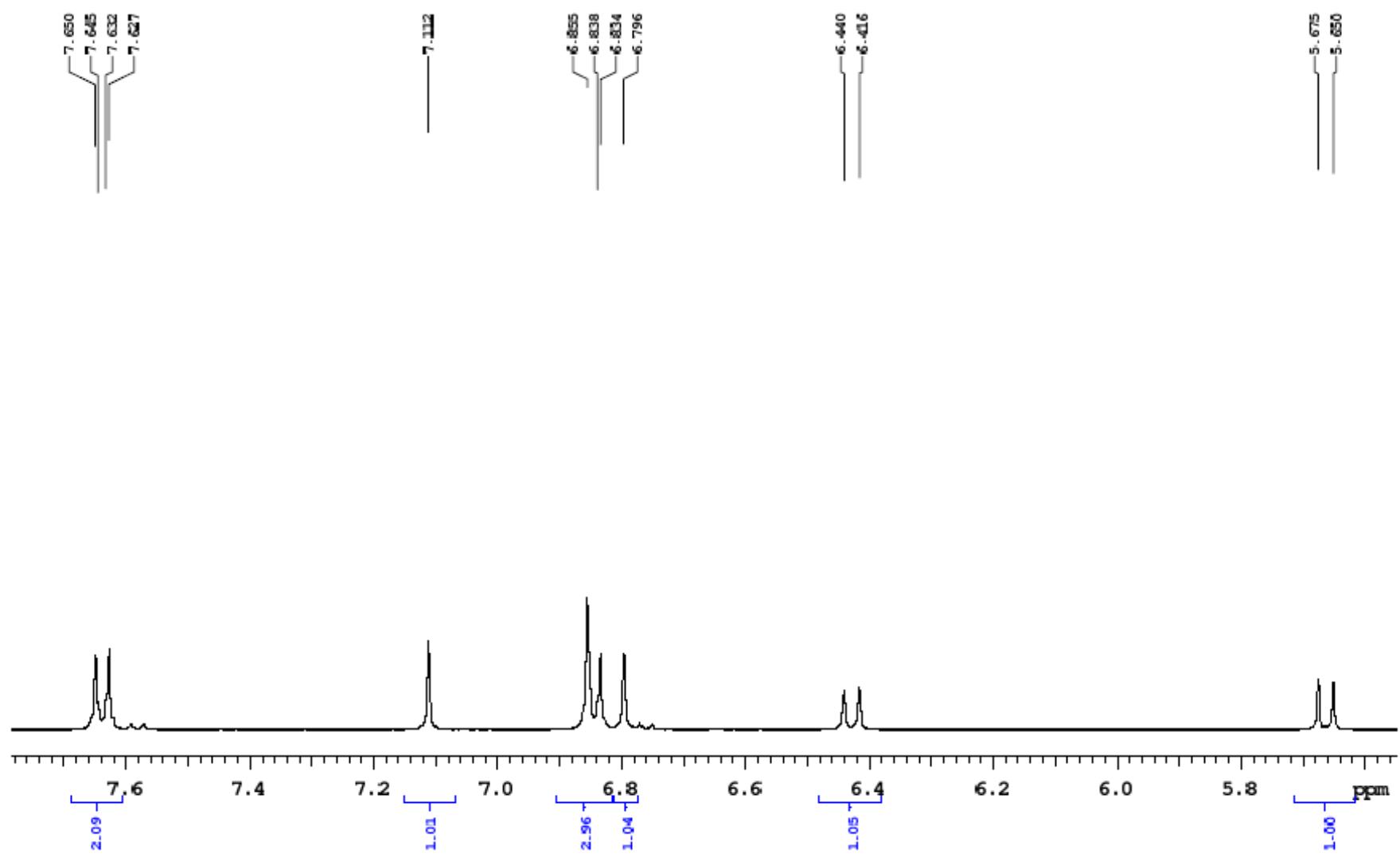
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-52-01  
Data Collected on:  
DRU400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-52-01MeOH  
  
Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Nov 7 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE HL, 399.8054829 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 28 sec





<sup>13</sup>C NMR (100 MHz, methanol-*d*4) spectrum of grammiphenol F (**8**).

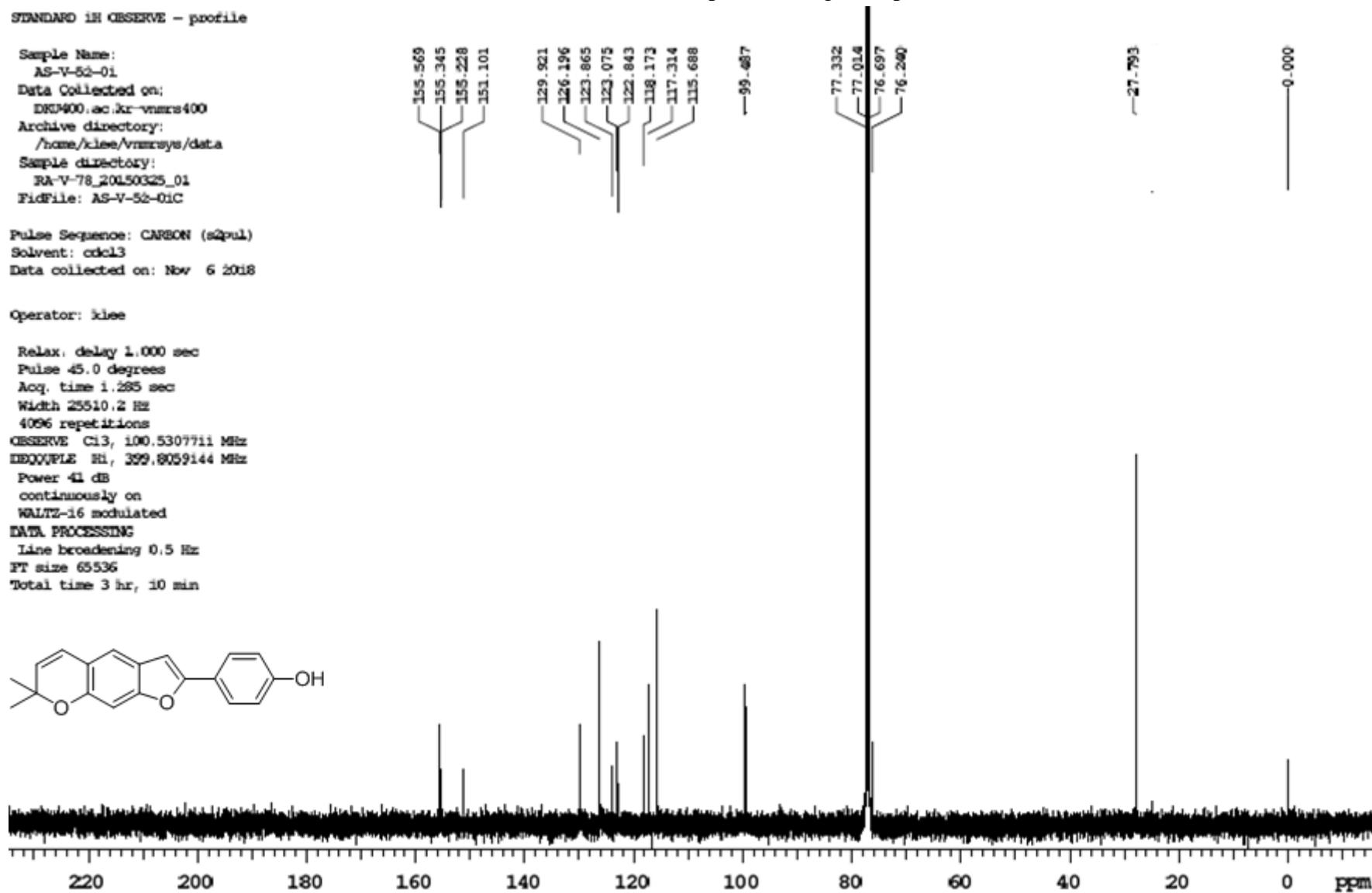
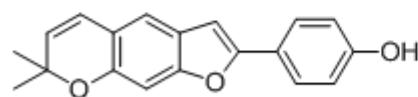
STANDARD IN OBSERVE - profile

