

**Asymmetric Synthesis of Chiral 9,10-Dihydrophenanthrenes Using Pd-Catalyzed Asymmetric Intramolecular Friedel-Crafts Allylic Alkylation of Phenols**

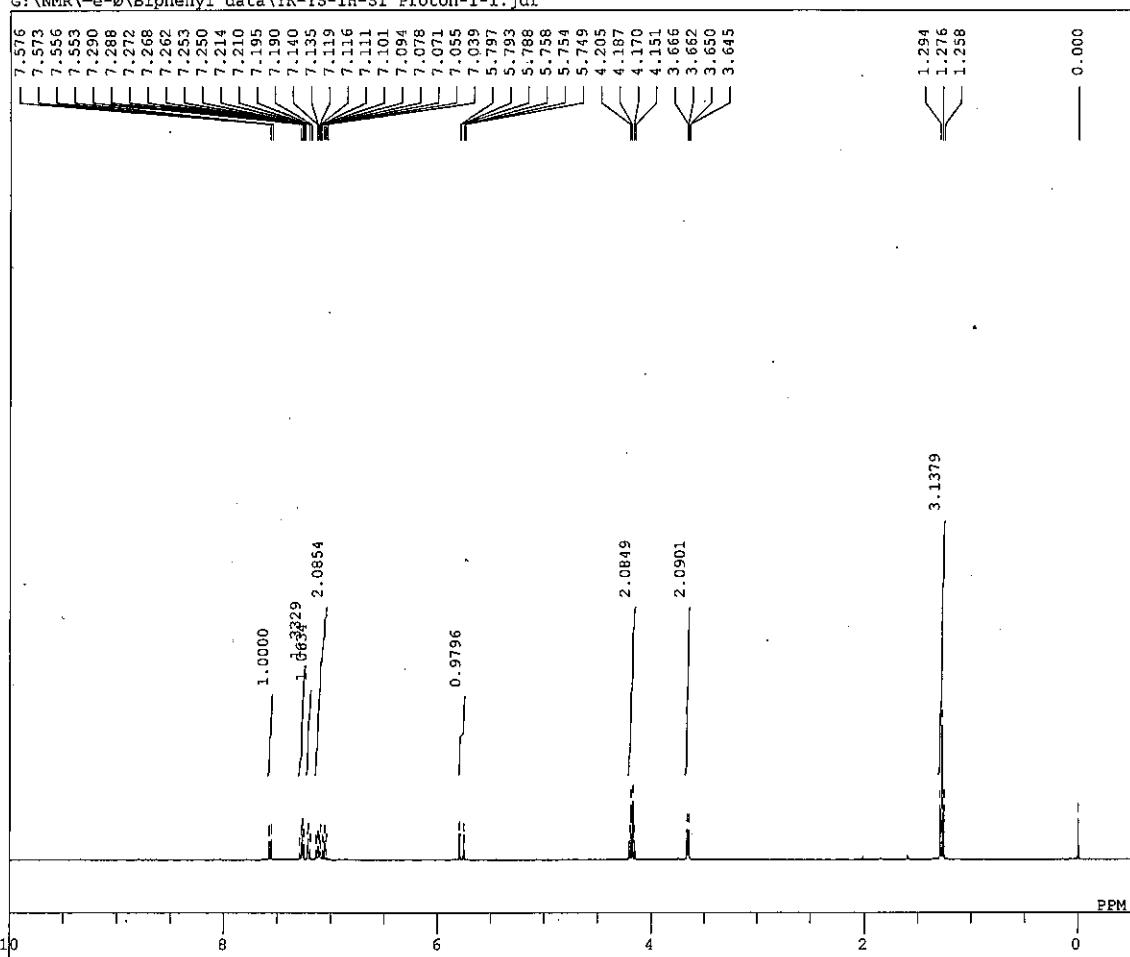
Yuta Suzuki, Tetsuhiro Nemoto, Kazumi Kakugawa, Akinari Hamajima, and Yasumasa Hamada\*

**Supporting Information 2**

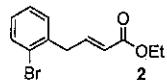
**5.  $^1\text{H}$  and  $^{13}\text{C}$  NMR Charts of New Compounds (Page S-20–S-59)**

single\_pulse

G:\NMR\é-Ø\Biphenyl data\YK-YS-1H-S1 Proton-1-1.jdf

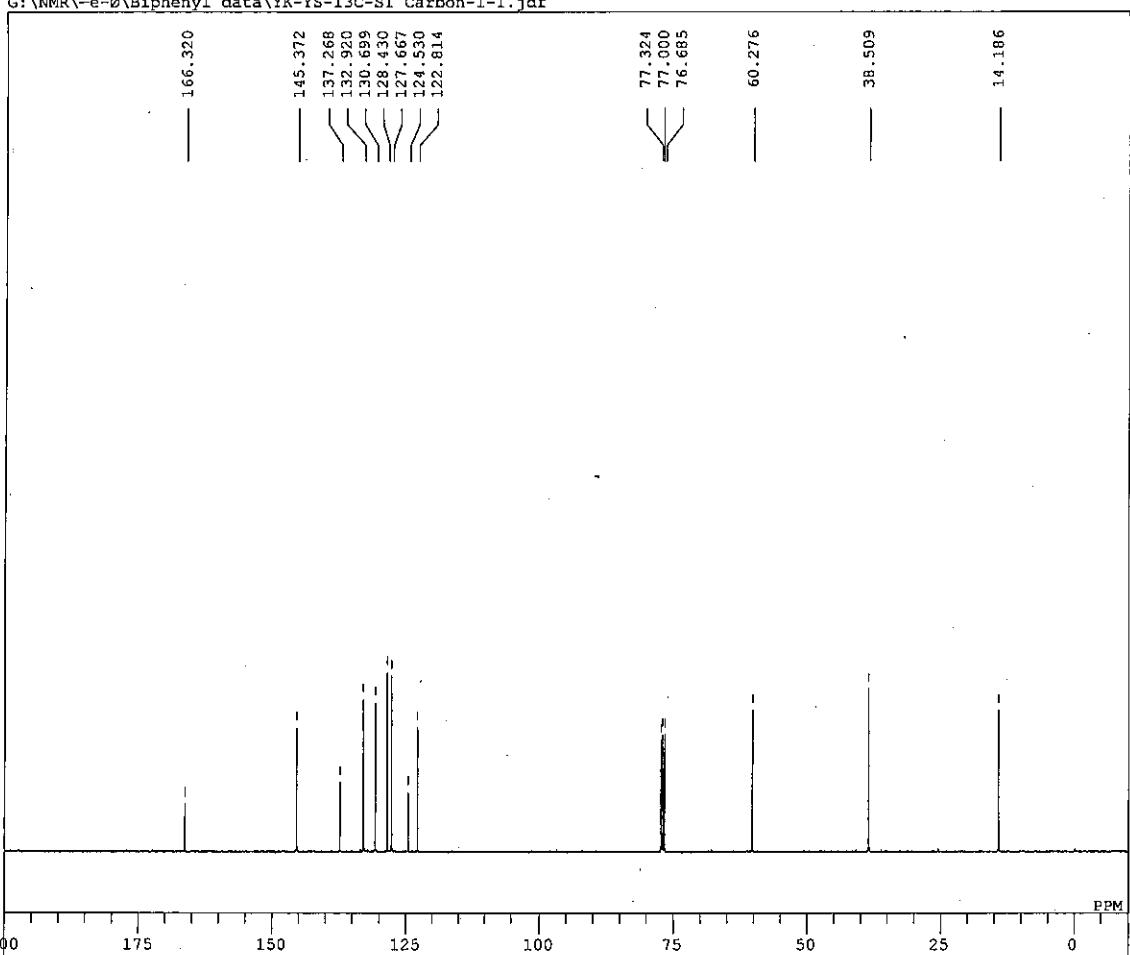


DFILE YK-YS-1H-S1\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-01-19 16:35:13  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usedc  
IRNUC 1H  
CTEMP CDCL3 19.8 c  
SLVNT EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 42

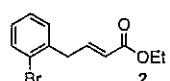


single pulse decoupled gated NOE

G:\NMR\é-Ø\Biphenyl data\YK-YS-13C-S1 Carbon-1-1.jdf

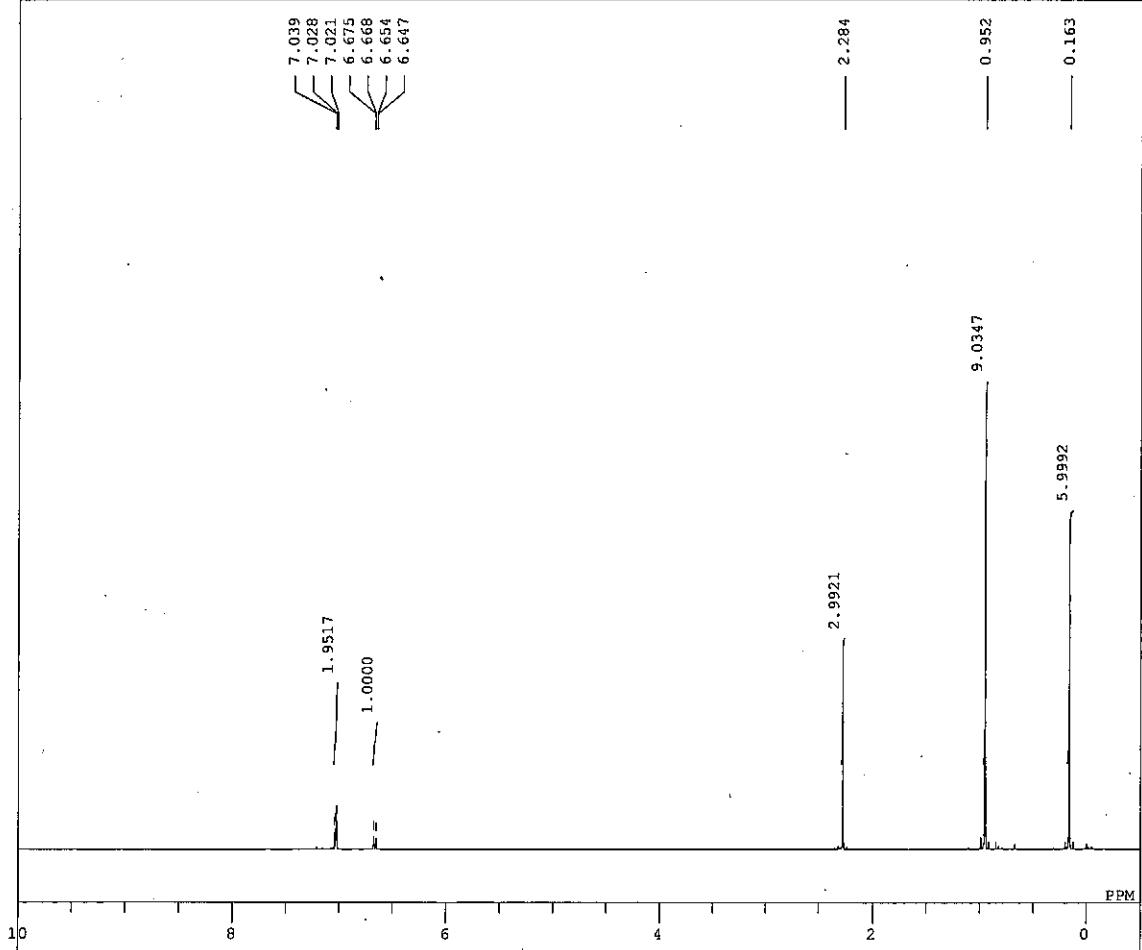
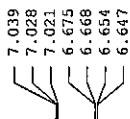


DFILE YK-YS-13C-S1\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-01-20 23:33:46  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 512  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP CDCL3 20.3 c  
SLVNT EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

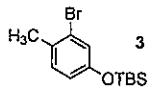


**single\_pulse**

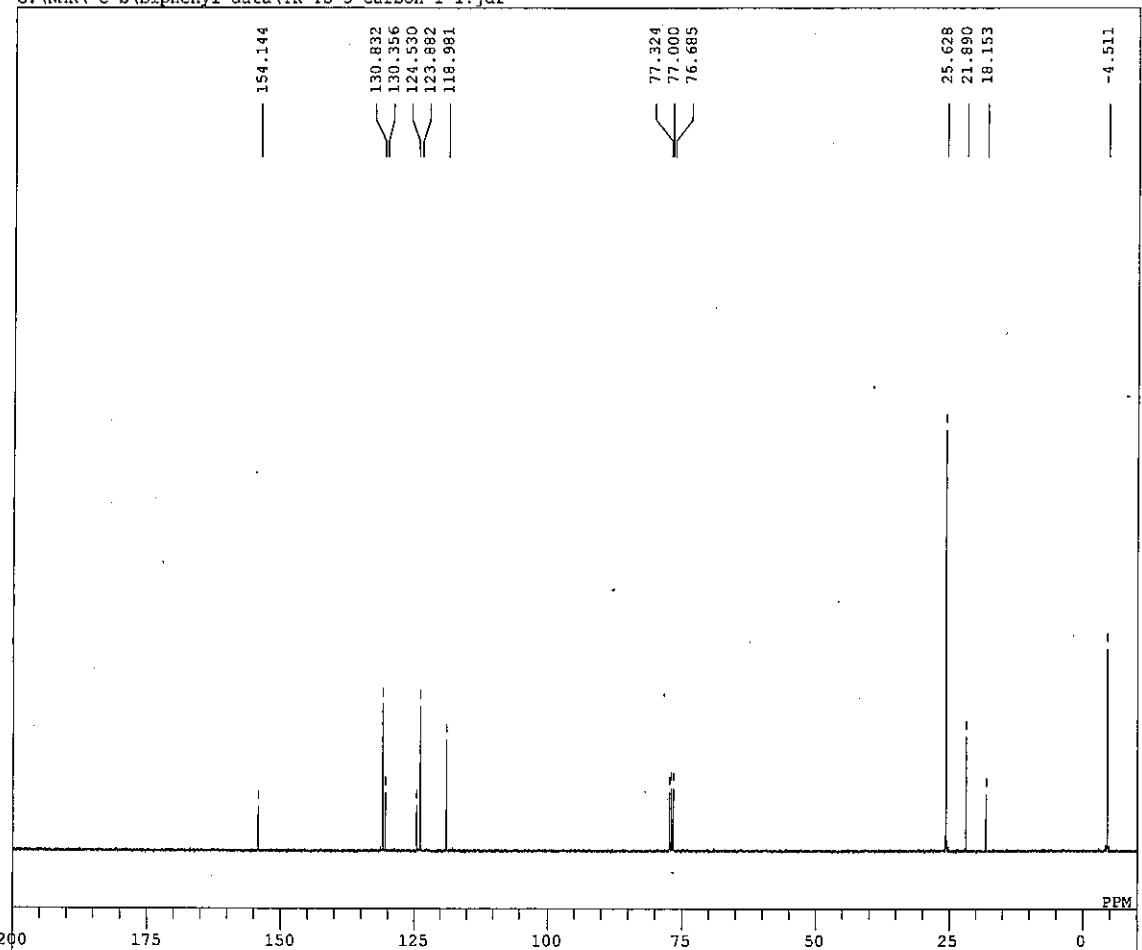
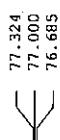
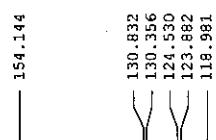
G:\NMR\é-Ø\Biphenyl data\YK-YS-3\_Proton-1-1.jdf



DFILE YK-YS-3\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-02-14 14:02:19  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 21.9 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 22

**single pulse decoupled gated NOE**

G:\NMR\é-Ø\Biphenyl data\YK-YS-3\_Carbon-1-1.jdf

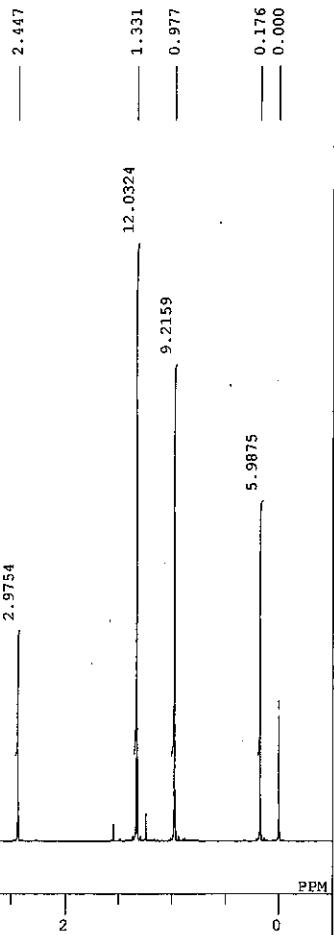
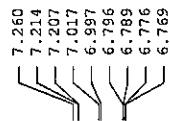


DFILE YK-YS-3\_Carbon-1-1.jdf  
COMNT single\_pulse decoupled gated  
DATIM 2012-02-14 14:03:39  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 32  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 22.1 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

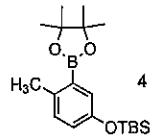


**single\_pulse**

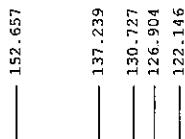
G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-1H-S3\_Proton-1-1.jdf



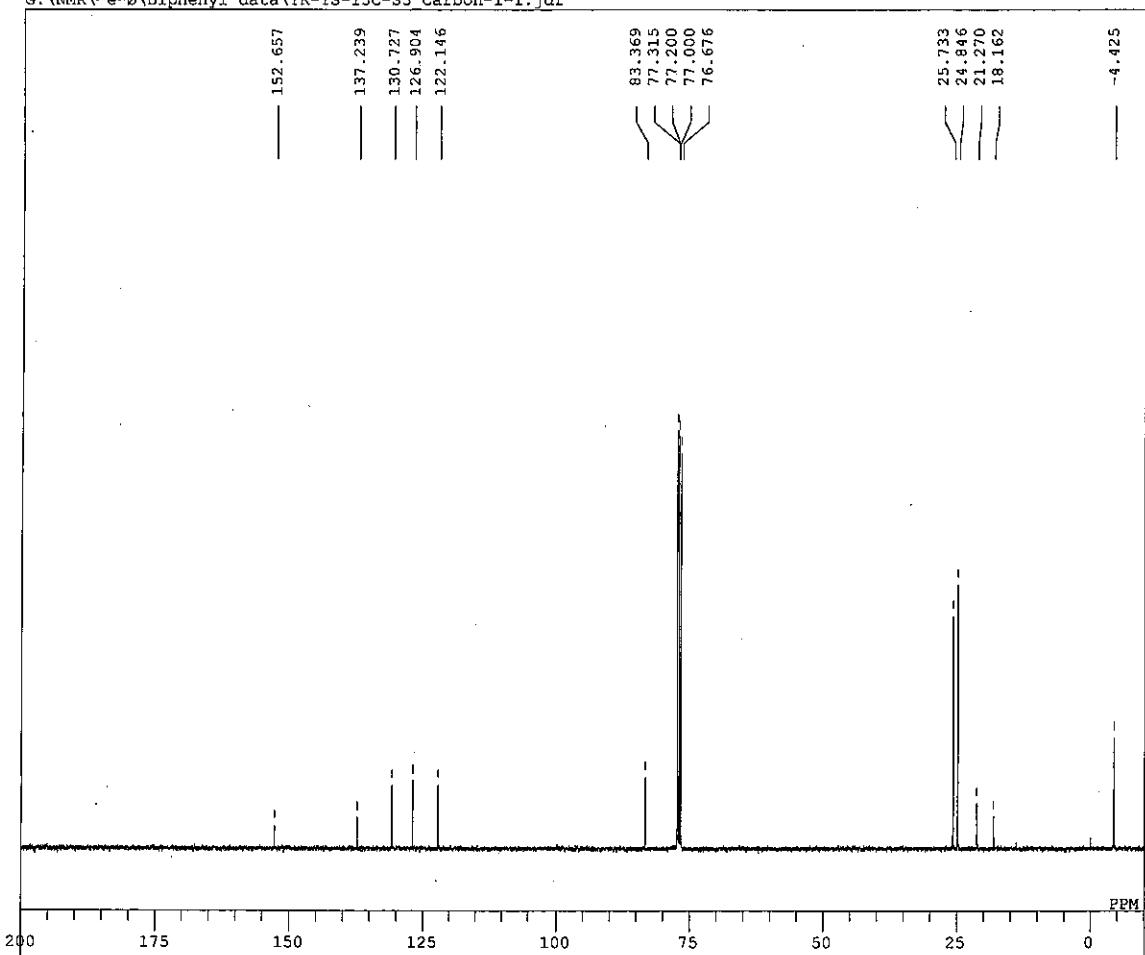
DFILE YK-YS-1H-S3\_Proton-1-1.jdf  
 COMNT single\_pulse  
 DATIM 2012-01-19 16:39:01  
 OBNUC 1H  
 EXMOD proton.jxp  
 OBFREQ 399.78 MHz  
 OBSET 4.19 KHz  
 OBFIN 7.29 Hz  
 POINT 16384  
 FREQU 7503.00 Hz  
 SCANS 8  
 ACQTM 2.1837 sec  
 PD 5.0000 sec  
 PW1 5.00 usec  
 IRNUC 1H  
 CTEMP 19.8 c  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF 0.12 Hz  
 RGAIN 46