Sample Name:  
AS-V-52-01  
Data Collected on:  
DNP400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-52-01C

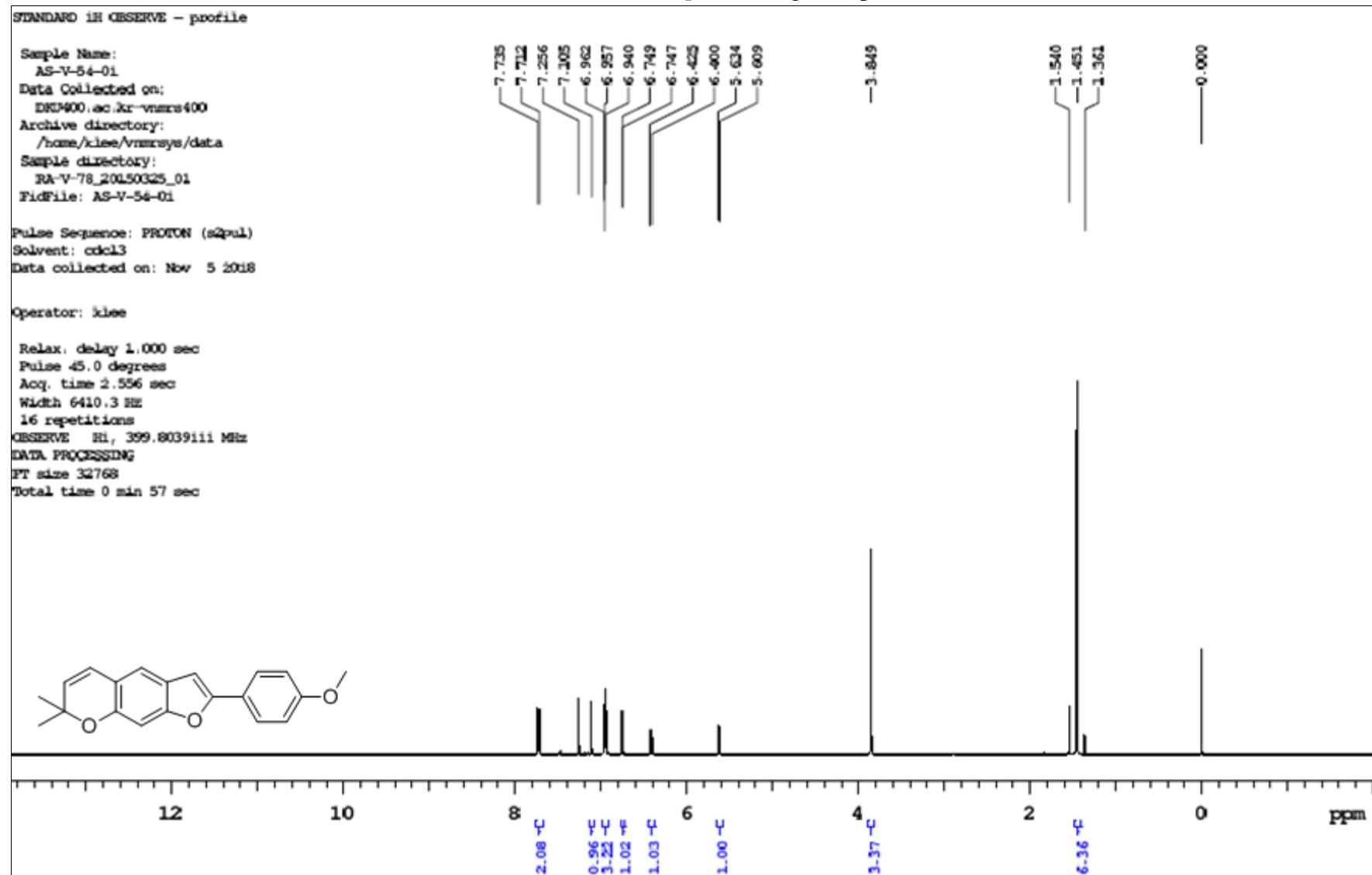
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 6 2015