**single pulse decoupled gated NOE**

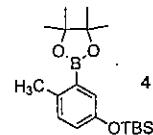
G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-13C-S3\_Carbon-1-1.jdf



-4.425

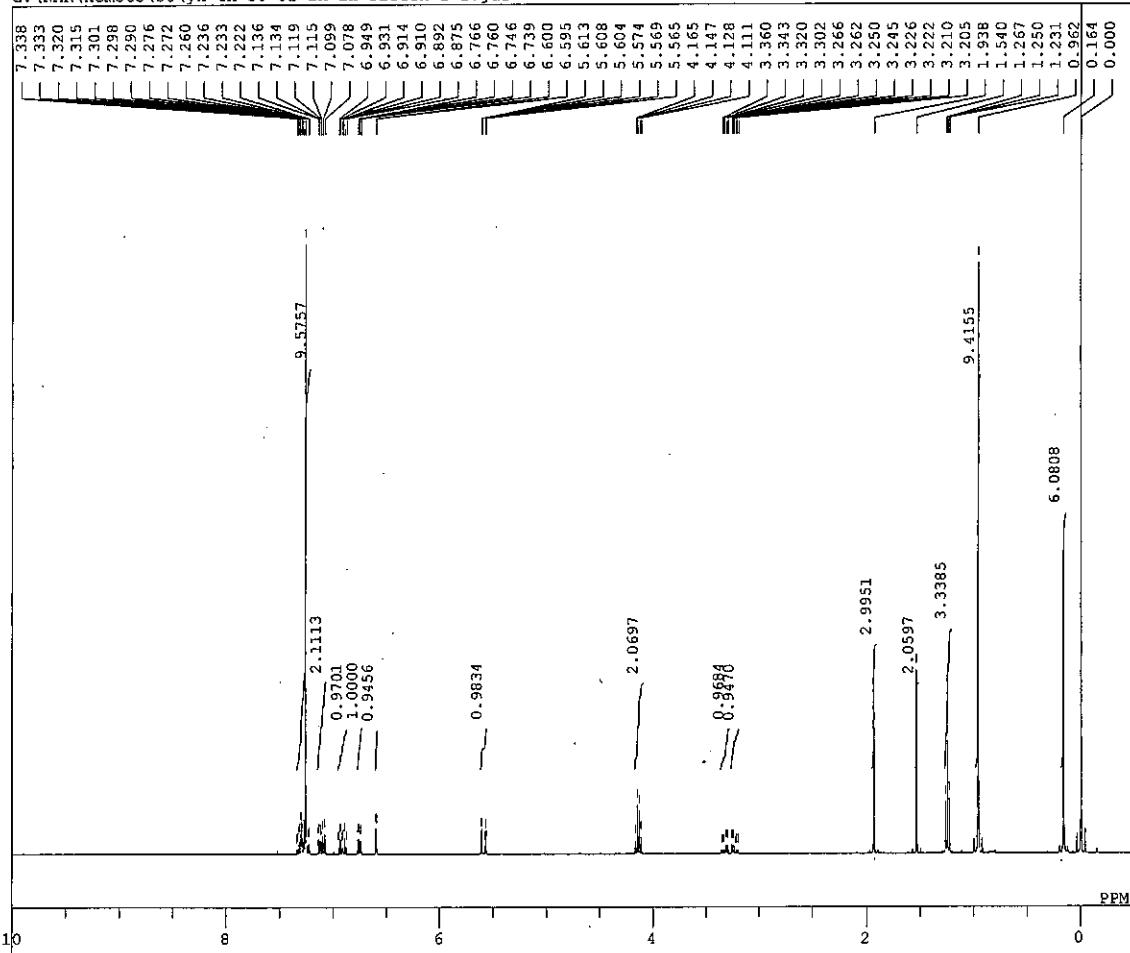


DFILE YK-YS-13C-S3\_Carbon-1-1.jdf  
 COMNT single pulse decoupled gated  
 DATIM 2012-01-21 00:01:53  
 OBNUC 13C  
 EXMOD carbon.jxp  
 OBFREQ 100.53 MHz  
 OBSET 5.35 KHz  
 OBFIN 5.86 Hz  
 POINT 32767  
 FREQU 31407.04 Hz  
 SCANS 512  
 ACQTM 1.0433 sec  
 PD 2.0000 sec  
 PW1 3.07 usec  
 IRNUC 1H  
 CTEMP 20.2 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 1.20 Hz  
 RGAIN 50

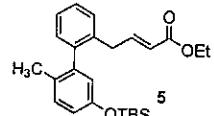


single\_pulse

G:\NMR\nemoto\30\yk-tn-30-02-SM-1H\_Proton-1-1.jdf

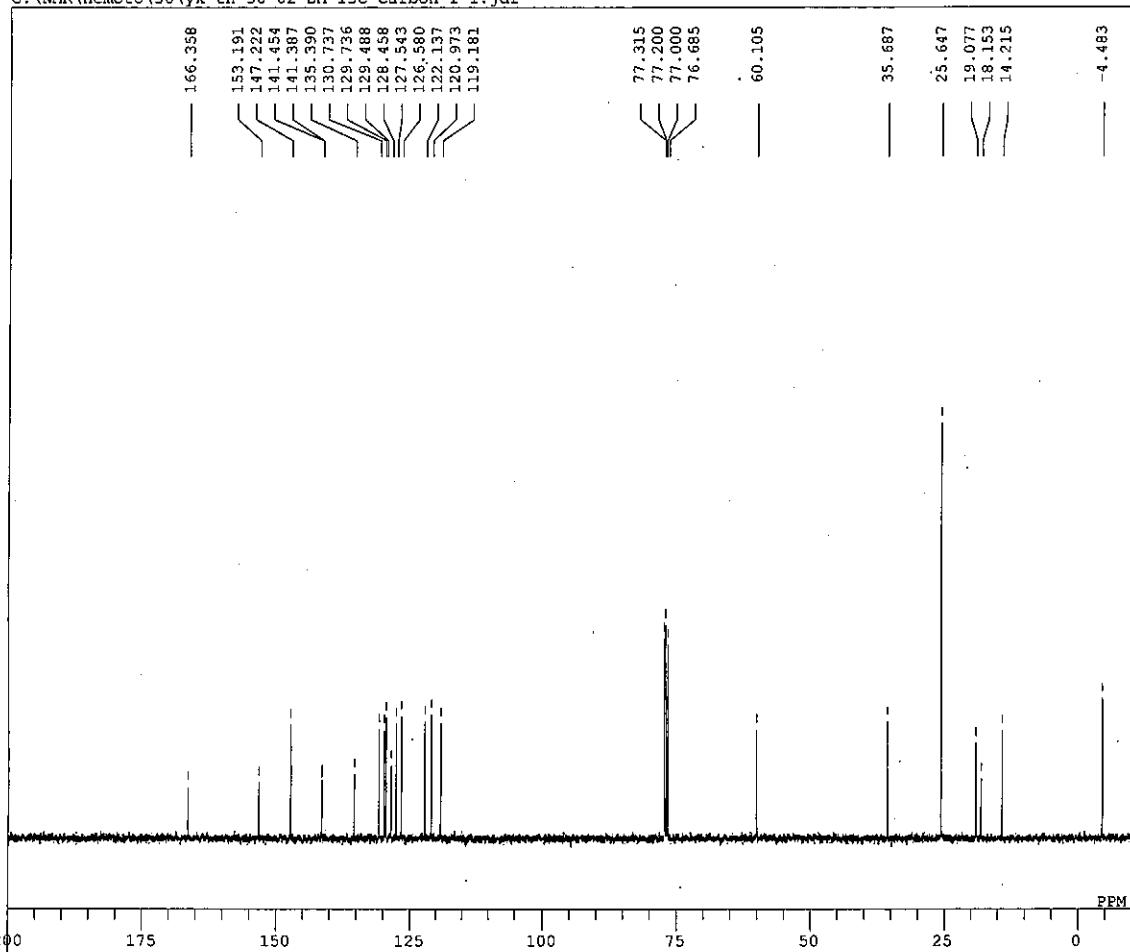


DFILE yk-tn-30-02-SM-1H\_Proton-1-1  
COMNT single\_pulse  
DATIM 2012-02-15 19:05:35  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 22.8 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 54

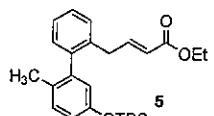


single pulse decoupled gated NOE

G:\NMR\nemoto\30\yk-tn-30-02-SM-13C\_Carbon-1-1.jdf

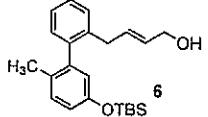
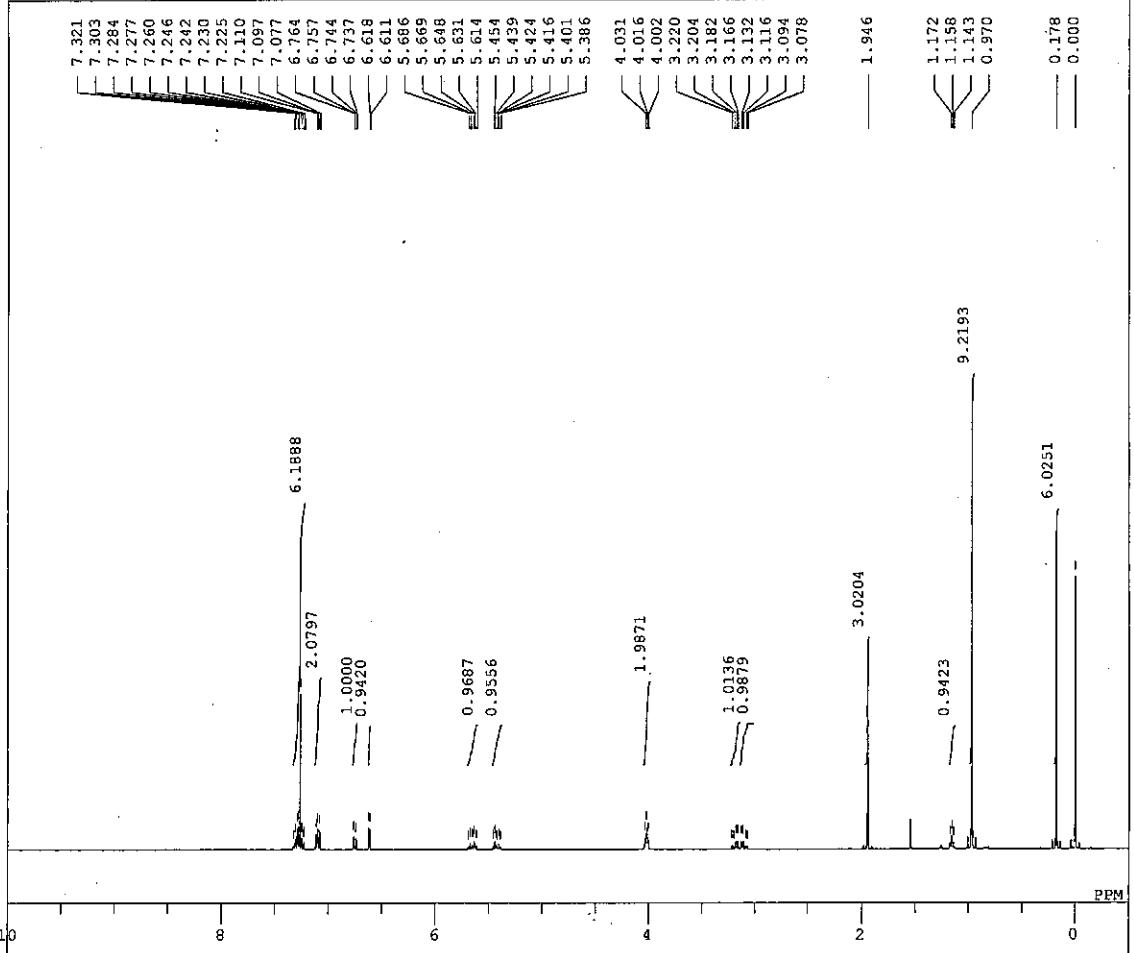


DFILE yk-tn-30-02-SM-13C\_Carbon-1-1  
COMNT single pulse decoupled gated  
DATIM 2012-02-15 19:16:20  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 32  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 22.9 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



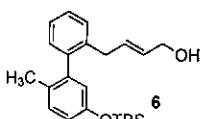
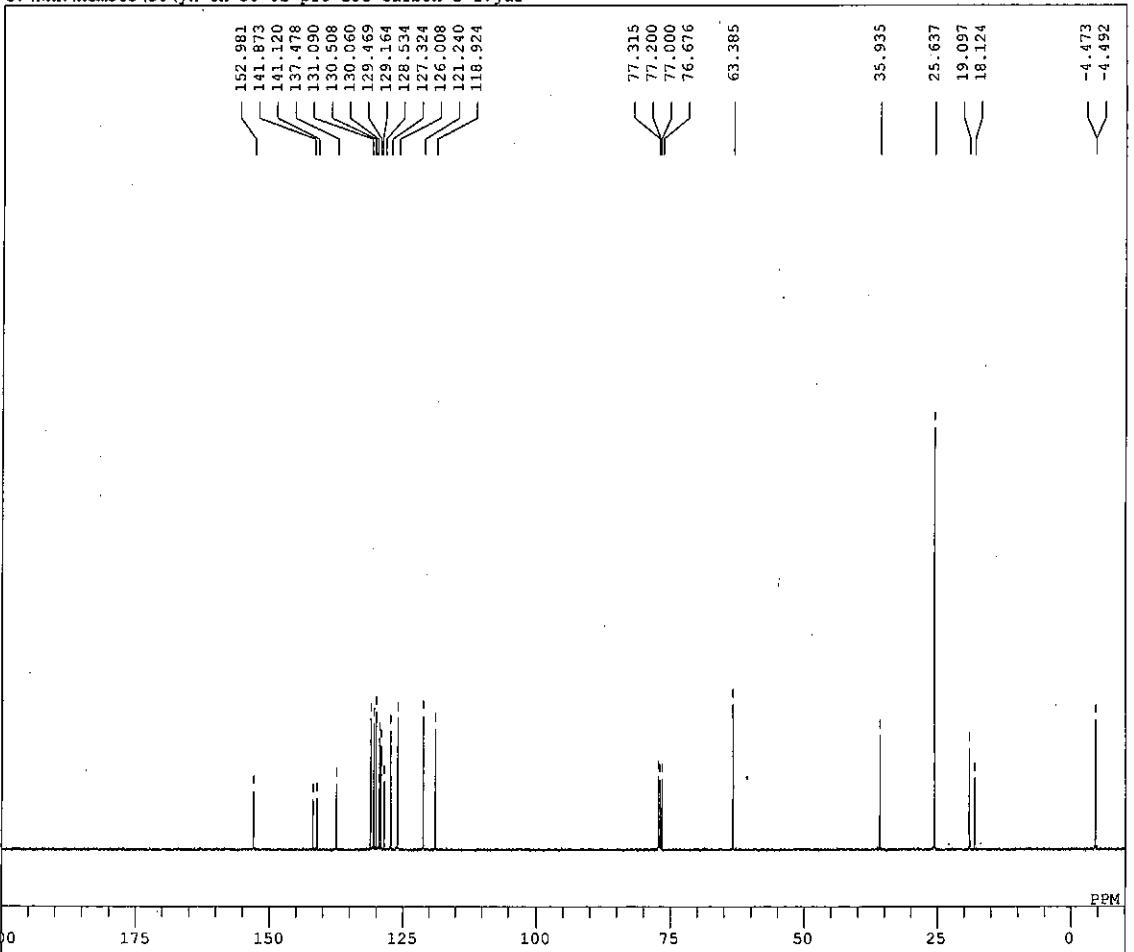
### single\_pulse

G:\NMR\nemoto\30\yk-tn-30-02-pro-1H\_Proton-1-1.jdf



#### **single pulse decoupled gated NOE**

G:\NMR\nemoto\30\yk-tn-30-02-pro-13C Carbon-1-1.jdf



```

DTFILE yk-tn-30-02-pro-1H_Proton-1-
COMNT single_pulse
DATIM 2012-02-20 15:03:19
OBNUC 1H
EXMOD proton.jxp
OBFRQ      399.78 MHz
OBSET      4.19 kHz
OBFIN      7.29 Hz
POINT      16384
FREQU 7503.00 Hz
SCANS      16
ACQTM      2.1837 sec
PD         5.0000 sec
PW1        5.00 usec
IRNUC     1H
CTEMP      22.1 c
SLVNT    CDCL3
EXREF      0.00 ppm
BF         0.12 Hz
RGAIN      50

```

```

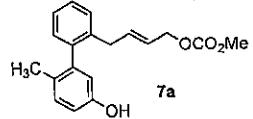
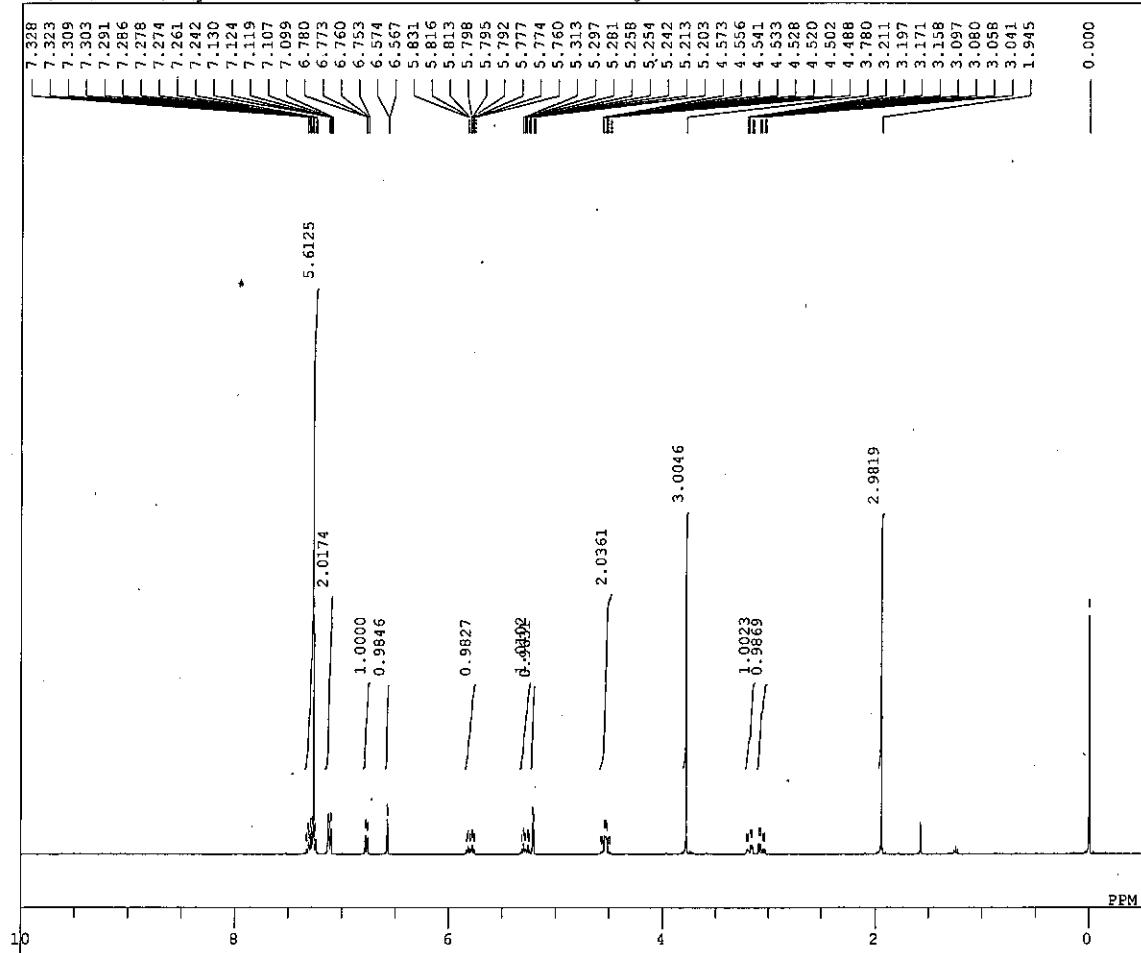
DFILE yk-tn-30-02-pro-13C_Carbon-1
COMNT single pulse decoupled gated
DATIM 2012-02-20 15:10:02
OBNUC 13C
EXMOD carbon.jxp
OBPRQ      100.53 MHz
OBSET      5.35 KHz
OBSEIN     5.86 Hz
POINT      32767
FREQU     31407.04 Hz
SCANS       64
ACOTM      1.0433 sec
PD        2.0000 sec
PW1       3.07 usec
IRNUC     1H
CTEMP      22.3 c
SLVNT    CDCL3
EXREF      77.00 ppm
BF        1.20 Hz
PCAIN      50