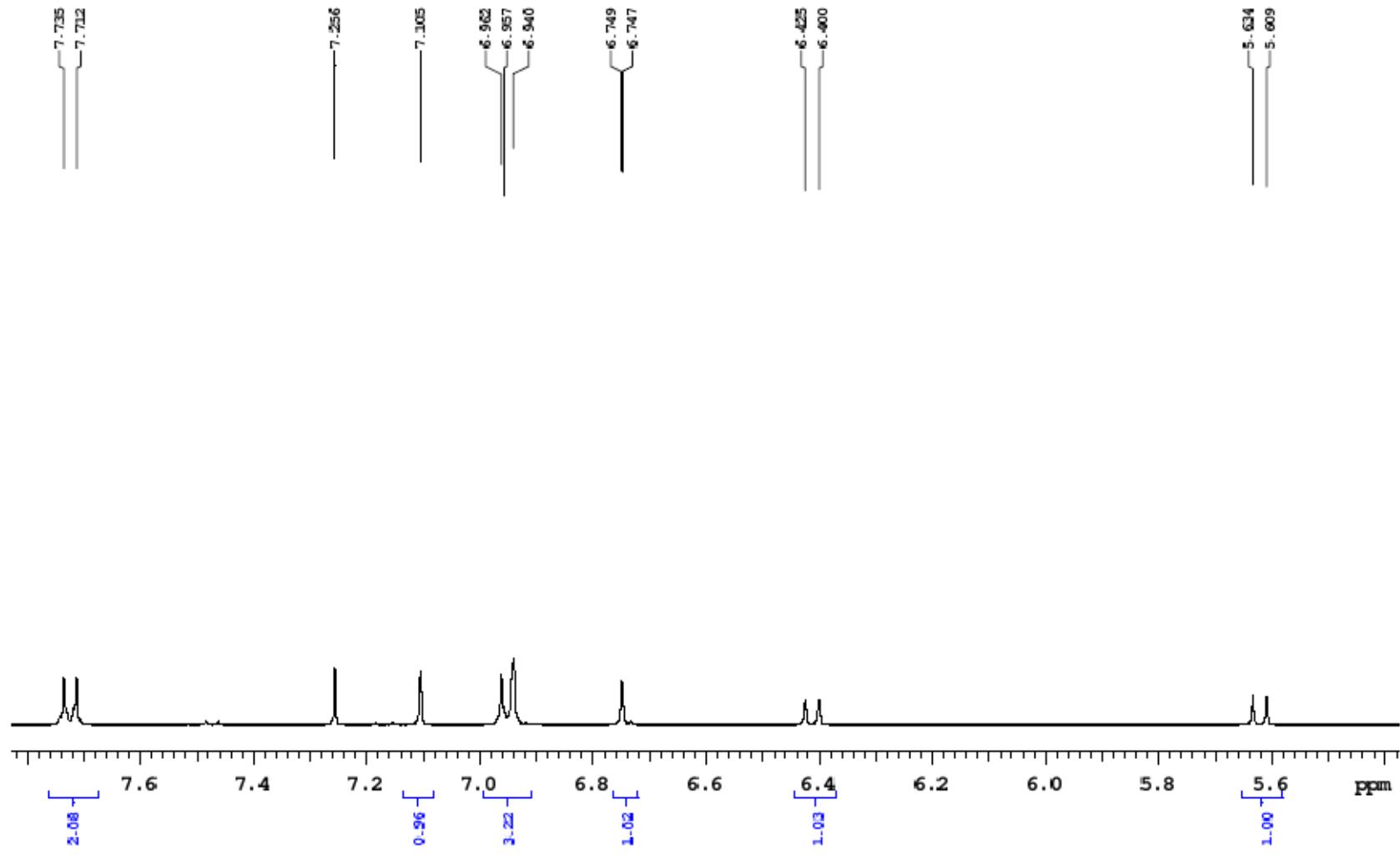
Operator: klee

Relax: delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
4096 repetitions  
OBSERVE Cl3, 100.5307711 MHz  
DECOUPLE HI, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 10 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of gramnipheno G (**9**).





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of grammiphenoL G (**9**).

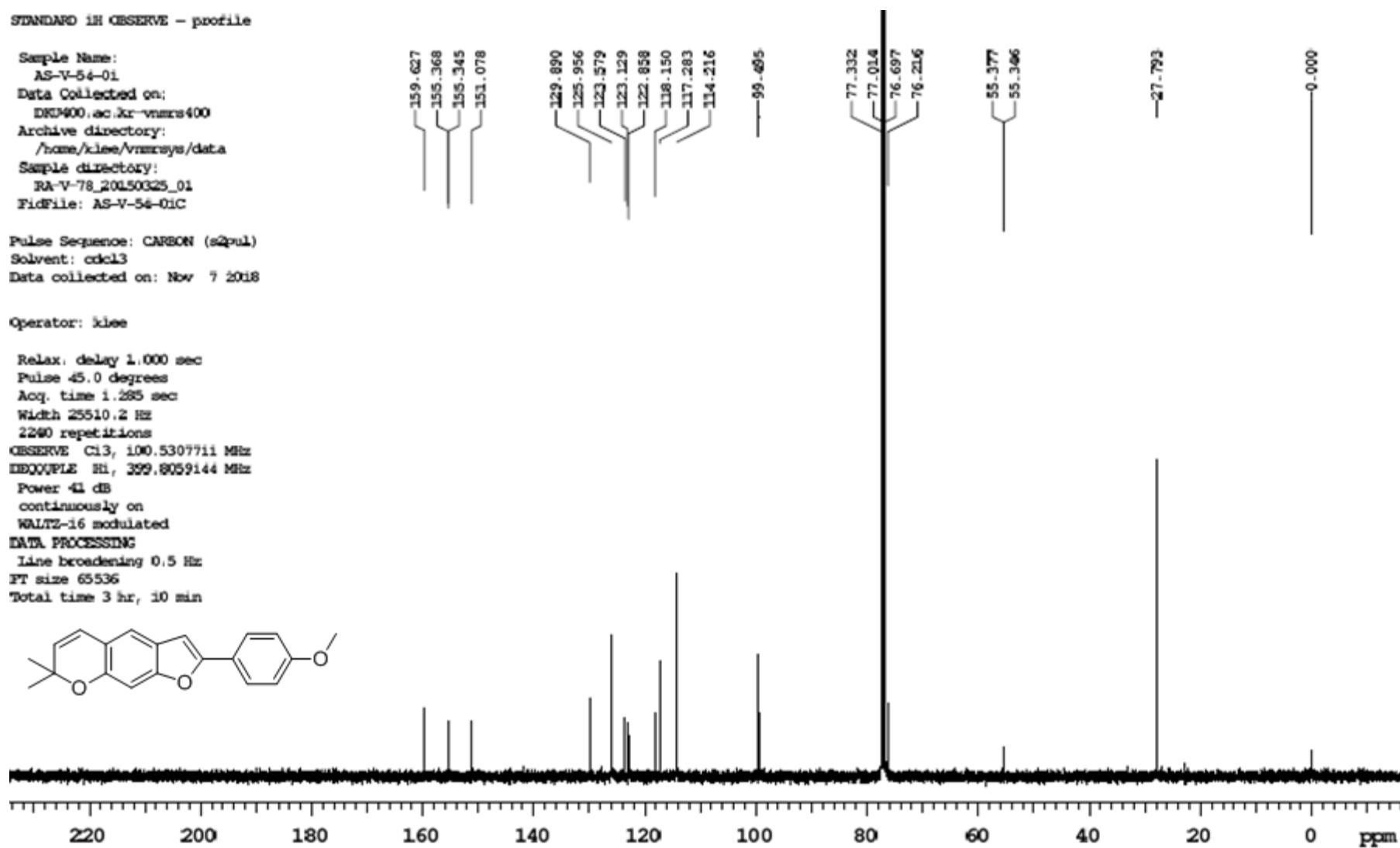
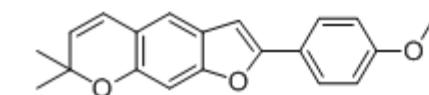
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-54-01  
Data Collected on:  
DEK400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-54-01C

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 7 2018

Operator: klee

Relax: delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
2240 repetitions  
OBSERVE Cl3, 100.5307711 MHz  
PROVIDE Si, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 10 min

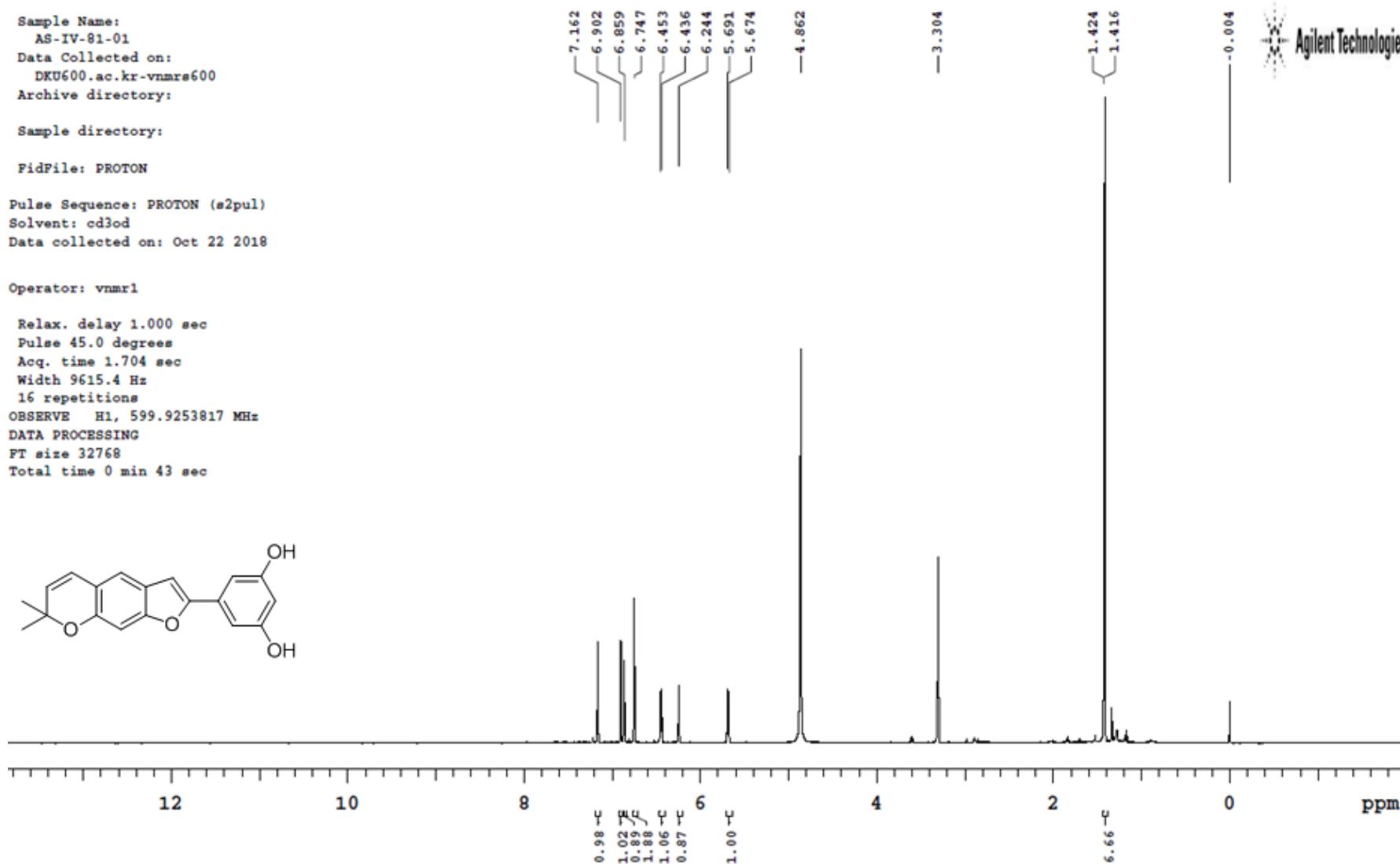
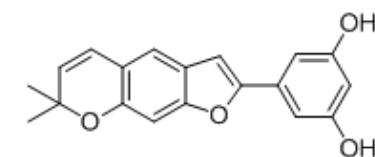


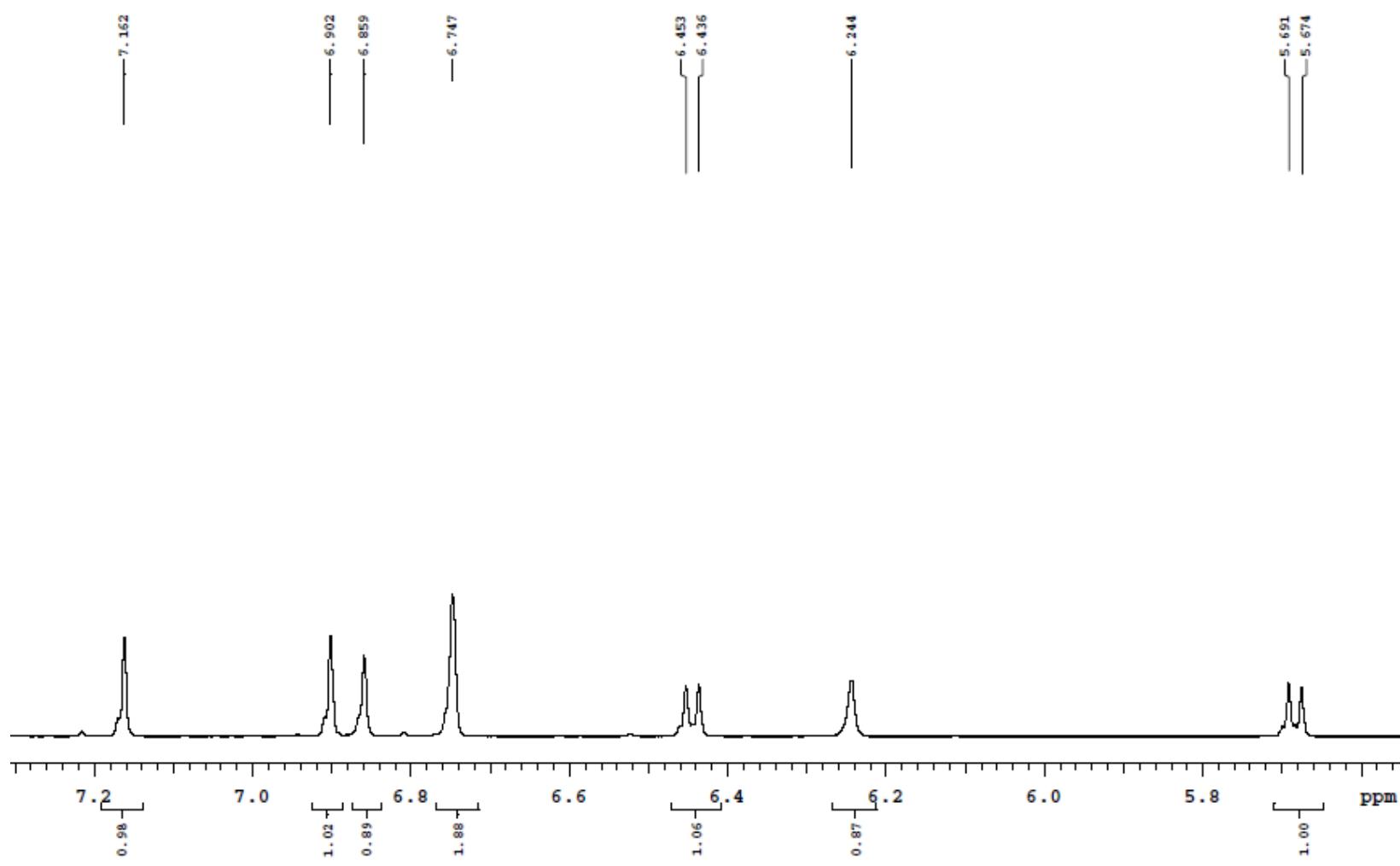
<sup>1</sup>H NMR (600 MHz, methanol-d<sub>4</sub>) spectrum of morunigrol C (**10**).

STANDARD PROTON PARAMETERS

Sample Name:  
AS-IV-81-01  
Data Collected on:  
DKU600.ac.kr-vnmrs600  
Archive directory:  
  
Sample directory:  
  
PidFile: PROTON  
  
Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Oct 22 2018

Operator: vnmrl  
  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.704 sec  
Width 9615.4 Hz  
16 repetitions  
OBSERVE H1, 599.9253817 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 43 sec





<sup>13</sup>C NMR (150 MHz, methanol-*d*<sub>4</sub>) spectrum of morunigrol C (**10**).