```

S-24

### **single\_pulse**

G:\NMR\nemoto\29\yk-tn-29-120120-model-substrate Proton-1-1.jdf



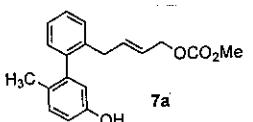
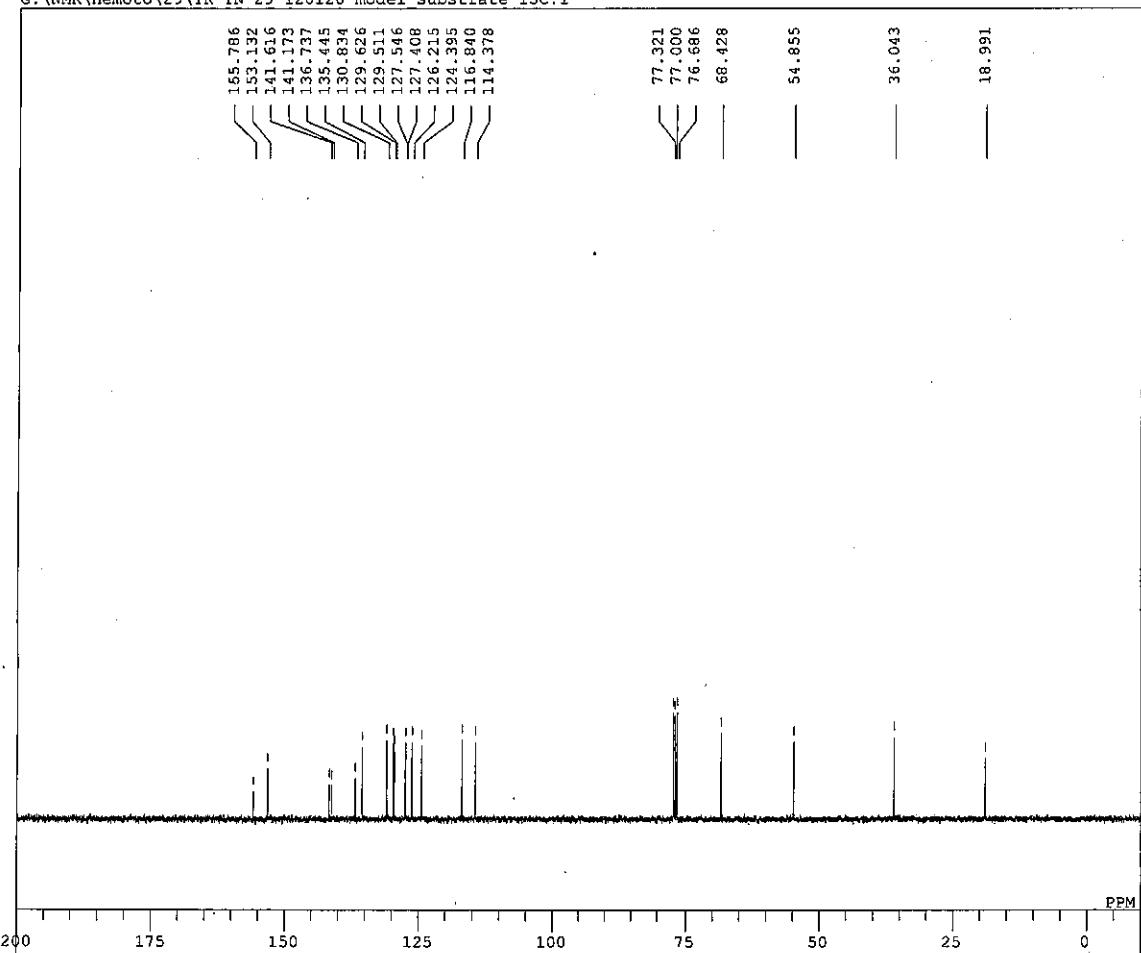
```

DFILE  yk-tn-29-120120-model-substr
COMMENT single_pulse
DATIM  2012-01-20 13:37:03
OBNUC  1H
EXMOD proton.jxp
OBFREQ 399.78 MHz
OBSET   4.19 kHz
OBFIN   7.29 Hz
POINT   16384
FREQU  7503.00 Hz
SCANS   8
ACQTM   2.1837 sec
PD      5.0000 sec
PW1     5.00 usec
IRNUC  1H
CTEMP   20.1 c
SLVNT   CDCL3
EXREF   0.00 ppm
BF      0.12 Hz
RGAIN   50

```

YK-TN-29-120120-model substrate-13C

G:\NMR\nemoto\29\YK-TN-29-120120-model substrate-13C.1



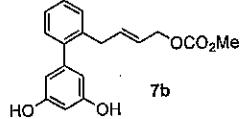
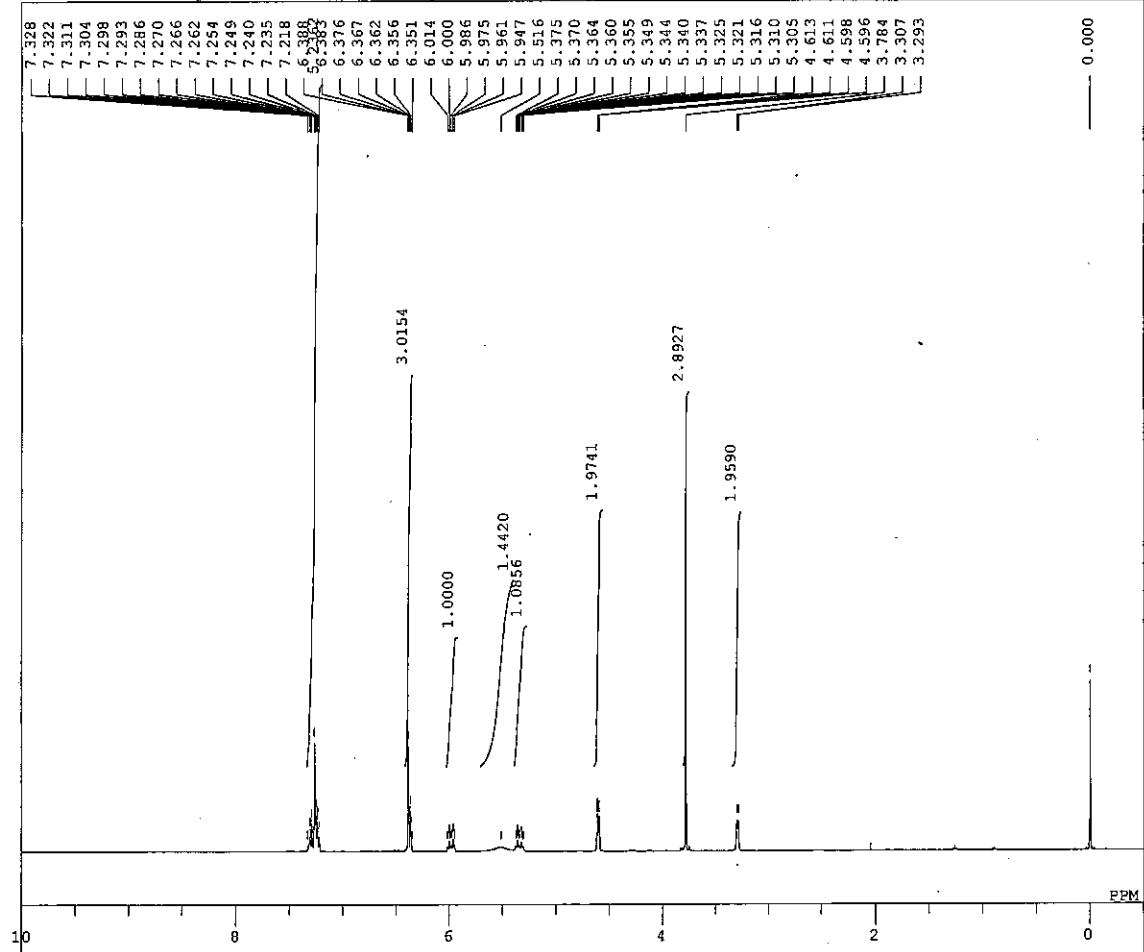
```

DFILE YK-TN-29-120120-model_substr
COMMT YK-TN-29-120120-model substr
DATIM 2012-01-20 14:57:12
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 54
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.17 usec
IRNUC 1H
CTEMP 23.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

```

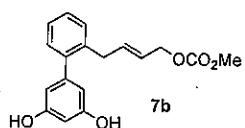
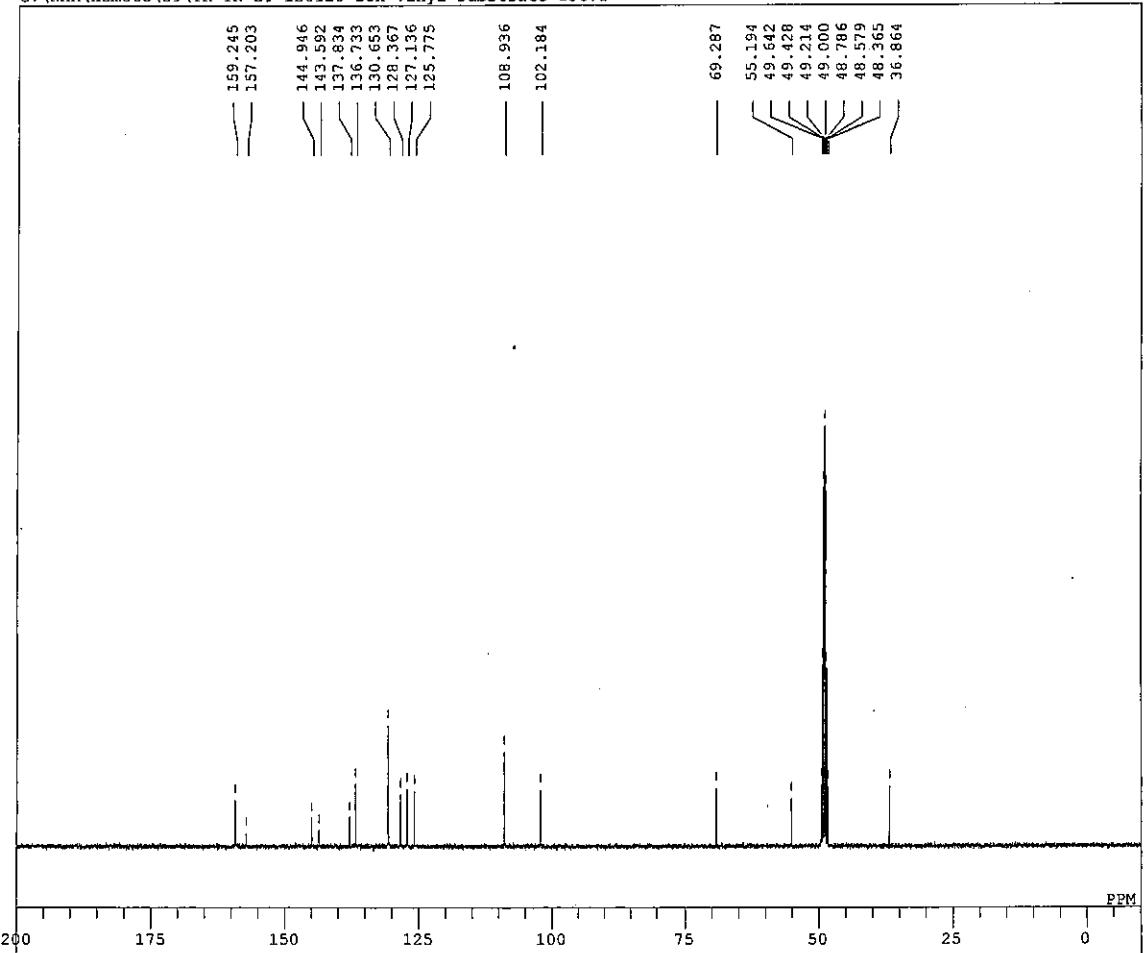
### single\_pulse

G:\NMR\nemoto\29\yk-tn-29-120120-2OH-vinyl-substrate\_Proton-1-1.jdf



## YK-TN-29-120120-2OH-vinyl-substrate-13C

G:\NMR\nemoto\29\YK-TN-29-120120-2OH-vinyl-substrate-13C.1



```

DFILE yk-tn-29-120120-20H-vinyl-su
COMNT single_pulse
DATIM 2012-01-20 13:47:45
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 kHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 16
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50

```

```

YK-TN-29-120120-20H-vinyl-su
YK-TN-29-120120-20H-vinyl-su
2012-01-20 15:11:45
13C
single_pulse_dec
    100.53 MHz
      5.35 kHz
      5.86 Hz
    32768
  25188.92 Hz
    223
  1.3009 sec
  1.0000 sec
    3.17 usec

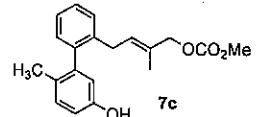
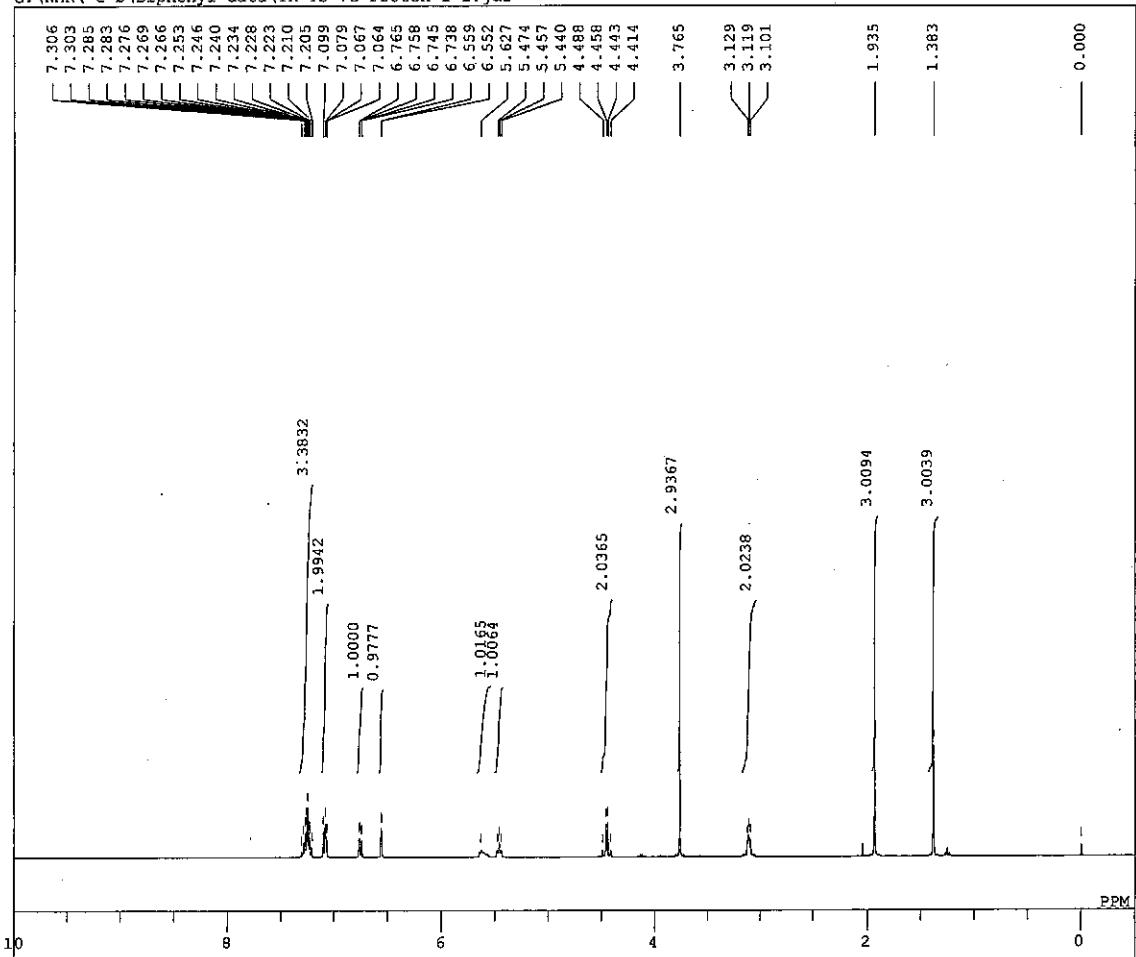
1H
    24.1 c
CD3OD
  49.00 ppm
  1.20 Hz
    23

```

S-26

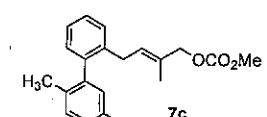
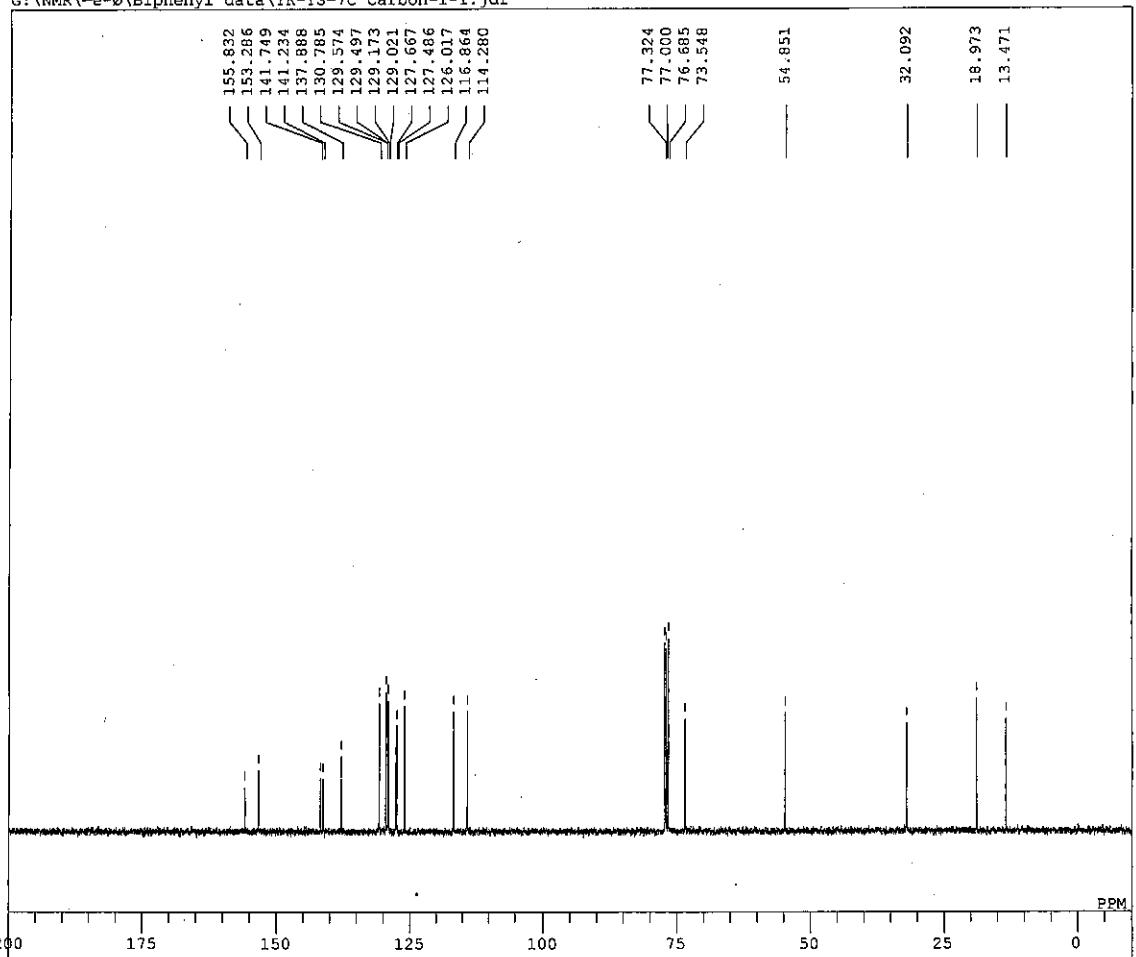
### **single\_pulse**