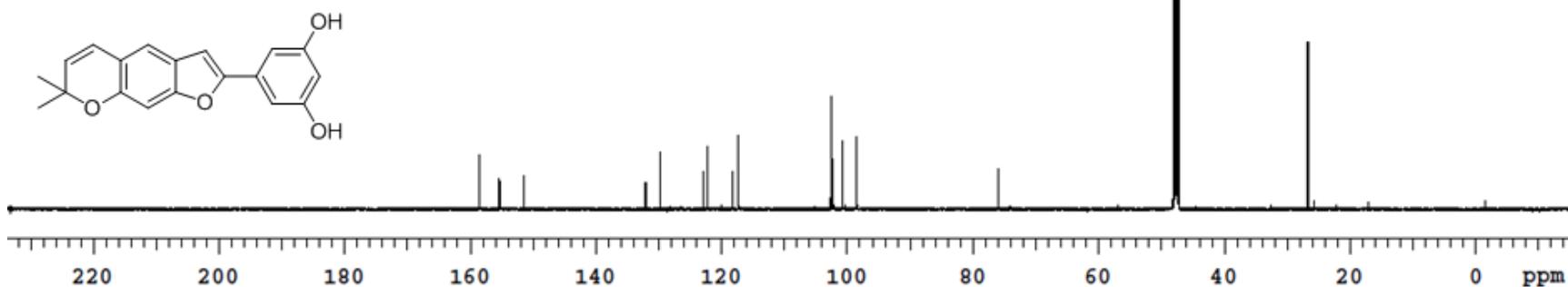
Calibration for 5mm\_One\_probe on 14Jul2017  
 Sample : C13 enriched CH3OH in doped D2O (autotest)

Sample Name:  
 AS-IV-81-01  
 Data Collected on:  
 DKU600.ac.kr-vnmrsys600  
 Archive directory:  
 /home/vnmr1/vnmrsys/probes/probe\_calibs  
 Sample directory:  
 5mm\_One\_probe\_calib  
 FidPile: CARBON

Pulse Sequence: CARBON (s2pul)  
 Solvent: cd3od  
 Data collected on: Oct 22 2018

Operator: vnmr1

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 0.865 sec  
 Width 37878.8 Hz  
 25000 repetitions  
 OBSERVE C13, 150.8513572 MHz  
 DECOUPLE H1, 599.9283813 MHz  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 12 hr, 57 min



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of 3',5'-di-O-methyl morunigrol C (**11**)

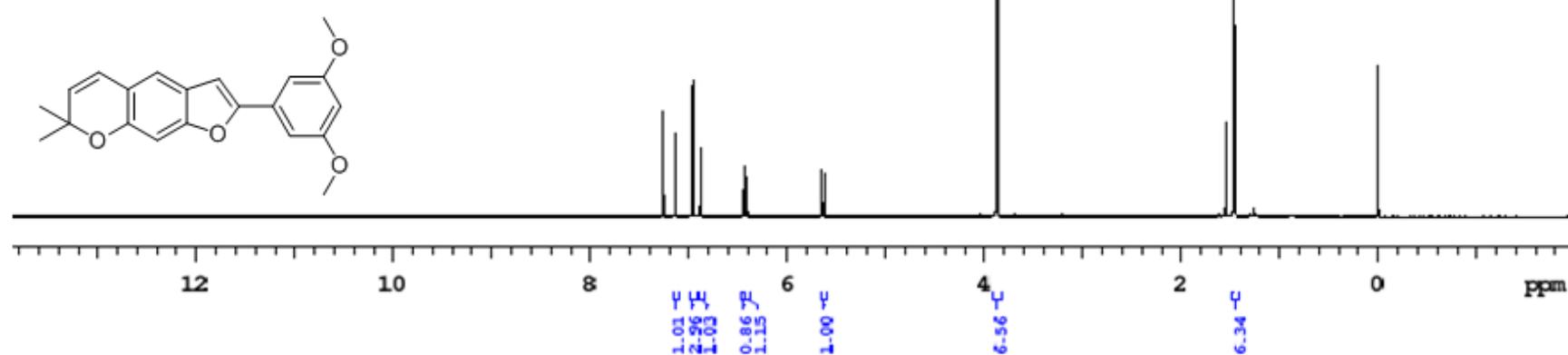
STANDARD IN OBSERVE - profile

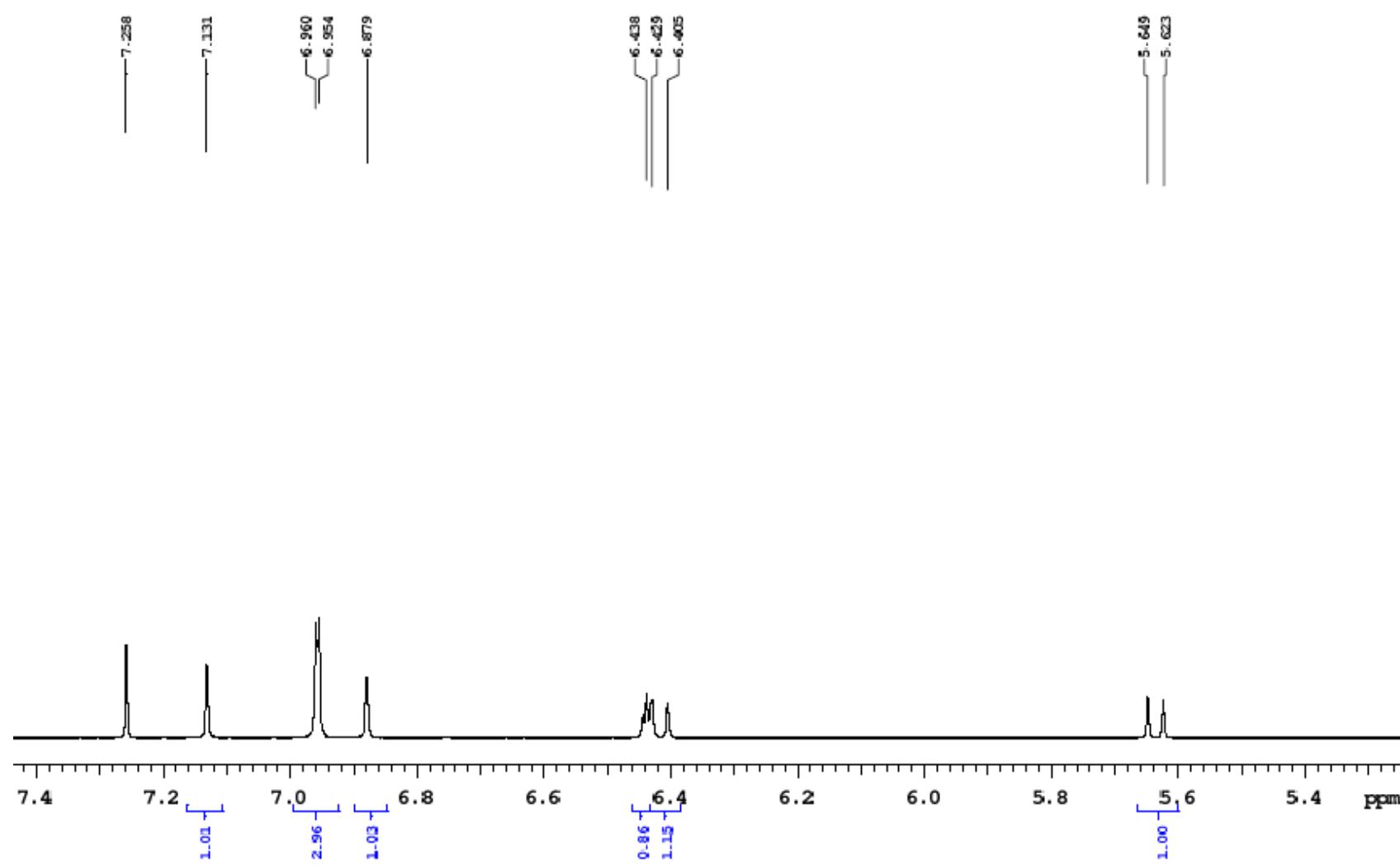
Sample Name:  
AS-V-53-01  
Data Collected on:  
DRX400.ac.kr-vnmrs400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-53-01

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 5 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE Hz, 399.8039104 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec





<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of 3',5'-di-*O*-methyl morunigrol C (**11**)

STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-53-01  
Data Collected on:  
DK0400.ac.kr-vnmrs400  
Archive directory:  
/home/kilee/vnmrsys/data  
Sample directory:  
RA-V-78\_20150325\_01  
FidFile: AS-V-53-01-i3c

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 7 2018

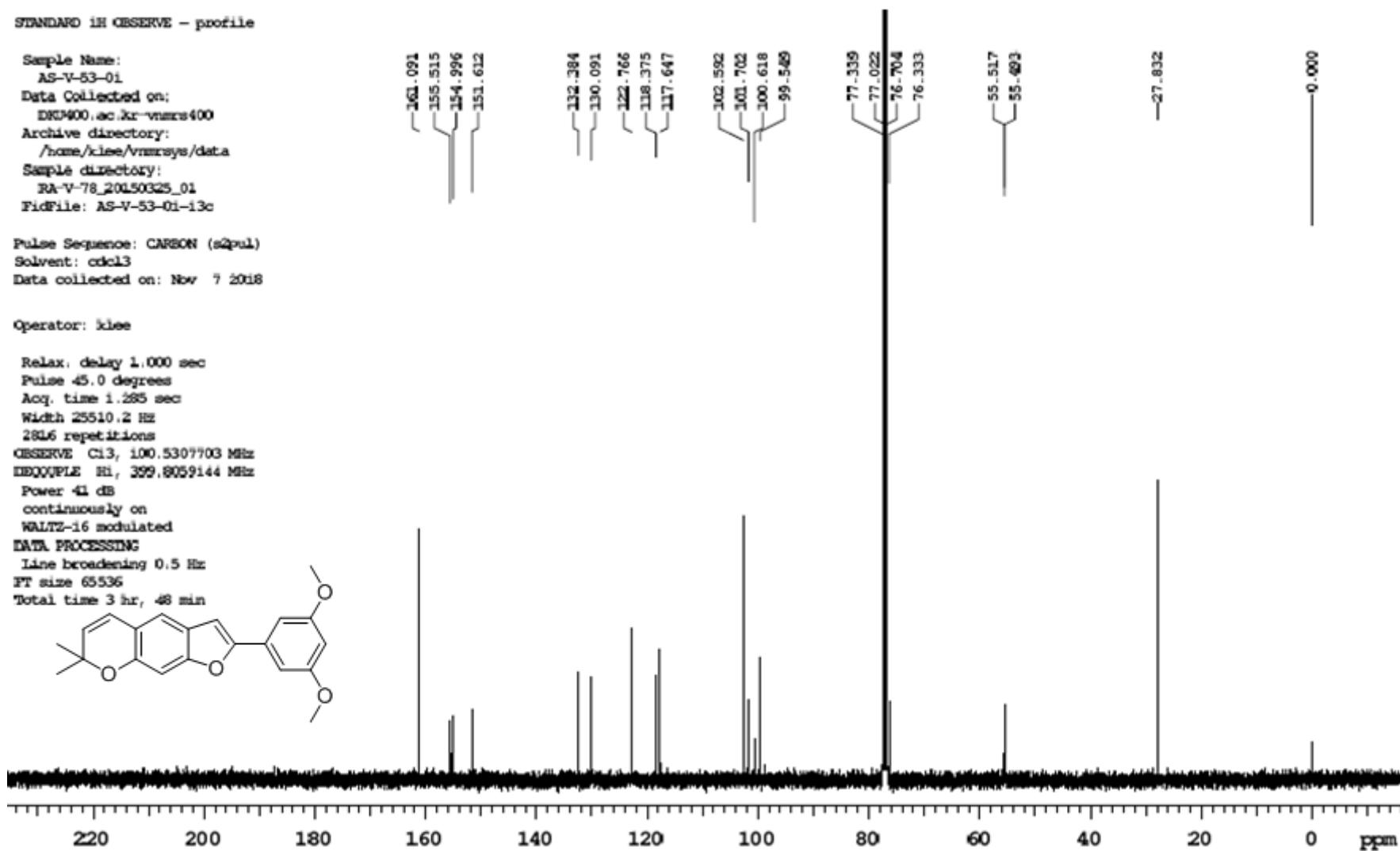
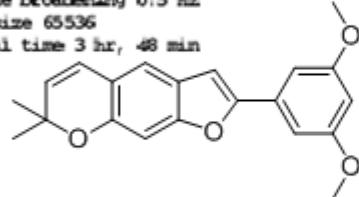
Operator: kilee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
2816 repetitions

OBSERVE C13, 100.5307703 MHz  
DECOUPLE H1, 399.8059144 MHz

Power +1 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 46 min



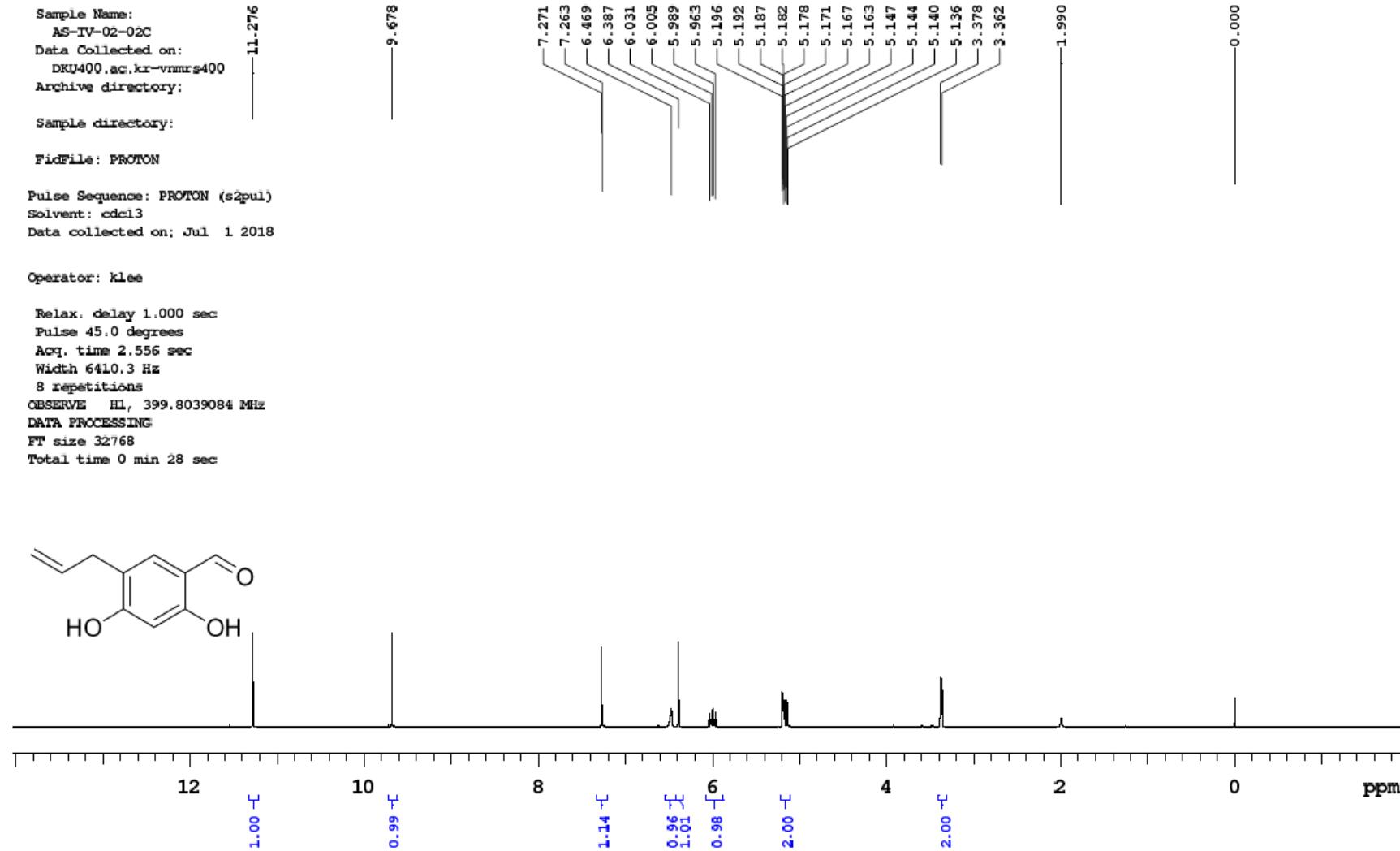
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of Compound 1g