G:\NMR\-\é-Ø\Biphenyl data\YK-YS-7c Proton-1-1.jdf



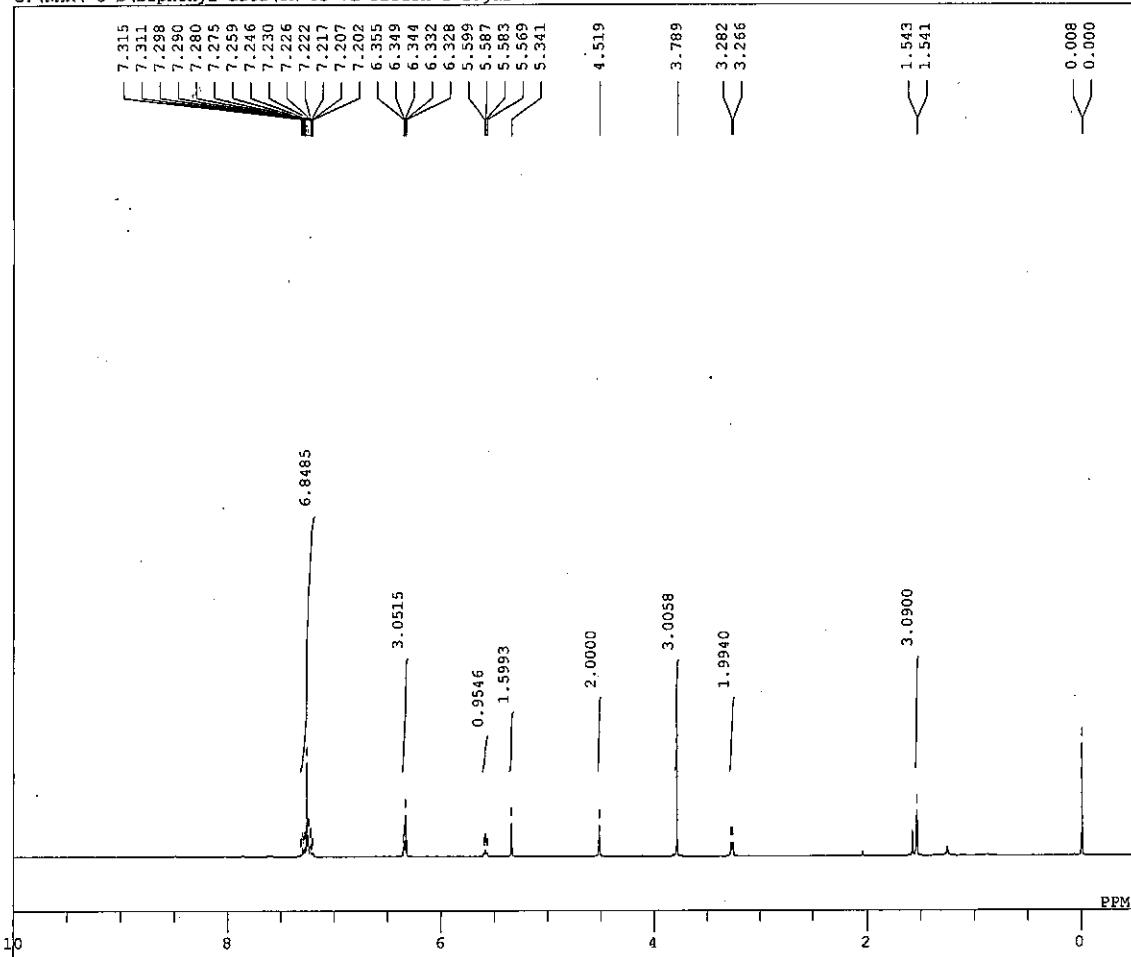
#### **single pulse decoupled gated NOE**

G:\NMR\-\é-Ø\Biphenyl data\YK-Y5-7c Carbon-1-1.jdf

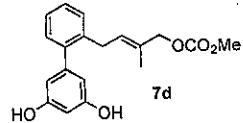


single\_pulse

G:\NMR\é-Ø\Biphenyl data\YK-YS-7d\_Proton-1-1.jdf

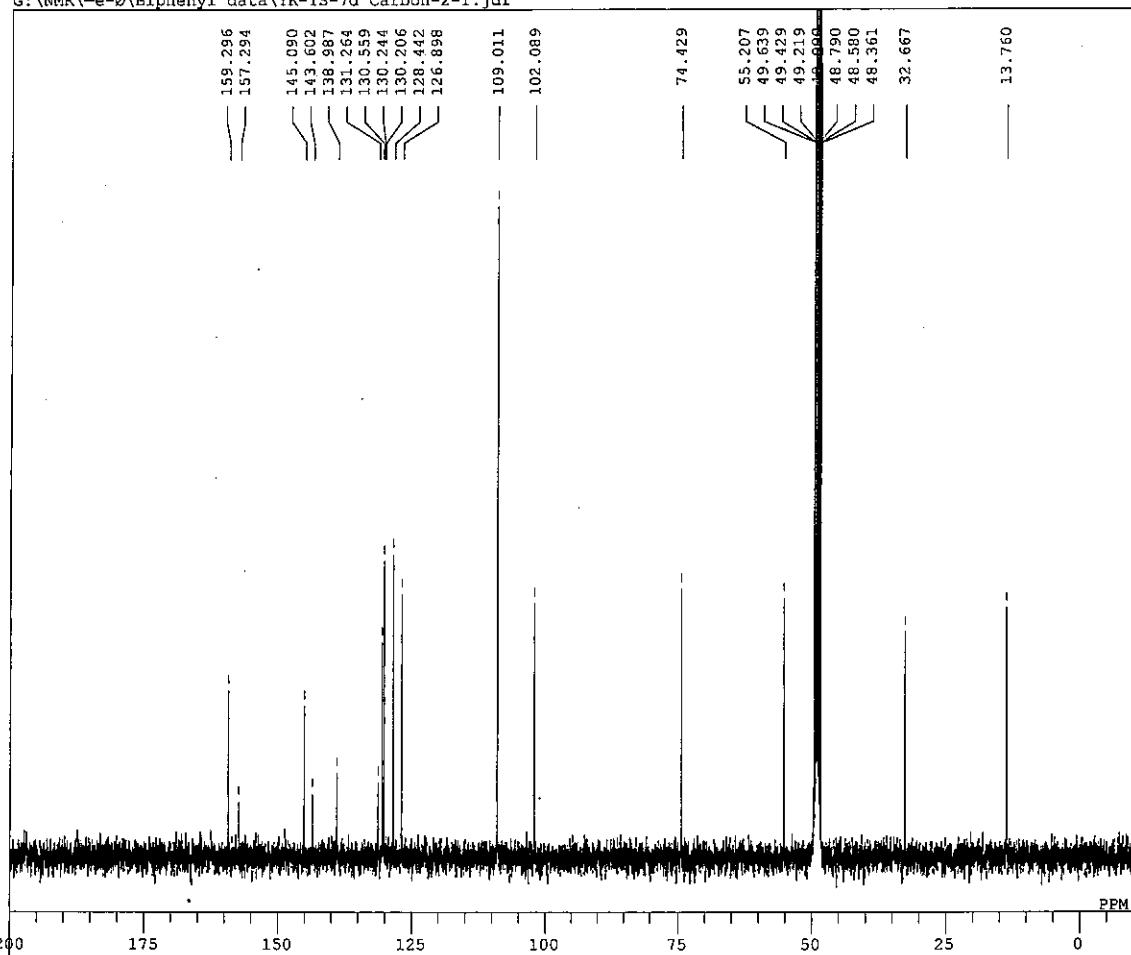


DFILE YK-YS-7d\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-03-13 18:01:44  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
FW1 5.00 usec  
IRNUC 1H  
CTEMP 24.6 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 50

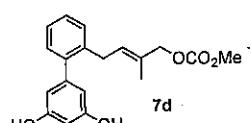


single pulse decoupled gated NOE

G:\NMR\é-Ø\Biphenyl data\YK-YS-7d\_Carbon-2-1.jdf

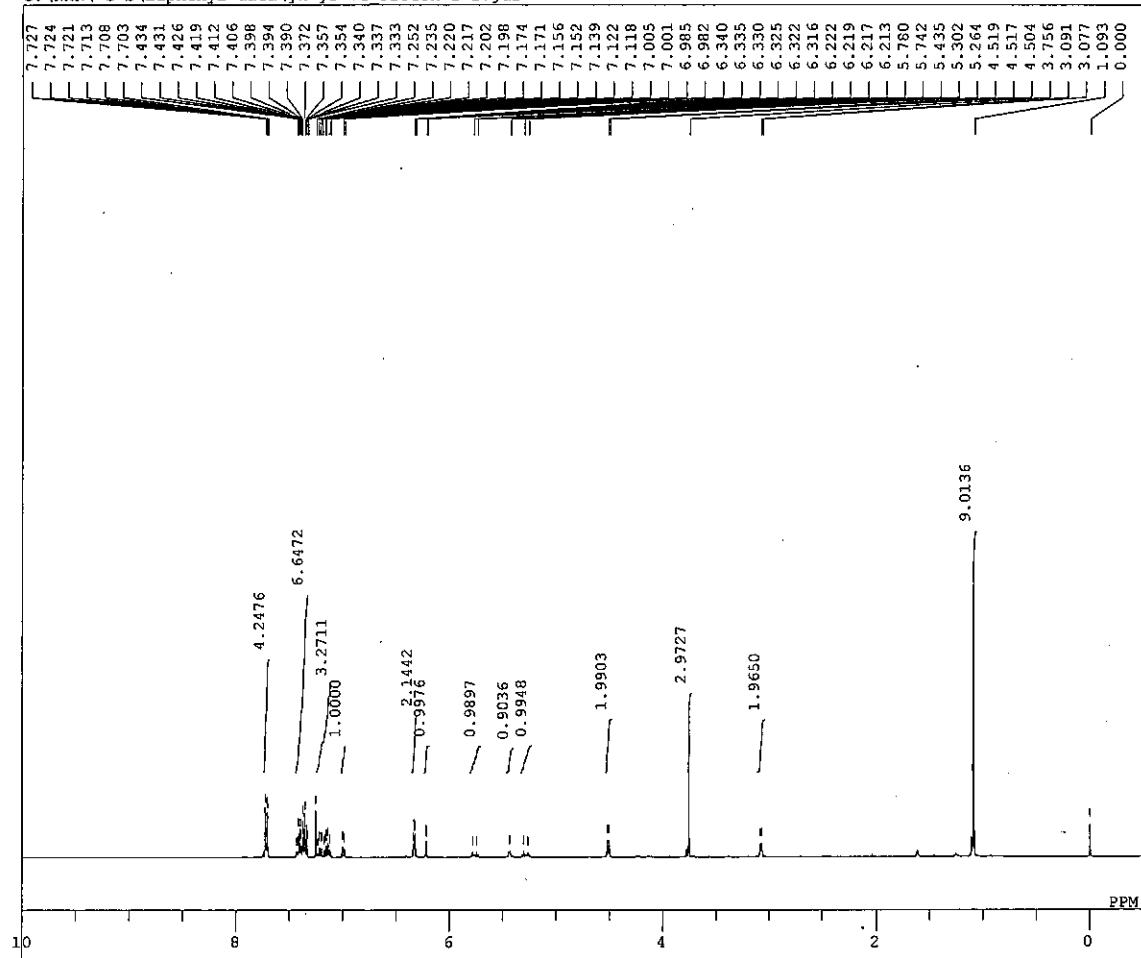


DFILE YK-YS-7d\_Carbon-2-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-03-13 22:48:59  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 257  
ACQTM 1.0433 sec  
PD 2.0000 sec  
FW1 3.07 usec  
IRNUC 1H  
CTEMP 24.6 c  
SLVNT CD3OD  
EXREF 49.00 ppm  
BF 1.20 Hz  
RGAIN 50

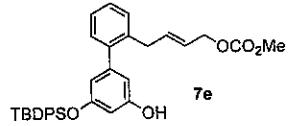


single\_pulse

G:\NMR\é-Ø\Biphenyl data\yk-ys-7e\_Proton-1-1.jdf

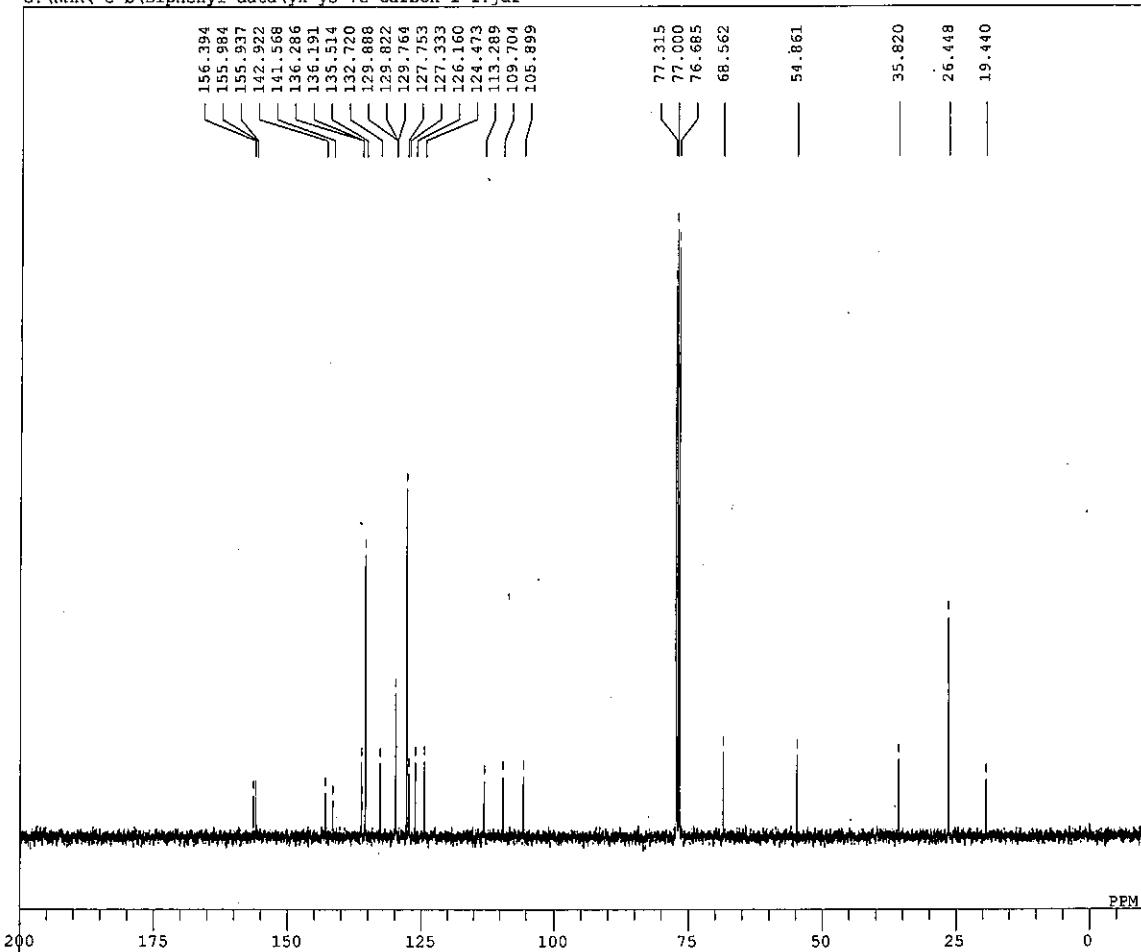


DFILE yk-ys-7e\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-02-29 15:19:58  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQ 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
FW1 5.00 usec  
IRNUC 1H  
CTEMP 21.9 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 40

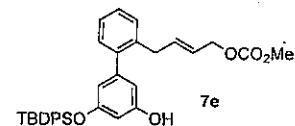


single pulse decoupled gated NOE

G:\NMR\é-Ø\Biphenyl data\yk-ys-7e\_Carbon-1-1.jdf

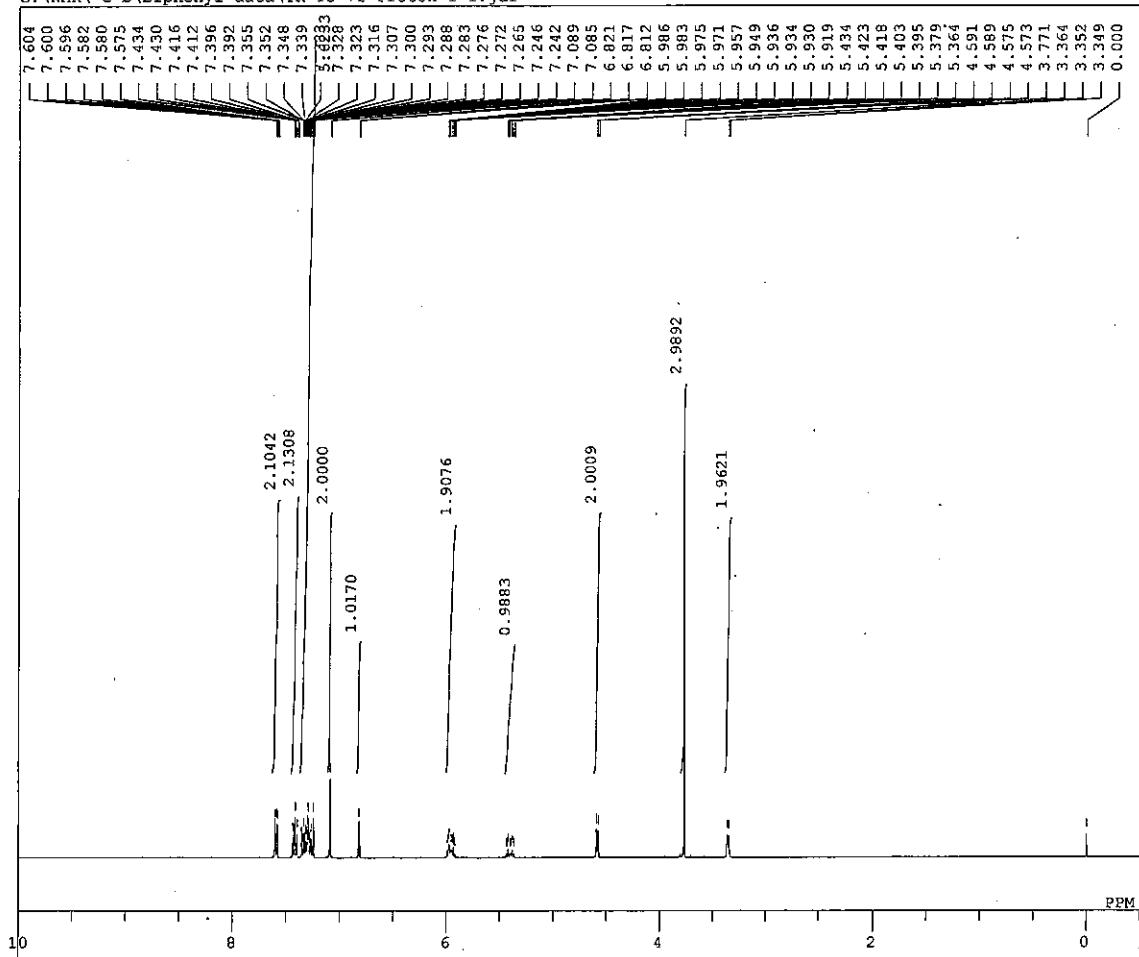


DFILE yk-ys-7e\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-02-29 15:21:17  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.66 Hz  
POINT 32767  
FREQ 31407.04 Hz  
SCANS 128  
ACQTM 1.0433 sec  
PD 2.0000 sec  
FW1 3.07 usec  
IRNUC 1H  
CTEMP 22.2 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

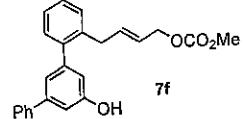


### single\_pulse

G:\NMR\-\é-\Biphenyl data\YK-YS-7f Proton-1-1.jdf

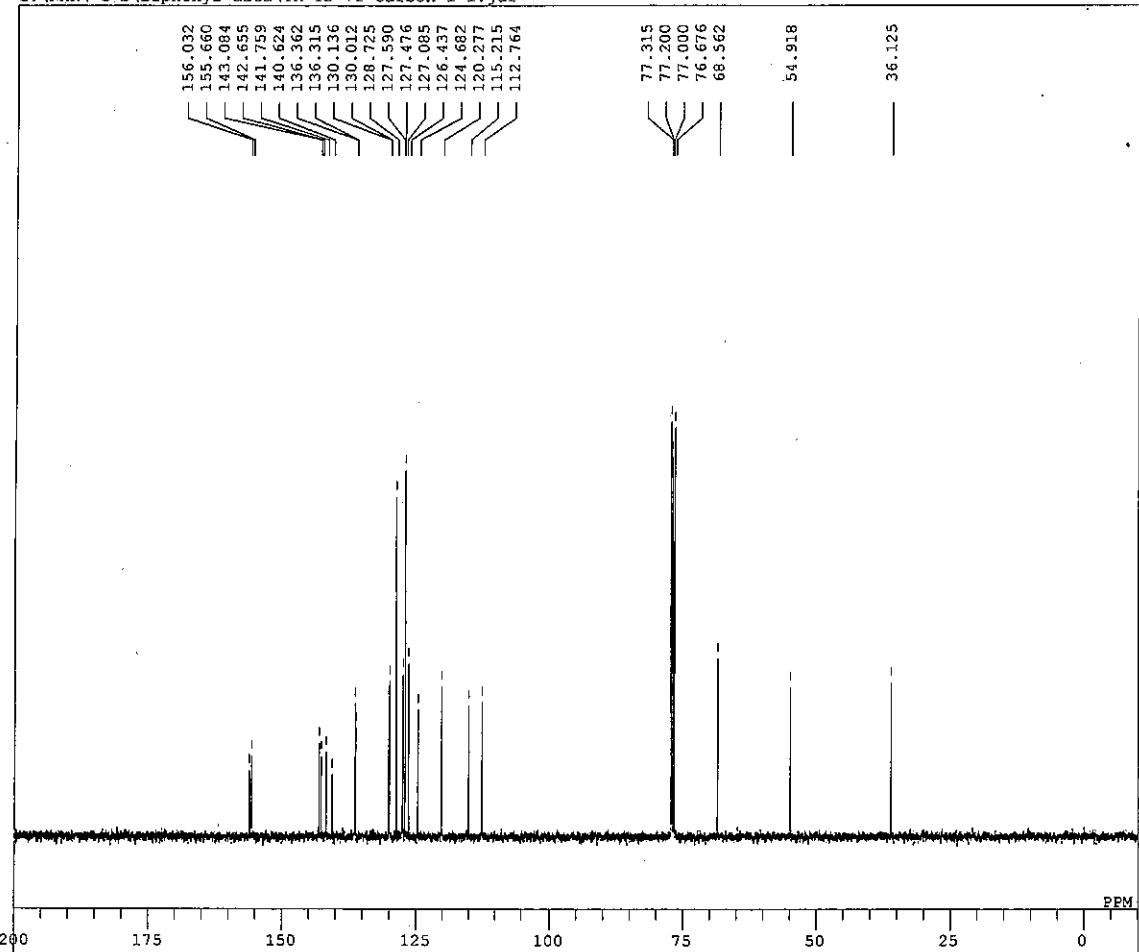


DFILE YK-YS-7f\_Proton-1-1.jdf  
single\_pulse  
DATIM 2012-02-28 23:32:44  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQ 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 22.7 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 34