new experiment

Sample Name:  
AS-TV-02-02C  
Data Collected on:  
DKU400.ac.kr-vnmrs400  
Archive directory:  
Sample directory:  
FidFile: PROTON  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 1 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE H1, 399.8039084 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 28 sec



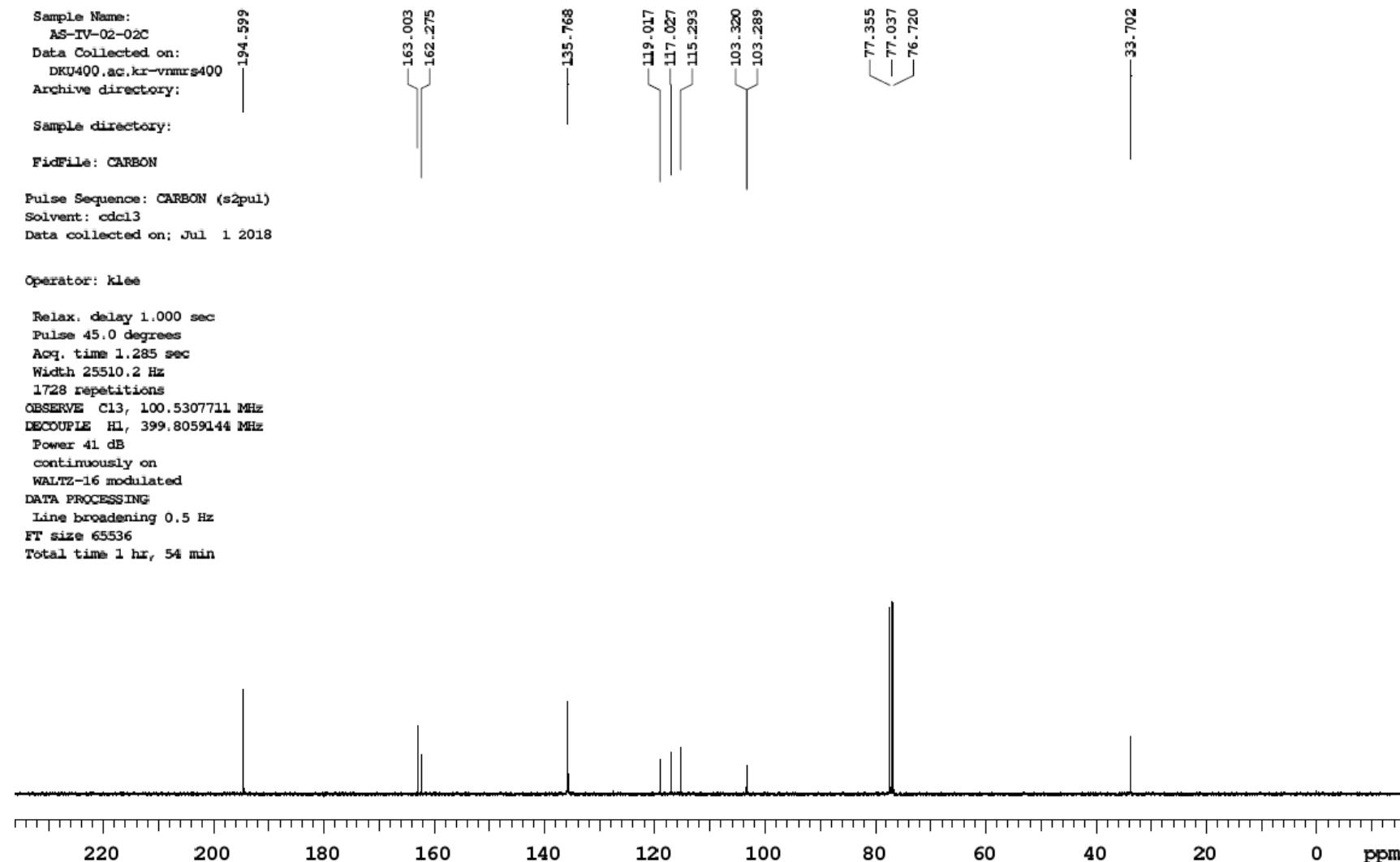
<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) spectrum of Compound 1g

new experiment

Sample Name: AS-TV-02-02C  
Data Collected on: DKU400.ac.kr-vnmrs400  
Archive directory:  
Sample directory:  
FidFile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jul 1 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1728 repetitions  
OBSERVE C13, 100.5307711 MHz  
DECOUPLE H1, 399.8059144 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