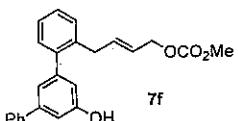


### single pulse decoupled gated NOE

G:\NMR\-\é-\Biphenyl data\YK-YS-7f Carbon-1-1.jdf

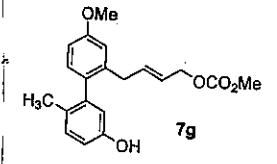
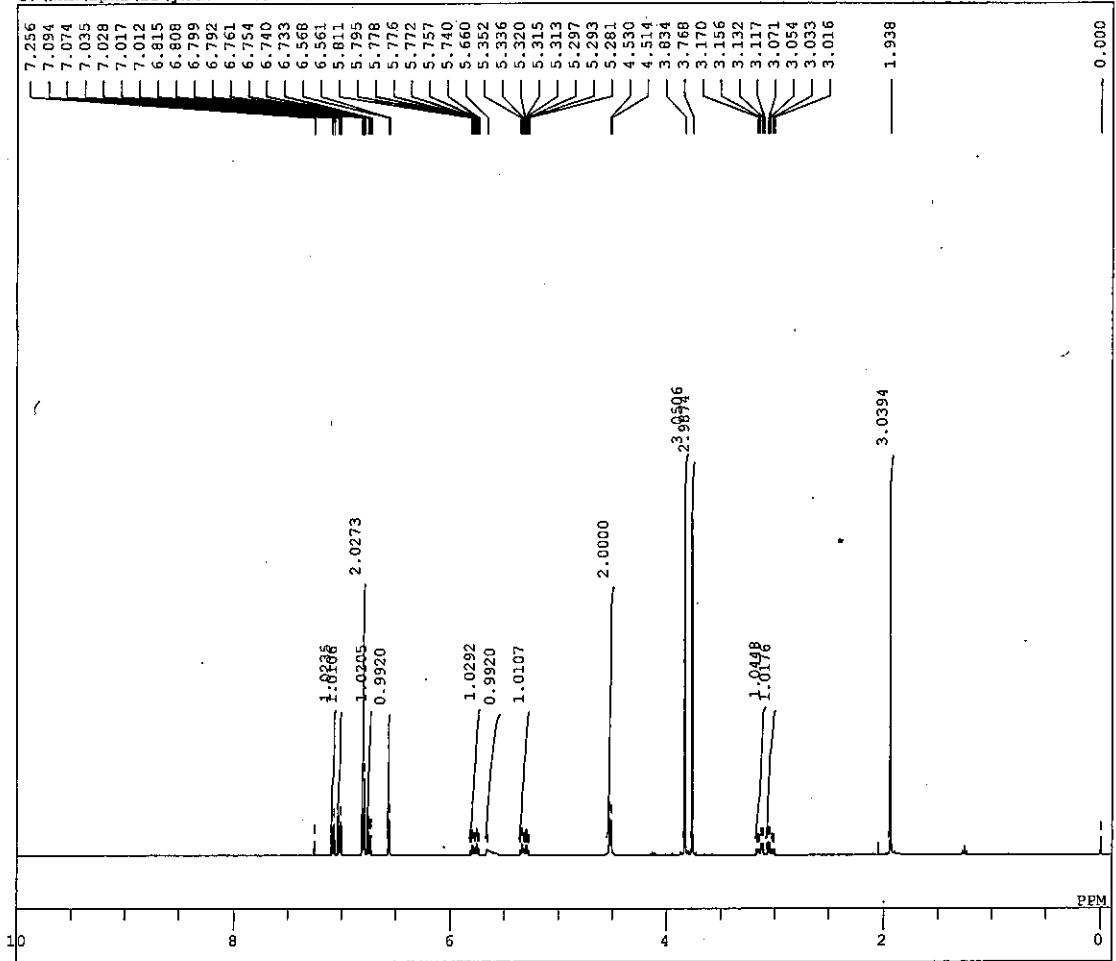


DFILE YK-YS-7f\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-02-28 23:34:03  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQ 31407.04 Hz  
SCANS 128  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 23.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



### single\_pulse

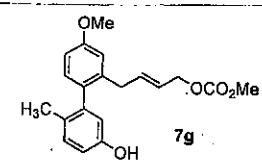
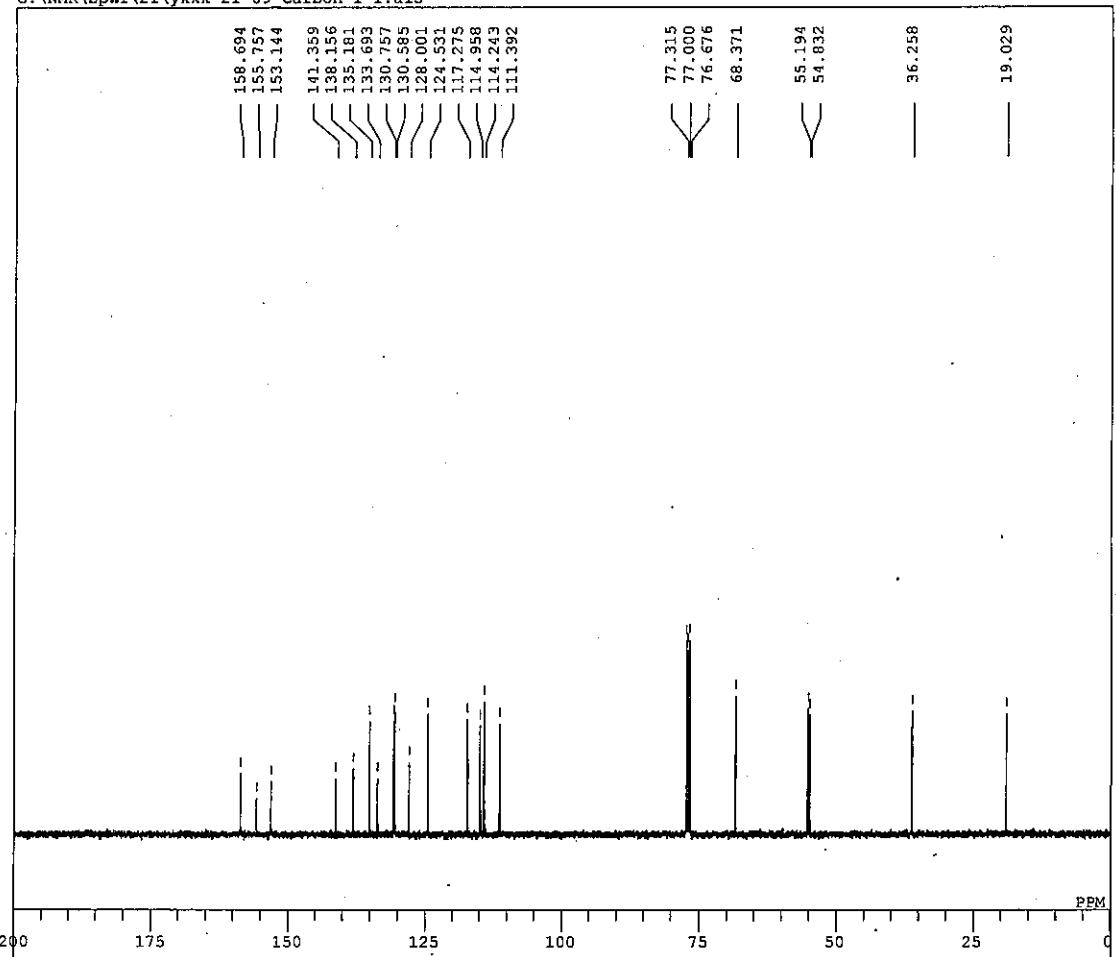
G:\NMR\Šp&f\21\ykkk-21-09\_Proton-1-1.als



Molecular Weight: 342.3857

### single pulse decoupled gated NOE

G:\NMR\Šp&f\21\ykkk-21-09\_Carbon-1-1.als

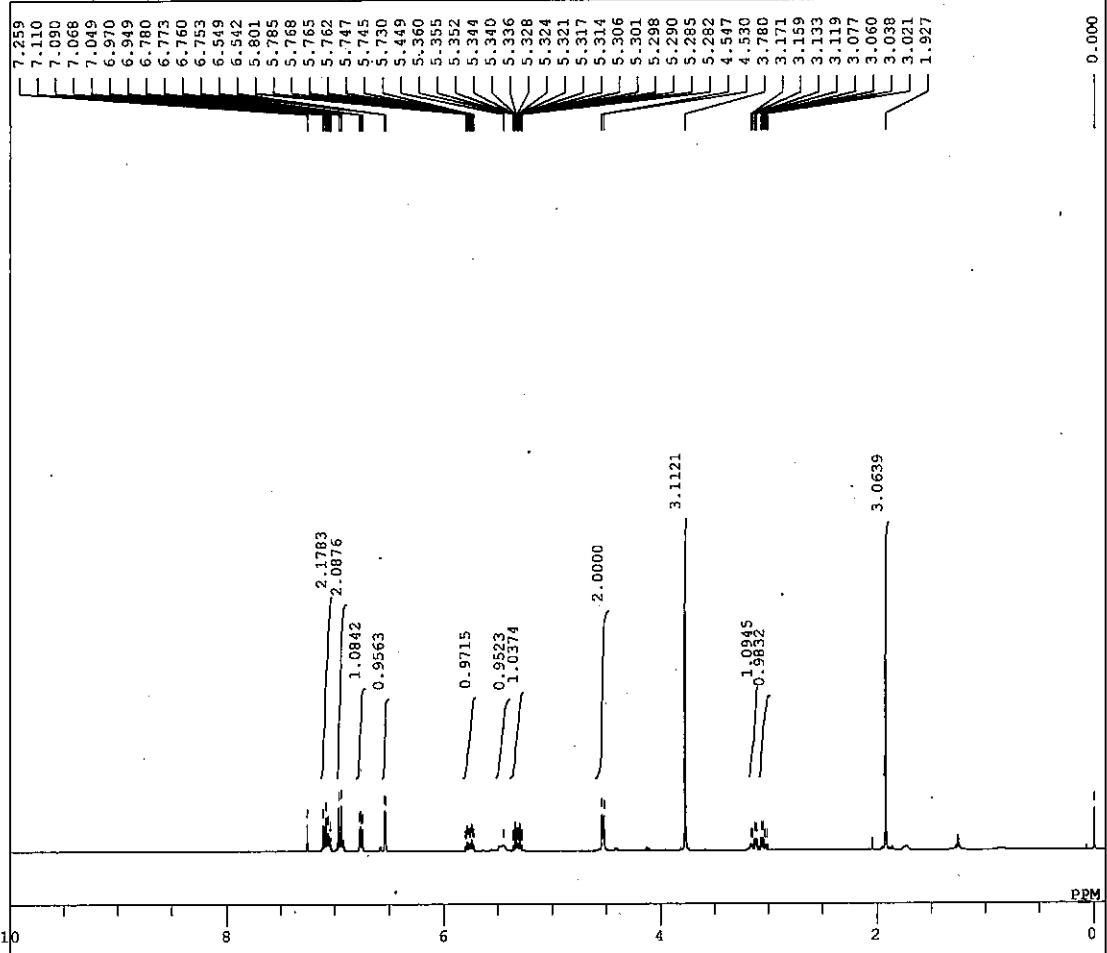


Molecular Weight: 342,3857

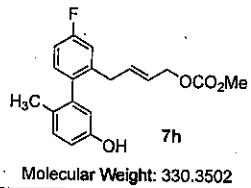
S-31

single\_pulse

G:\NMR\Šptí\21\ykkk-21-08\_Proton-1-1.als

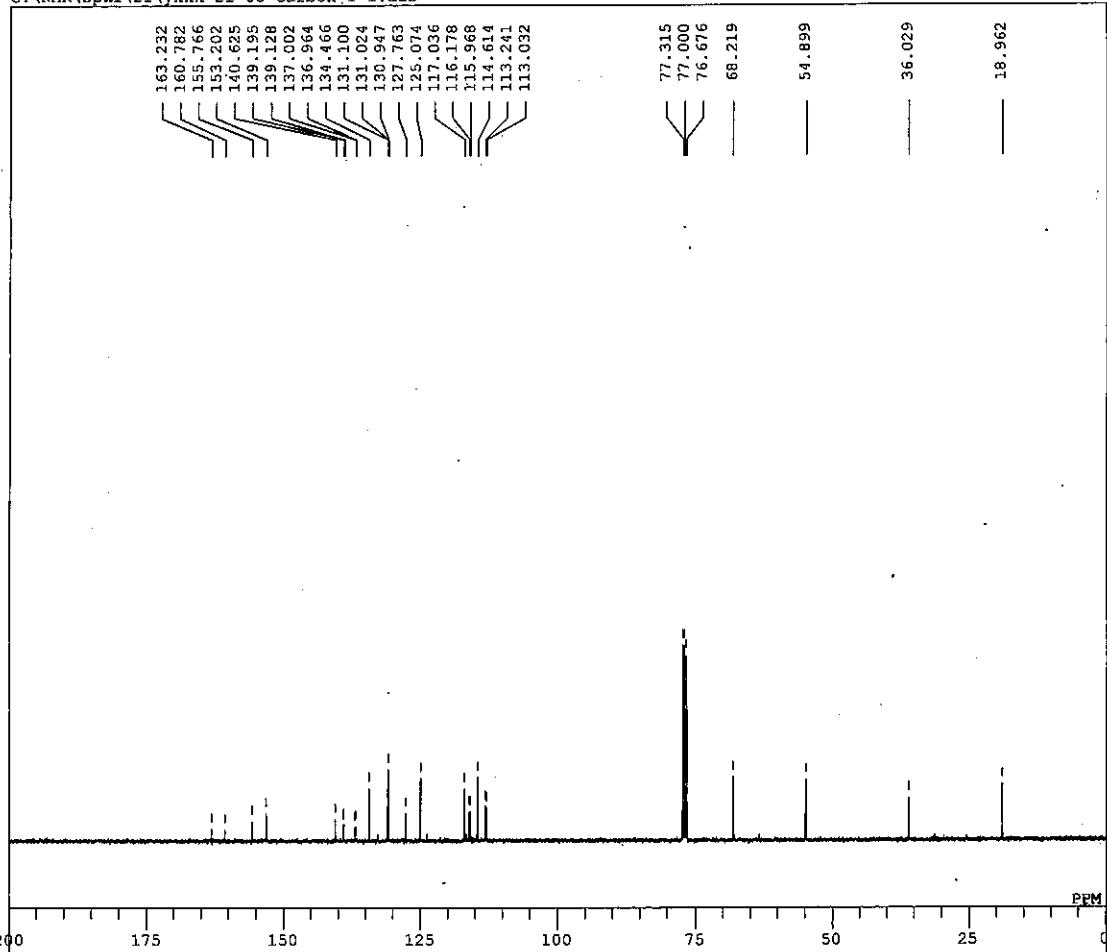


DFILE ykkk-21-08\_Proton-1-1.als  
COMNT single\_pulse  
DATIM 2012-03-07 07:43:48  
OBNUC 1H  
EXMOD proton.jxp  
OBFQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 13107  
FREQU 6002.40 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 23.5 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 38

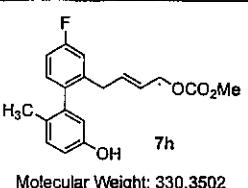


single pulse decoupled gated NOE

G:\NMR\Šptí\21\ykkk-21-08\_Carbon-1-1.als

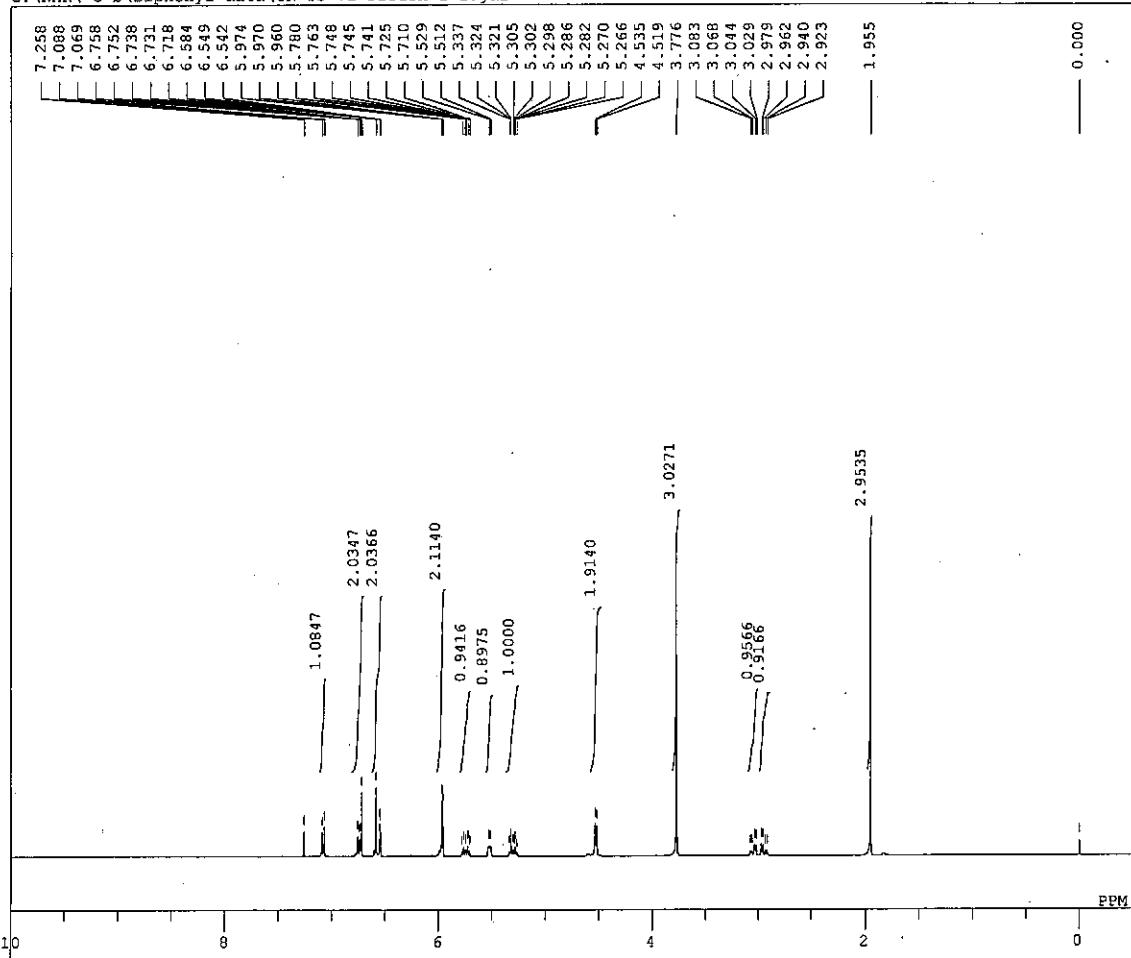


DFILE ykkk-21-08\_Carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2012-03-07 07:46:45  
OBNUC 13C  
EXMOD carbon.jxp  
OBFQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 26214  
FREQU 25125.63 Hz  
SCANS 318  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 23.7 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

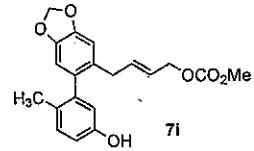


single\_pulse

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-7i Proton-1-1.jdf

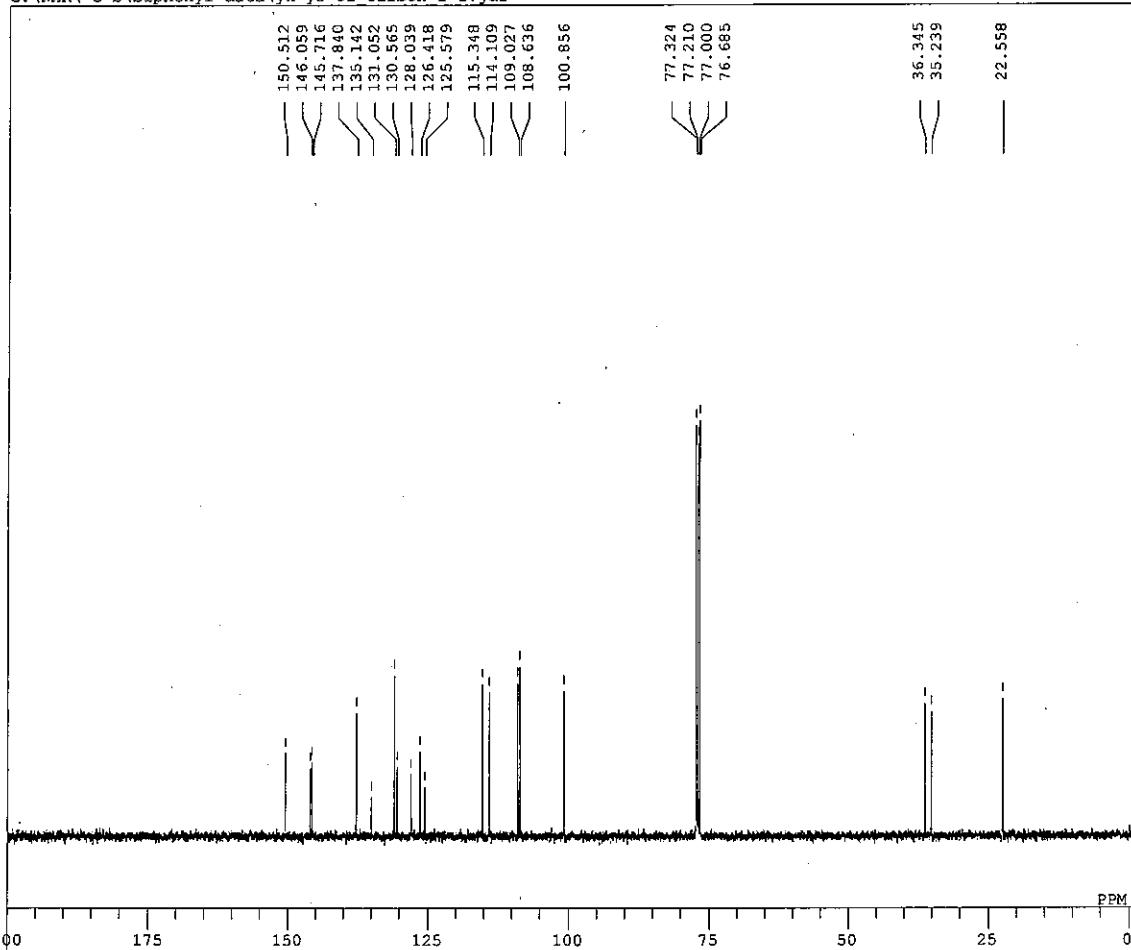


DFILE YK-YS-7i Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-02-28 23:46:17  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
FW1 5.00 usec  
IRNUC 1H  
CTEMP 22.7 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 34

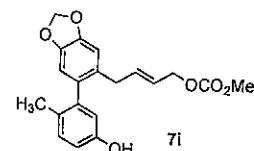


single pulse decoupled gated NOE

G:\NMR\-\é-\Ø\Biphenyl data\yk-ys-8i Carbon-1-1.jdf

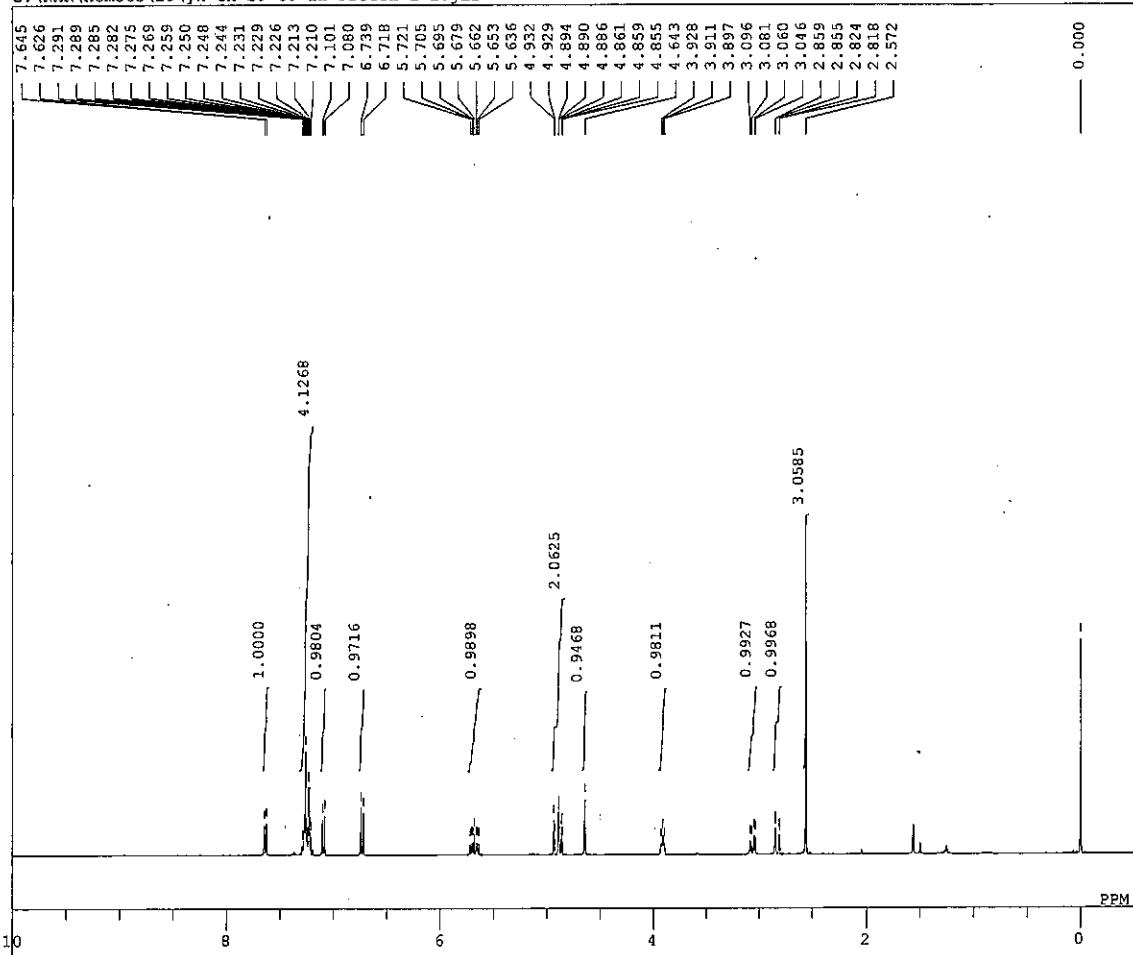


DFILE yk-ys-8i\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-02-29 22:53:06  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 128  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 22.0 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

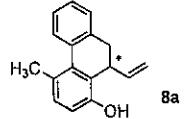


single\_pulse

G:\NMR\nemoto\29\yk-tn-29-60-1H\_Proton-1-1.jdf

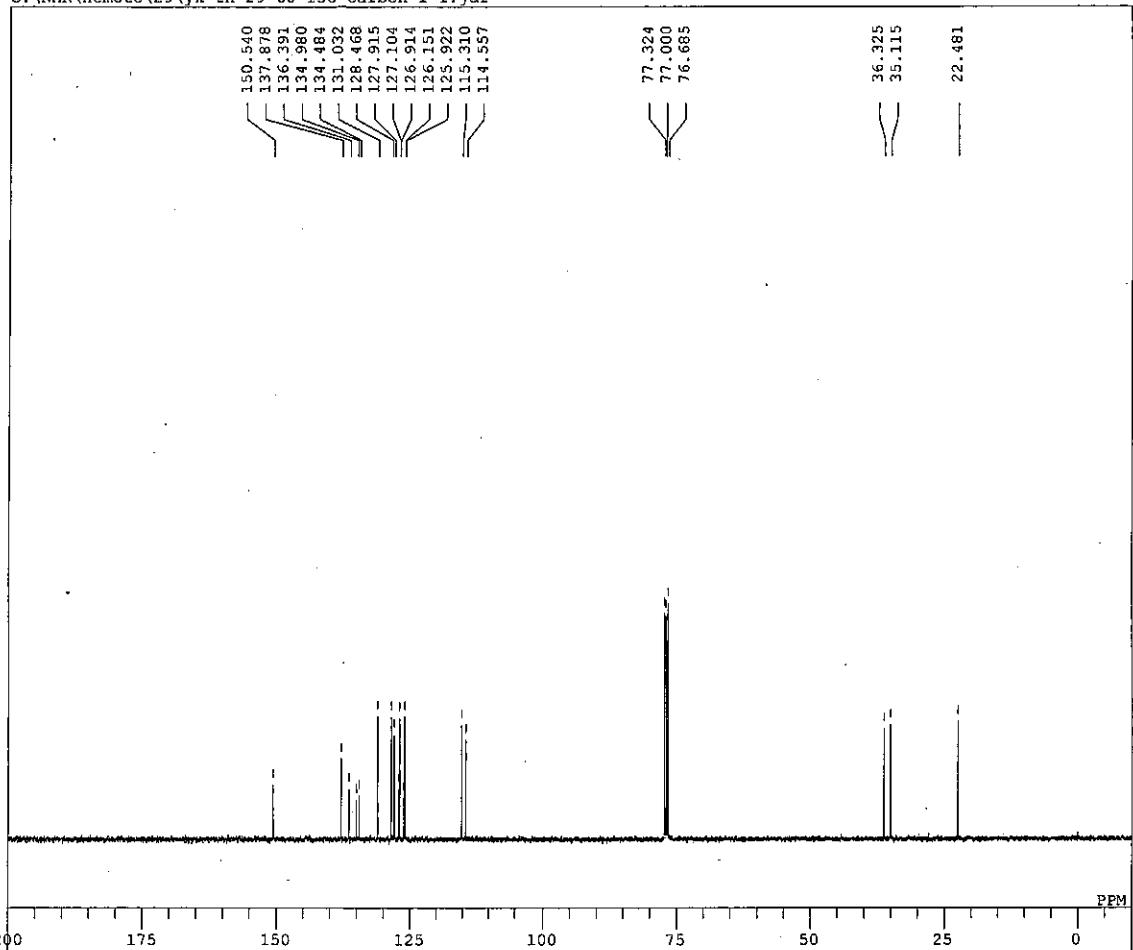


FILE yk-tn-29-60-1H\_Proton-1-1.jd  
COMMENT single\_pulse  
DATE 2012-01-21 15:05:16  
1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 20.1 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 50

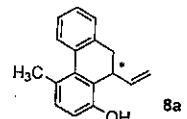


single pulse decoupled gated NOE

G:\NMR\nemoto\29\yk-tn-29-60-13C\_Carbon-1-1.jdf

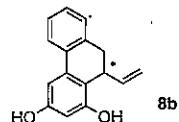
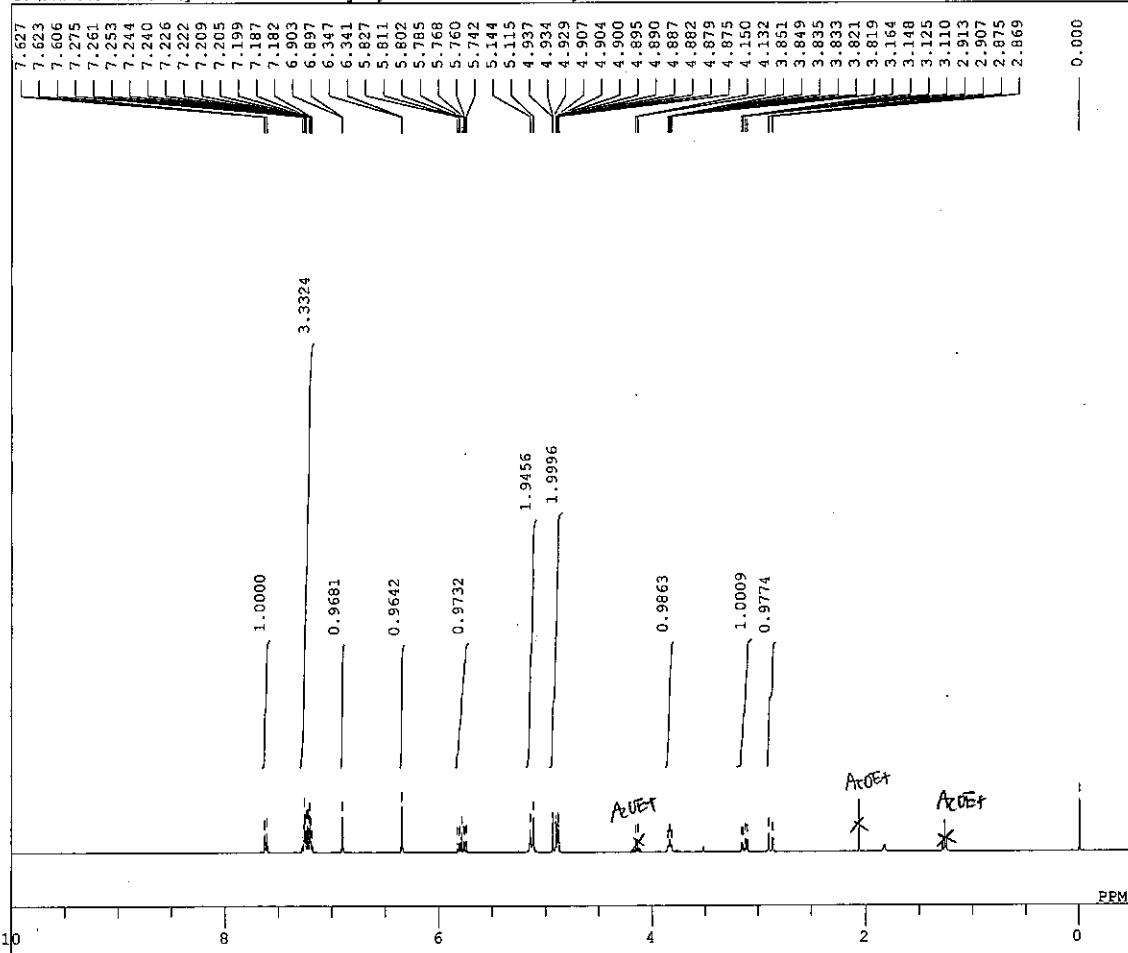


FILE yk-tn-29-60-13C\_Carbon-1-1.jd  
COMMENT single pulse decoupled gated  
DATE 2012-01-21 15:09:32  
13C  
carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 128  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 20.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



### single pulse

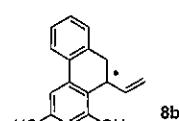
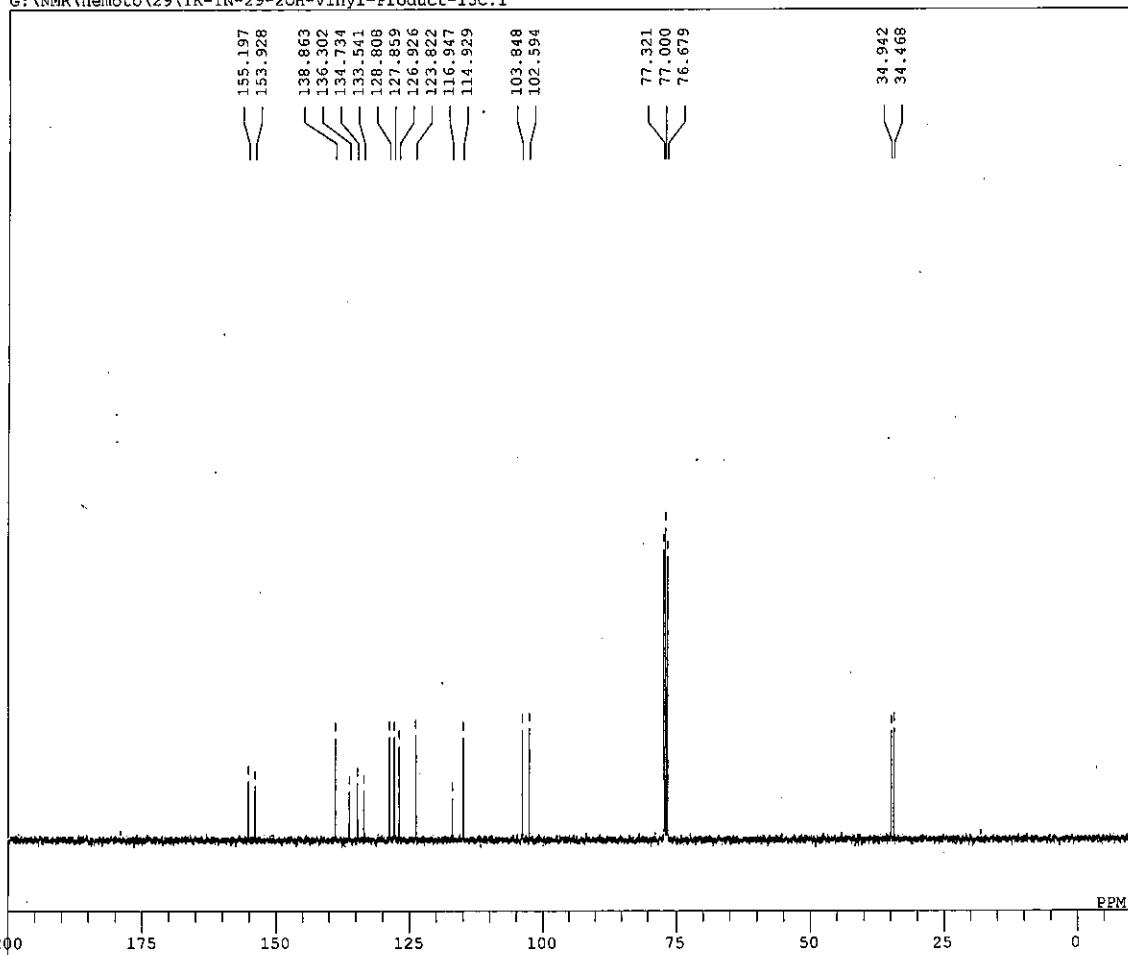
G:\NMR\nemoto\29\yk-tn-29-2OH-vinyl-product\_Proton-1-1.jdf



The chemical structure shows a benzene ring attached to a propenyl group at the para position and a methyl group at the meta position. A radical center is indicated by a dot above the carbon atom bonded to both the methyl and propenyl groups.