<sup>1</sup>HNMR (400 MHz, DMSO-d<sub>6</sub>) spectrum of Compound **1l**

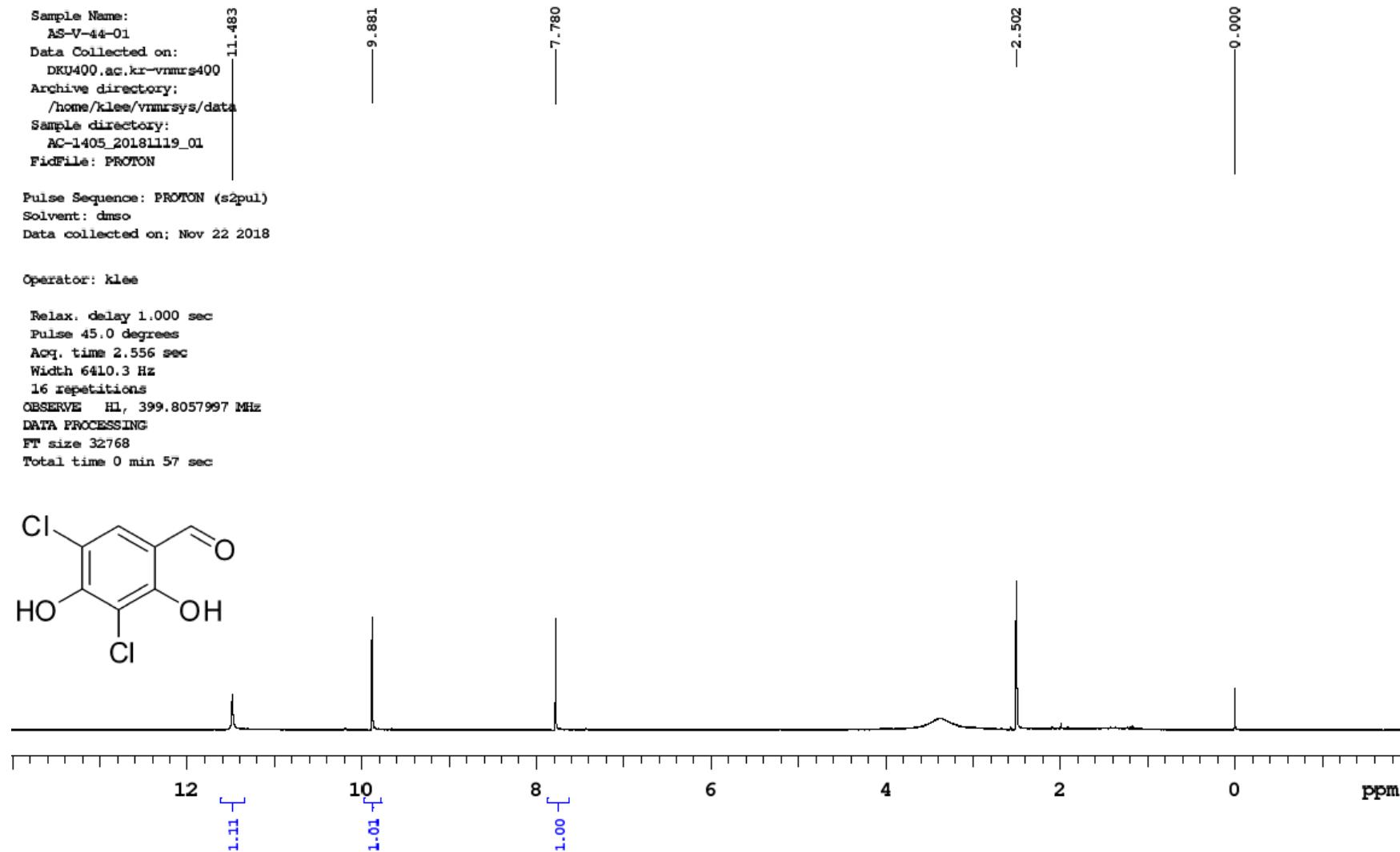
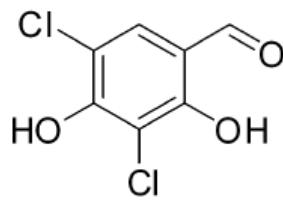
STANDARD 1H OBSERVE - profile

Sample Name: AS-V-44-01  
Data Collected on: 11.483  
Archive directory: /home/klee/vnmrsys/data  
Sample directory: AC-1405\_20181119\_01  
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: dmso  
Data collected on: Nov 22 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.556 sec  
Width 6410.3 Hz  
16 repetitions  
OBSERVE H1, 399.8057997 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min 57 sec



<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of Compound **1I**

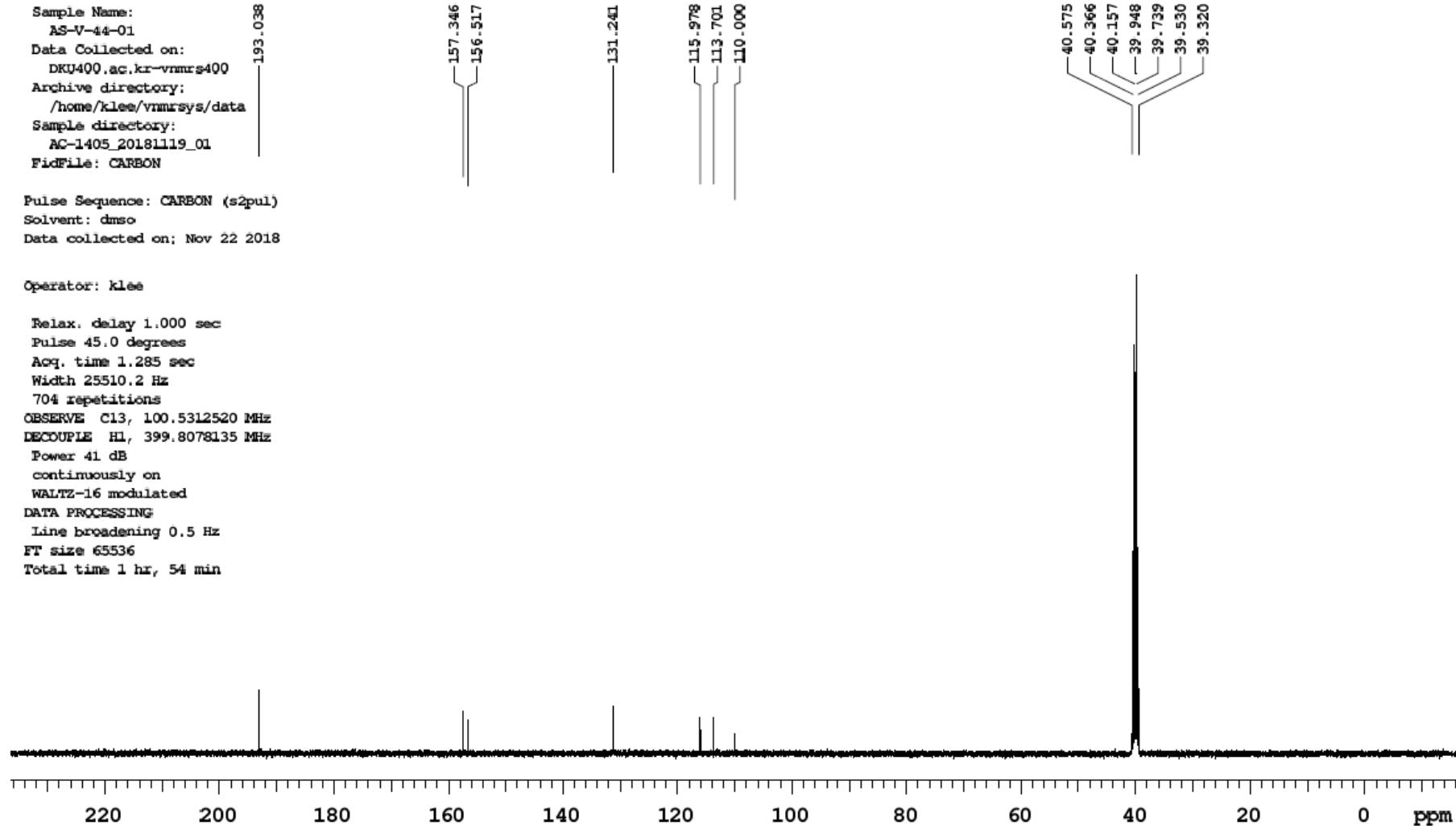
STANDARD 1H OBSERVE - profile

Sample Name:  
AS-V-44-01  
Data Collected on:  
DKU400.ac.kr-vnmrsys400  
Archive directory:  
/home/klee/vnmrsys/data  
Sample directory:  
AC-1405\_20181119\_01  
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: dmso  
Data collected on: Nov 22 2018

Operator: klee

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
704 repetitions  
OBSERVE C13, 100.5312520 MHz  
DECOUPLE H1, 399.8078135 MHz  
Power 41 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 54 min



## References

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8. WO 2011/017125 A1 10 February 2011 (10.02.2011) Inventors/Applicants (for US only): XIA, Yi [US/US];