## **YK-TN-29-2OH-vinyl-Product-13C**

G:\NMR\nemoto\29\YK-TN-29-20H-vinyl-Product-13C.1



8h

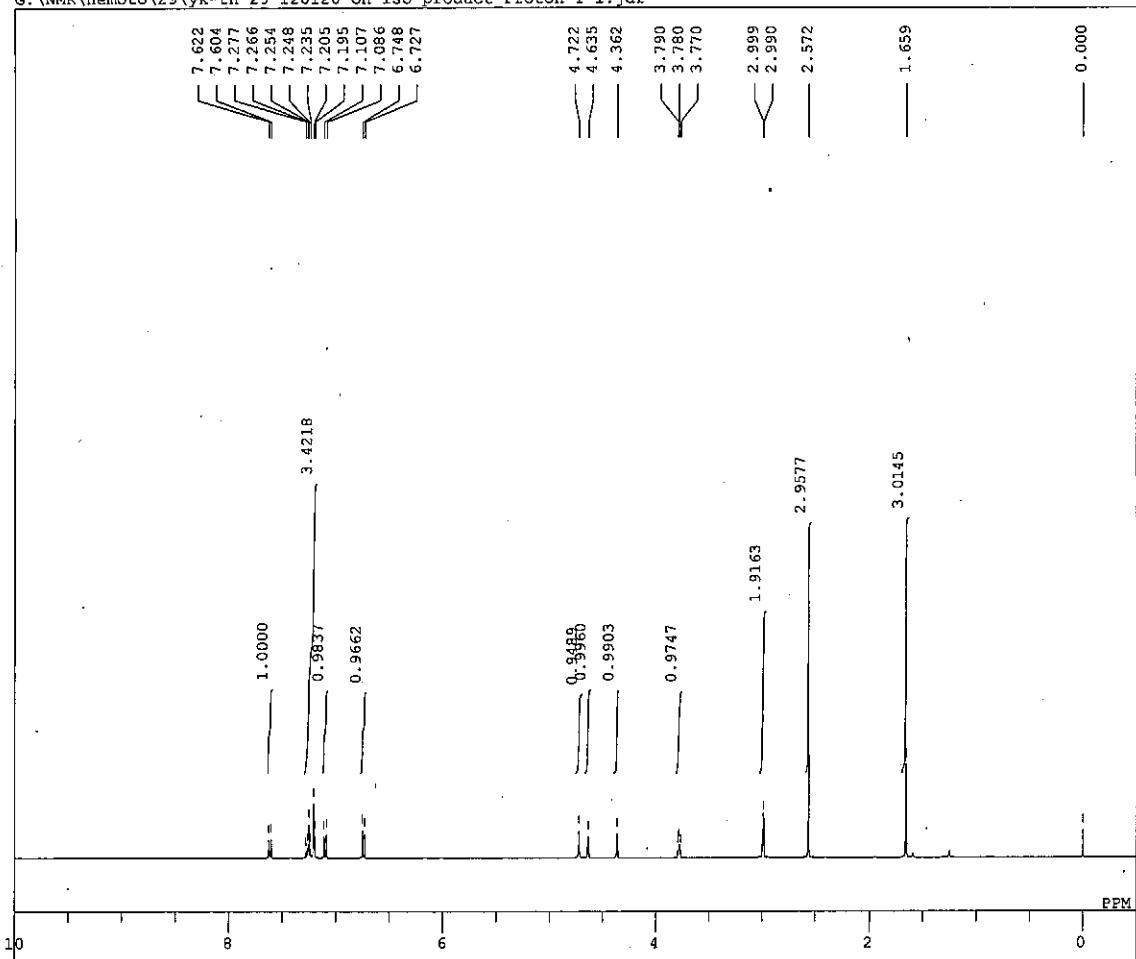
```

DFILE  yk-tn-29-20H-vinyl-product_P
COMNT  single_pulse
DATIM  2012-01-23 16:56:40
OBNUC  1H
EXMOD  proton.jxp
OBFRQ   399.78 MHz
OBSET    4.19 kHz
OBFIN    7.29 Hz
POINT    16384
FREQU   7503.00 Hz
SCANS     8
ACQTM    2.1837 sec
PD       5.0000 sec
PW1      5.00 usec
IRNUC   1H
CTEMP    20.0 c
SLVNT   CDCL3
EXREF    0.00 ppm
BF       0.12 Hz
PCATN    40

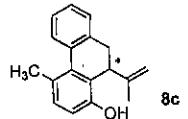
```

single\_pulse

G:\NMR\nemoto\29\yk-tn-29-120120-OH-iso-product\_Proton-1-1.jdf

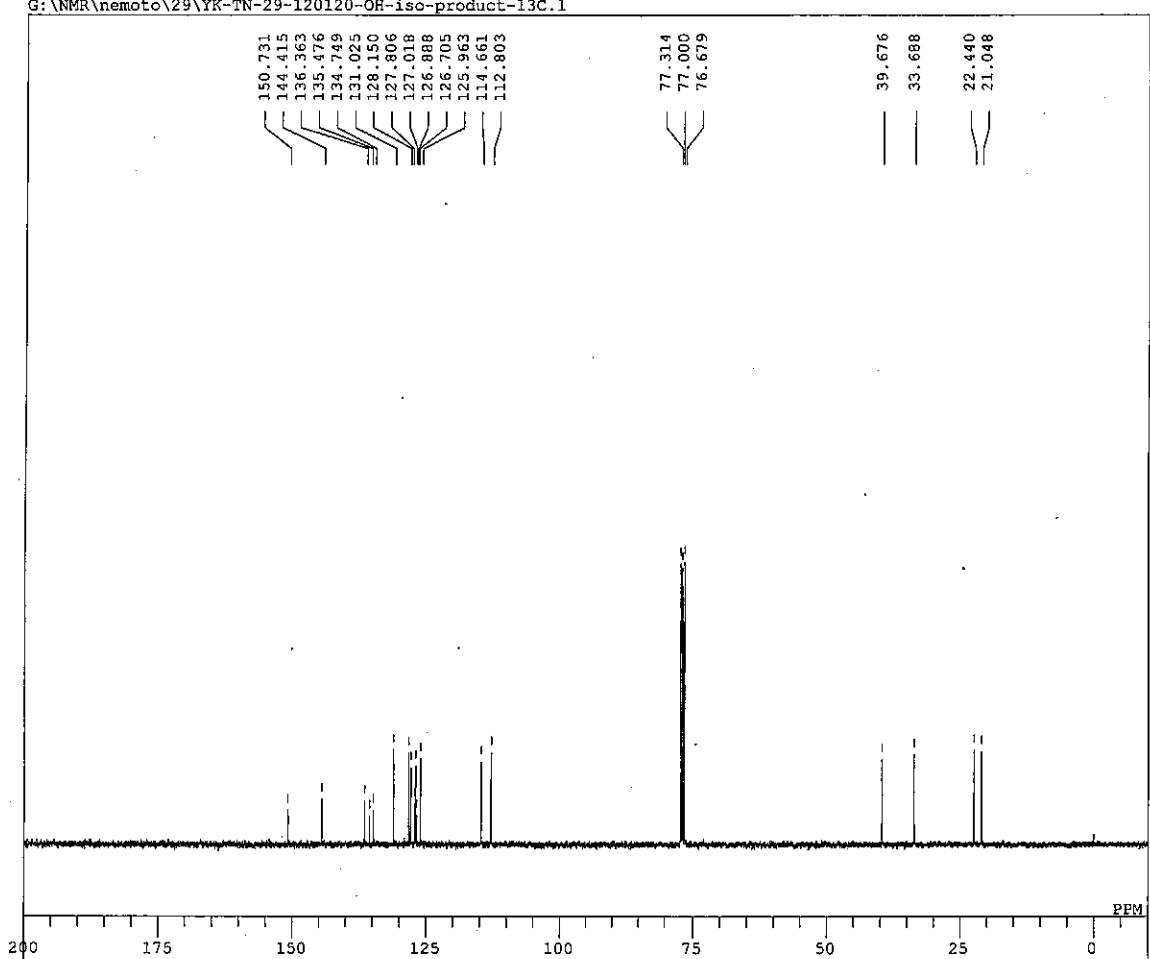


DFILE yk-tn-29-120120-OH-iso-produ  
COMM single\_pulse  
DATIM 2012-01-29 13:42:28  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 KHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 20.1 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 38

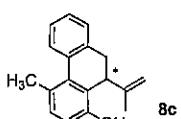


YK-TN-29-120120-OH-iso-product-13C

G:\NMR\nemoto\29\YK-TN-29-120120-OH-iso-product-13C.1

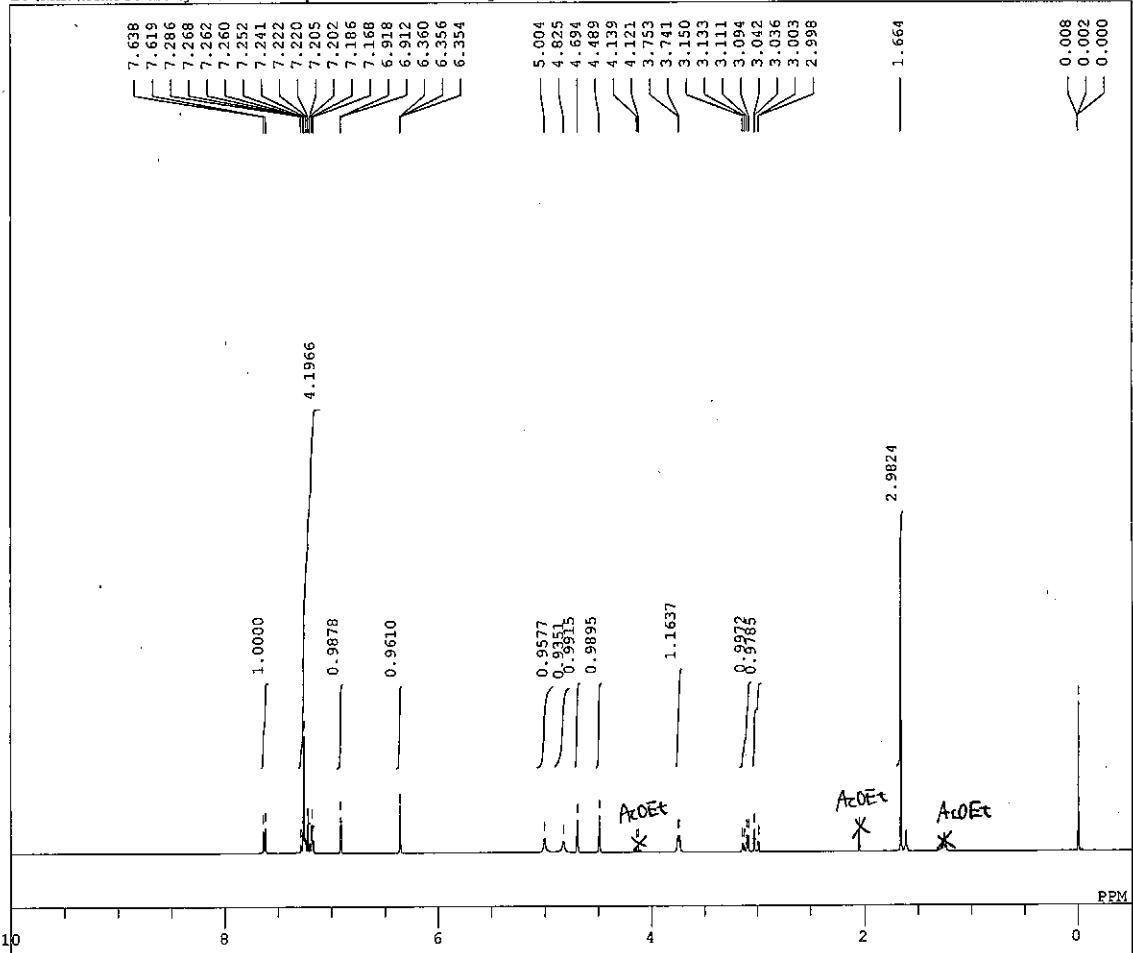


DFILE YK-TN-29-120120-OH-iso-produ  
COMM YK-TN-29-120120-OH-iso-produ  
DATIM 2012-01-20 15:32:56  
OBNUC 13C  
EXMOD single\_pulse\_dec  
OBFRQ 100.53 MHz  
OBSET 5.35 KHz  
OBFIN 5.86 Hz  
POINT 32768  
FREQU 25188.92 Hz  
SCANS 418  
ACQTM 1.3009 sec  
PD 1.0000 sec  
PWI 3.17 usec  
IRNUC 1H  
CTEMP 24.3 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 24

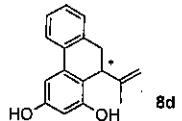


single\_pulse

G:\NMR\nemoto\29\yk-tn-29-61-pro-1H\_Proton-1-1.jdf

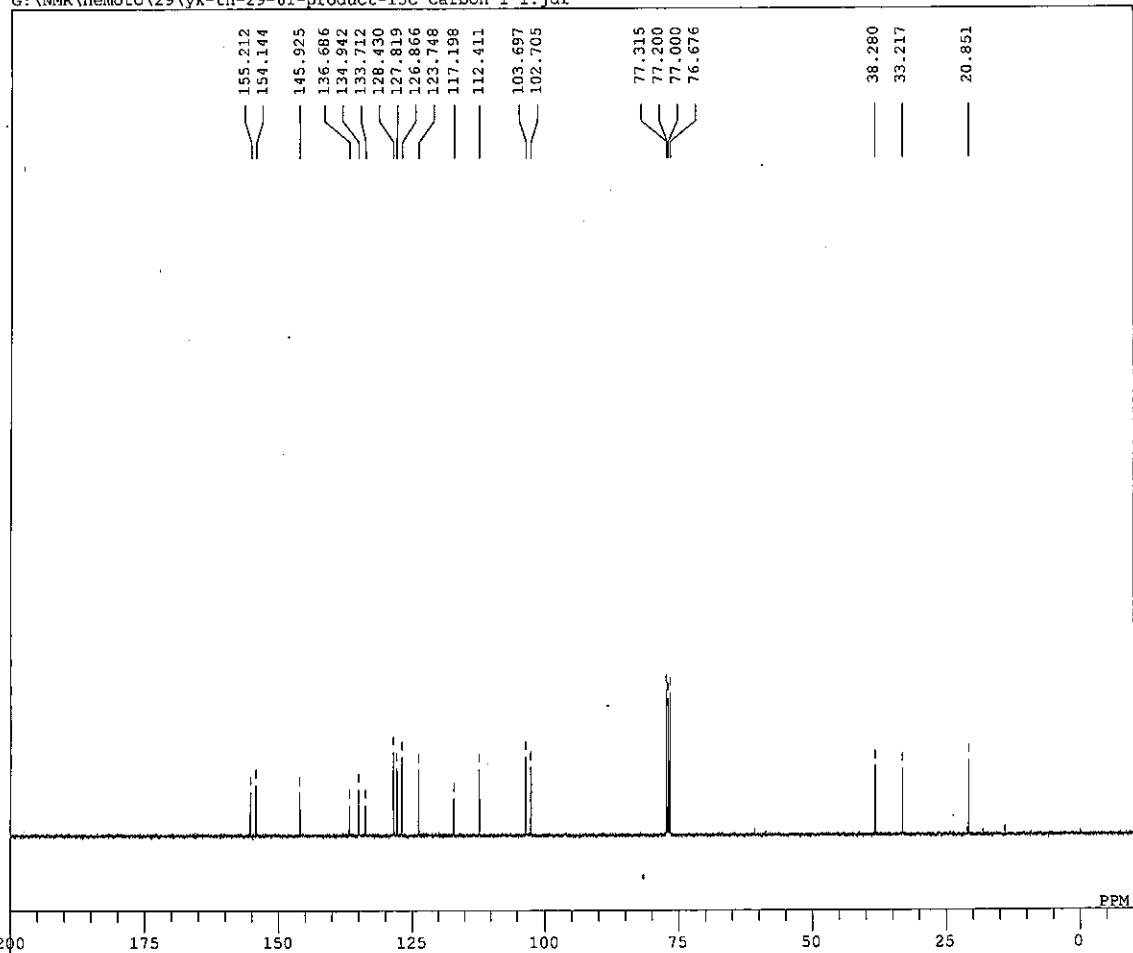


YK-tn-29-61-pro-1H\_Proton-1-1  
single\_pulse  
2012-01-24 15:03:29  
1H  
proton.jpx  
399.78 MHz  
4.19 kHz  
7.29 Hz  
16384  
7503.00 Hz  
8  
2.1837 sec  
5.0000 sec  
5.00 usec  
PWI 1H  
IRNUC 1H  
CTEMP 19.7 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 50

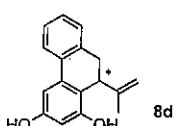


single pulse decoupled gated NOE

G:\NMR\nemoto\29\yk-tn-29-61-product-13C\_Carbon-1-1.jdf

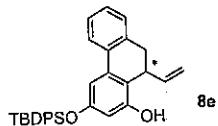
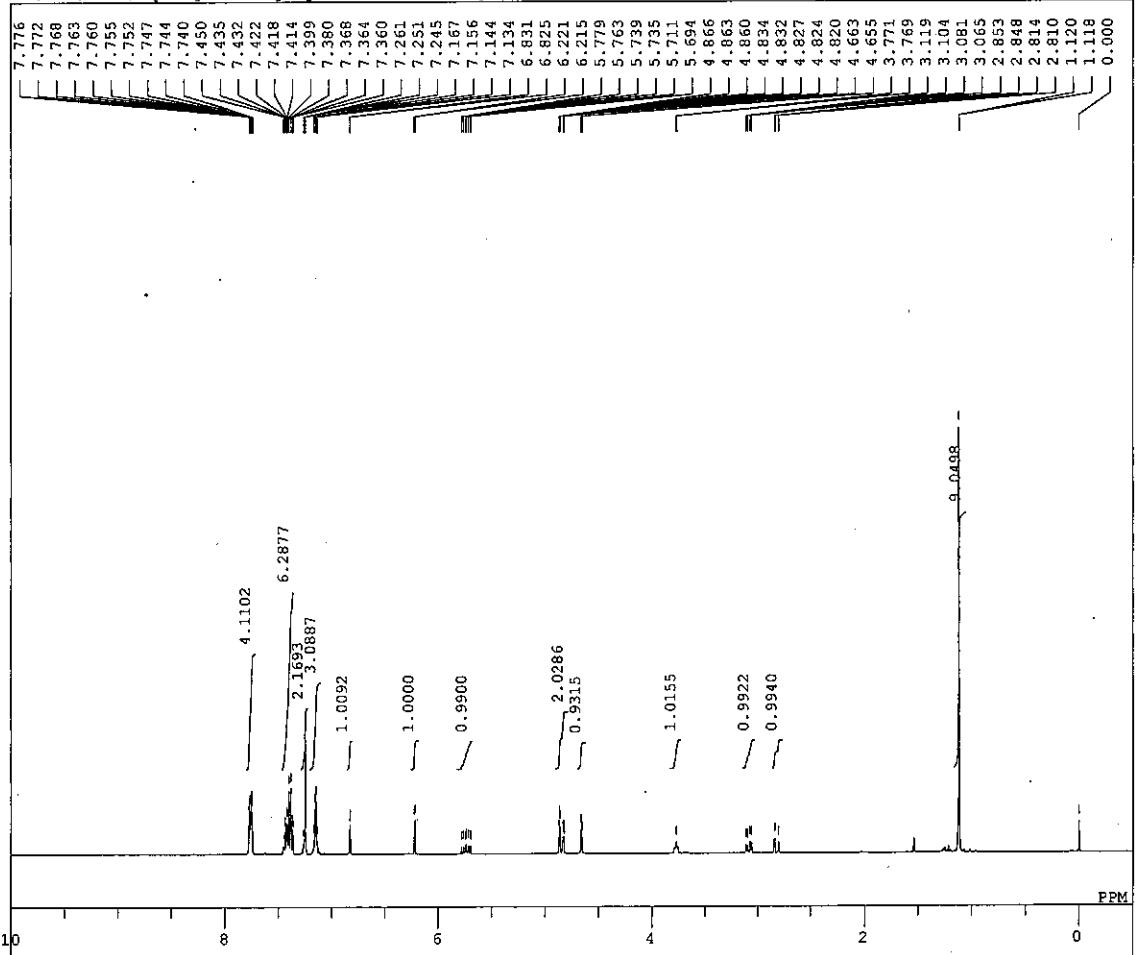


YK-tn-29-61-product-13C\_Carb  
single pulse decoupled gated  
2012-01-24 15:07:44  
13C  
carbon.jpx  
100.53 MHz  
5.35 kHz  
5.86 Hz  
32767  
31407.04 Hz  
128  
1.0433 sec  
2.0000 sec  
3.07 usec  
PWI 1H  
IRNUC 1H  
CTEMP 19.9 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



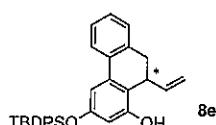
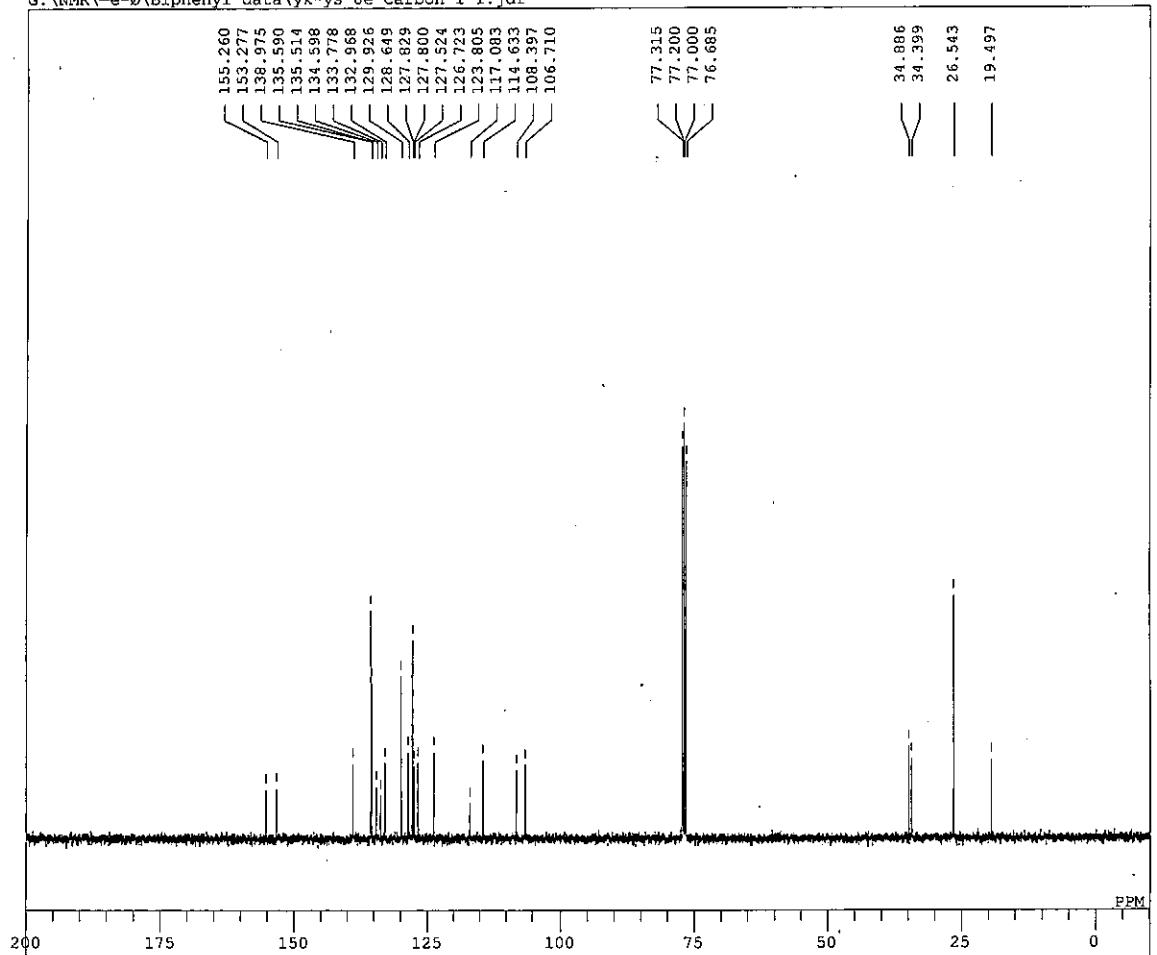
### single\_pulse

G:\NMR\-\é-\Ø\Biphenyl data\yk-ys-8e Proton-1-1.jdf



#### **single pulse decoupled gated NOE**

G:\NMR\-\é-\Ø\Biphenyl data\yk-ys-8e Carbon-1-1.jdf



```

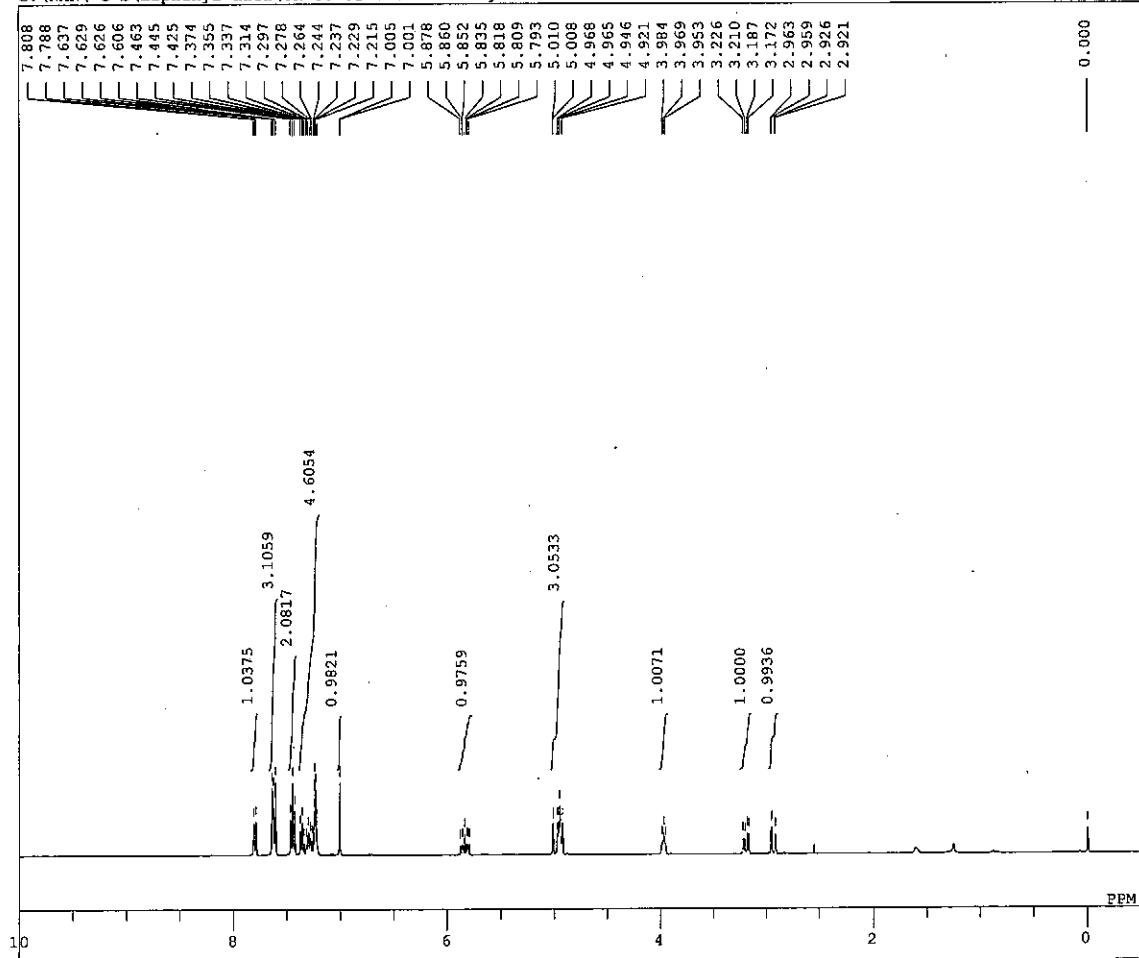
DFILE  yk-ys-8e_Carbon-1-1.jdf
COMNT  single pulse decoupled gated
DATIM  2012-02-29 22:41:23
OBNUC  13C
EXMOD carbon.jxp
OBERQ   100.53 MHz
OBSET    5.35 KHz
OBFIN    5.86 Hz
POINT    32767
FREQU   31407.04 Hz
SCANS    128
ACQTM    1.0433 sec
PD       2.0000 sec
PW1      3.07 usec
IRNUC   1H
CTEMP    22.1 c
SLVNT    CDCL3
EXREF   77.00 ppm
BF       1.20 Hz
RGAIN   50

```

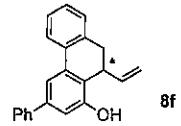
38

single\_pulse

G:\NMR\-\é-\Biphenyl data\YK-YS-8f\_Proton-2-1.jdf

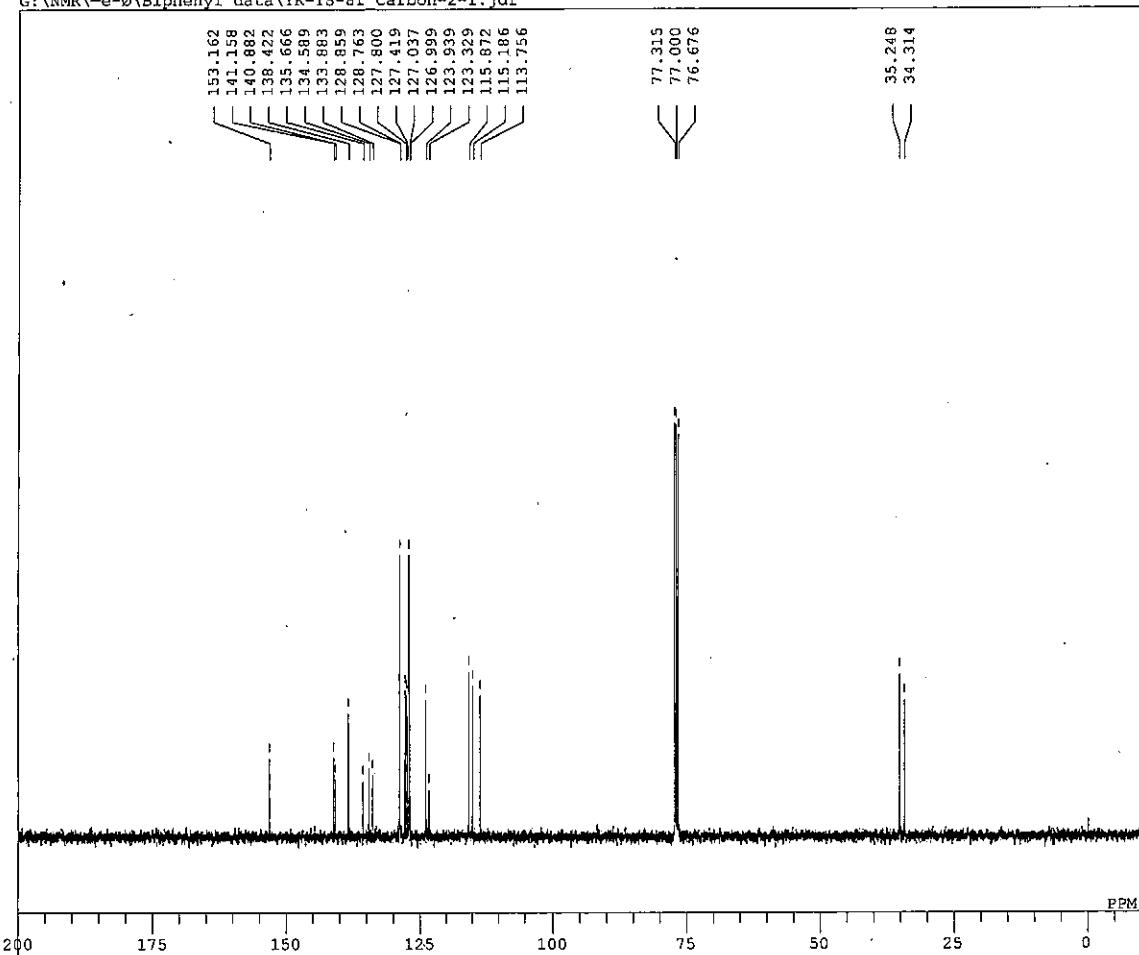


DFILE YK-YS-8f\_Proton-2-1.jdf  
COMNT single\_pulse  
DATIM 2012-03-24 18:12:46  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 KHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 25.2 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 38

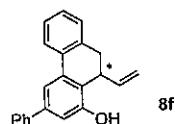


single pulse decoupled gated NOE

G:\NMR\-\é-\Biphenyl data\YK-YS-8f\_Carbon-2-1.jdf

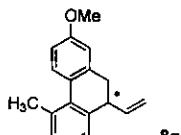
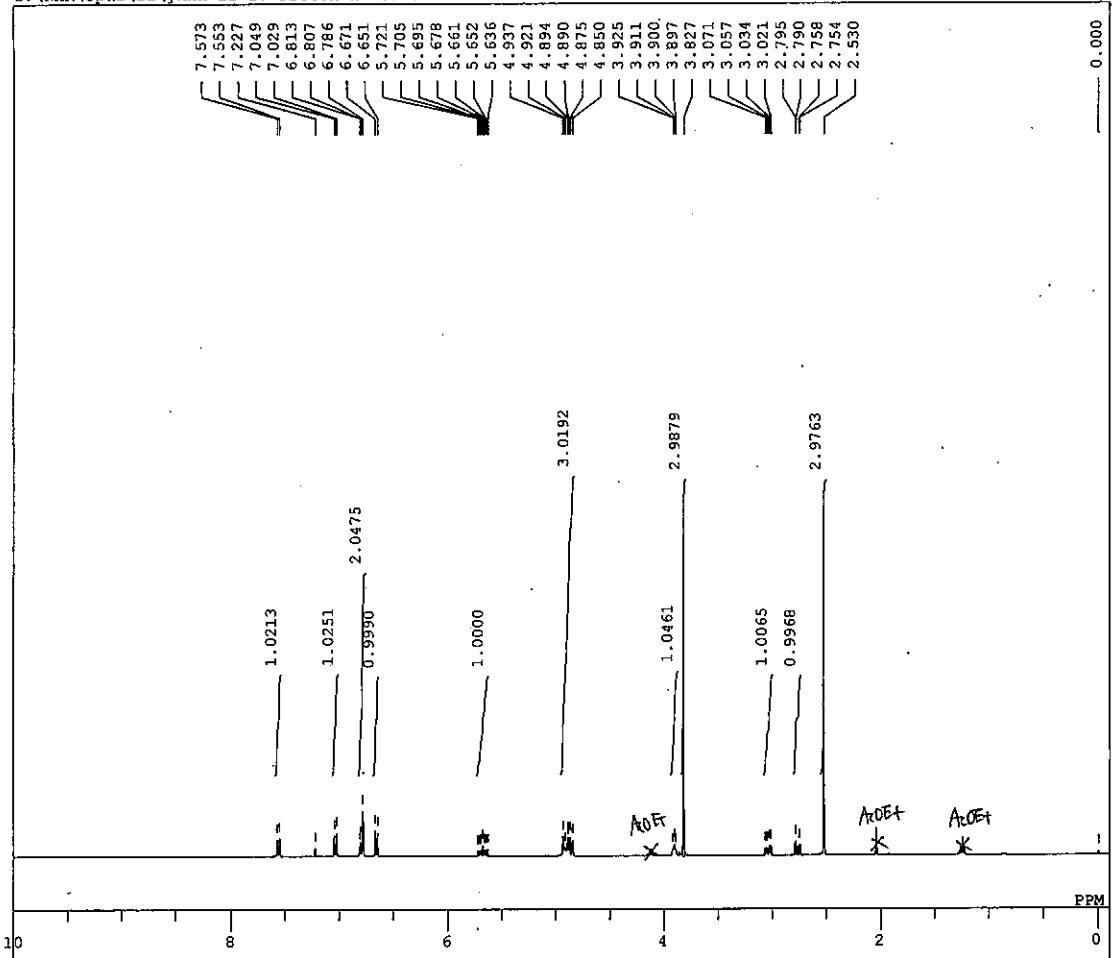


DFILE YK-YS-8f\_Carbon-2-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-03-24 18:14:06  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 KHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 128  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 25.5 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



## single\_pulse

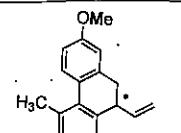
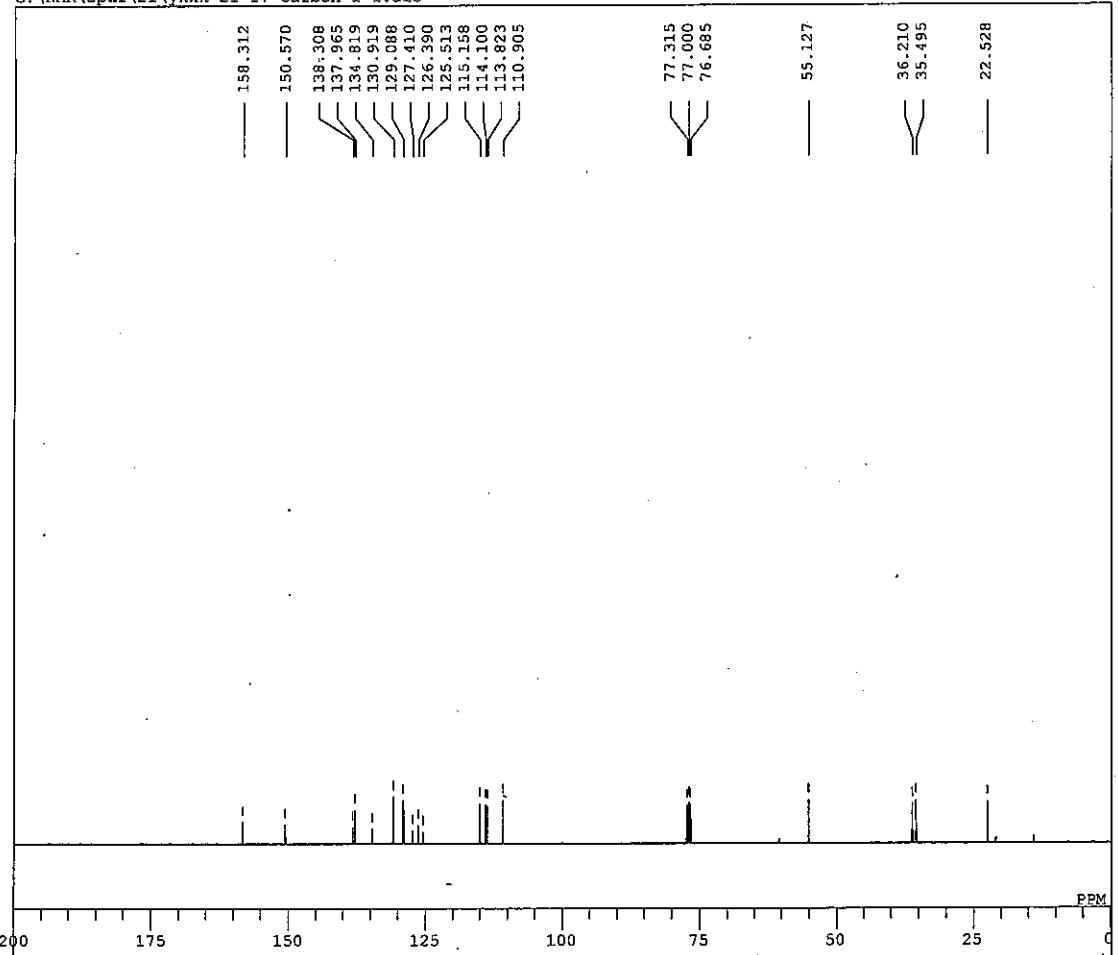
G:\NMR\Špkf\21\ykkk-21-17\_Proton-1-1.als



Molecular Weight: 265,3264

### single pulse decoupled gated NOE

G:\NMR\Sp\ff\21\ykkk-21-17 Carbon-1-1.als

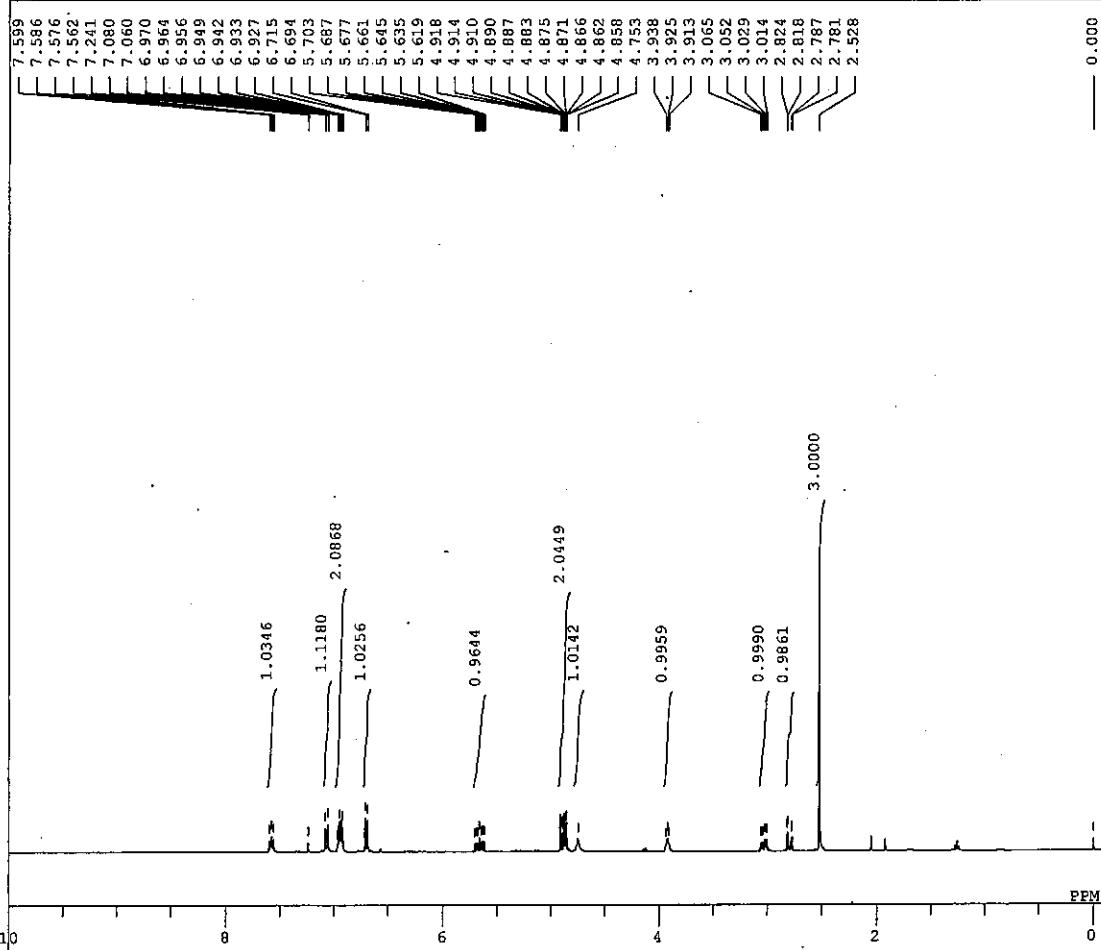


Molecular Weight: 265-326

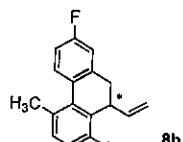
S-40

single\_pulse

G:\NMR\Sp\ff\21\ykkk-21-14\_Proton-1-1.als



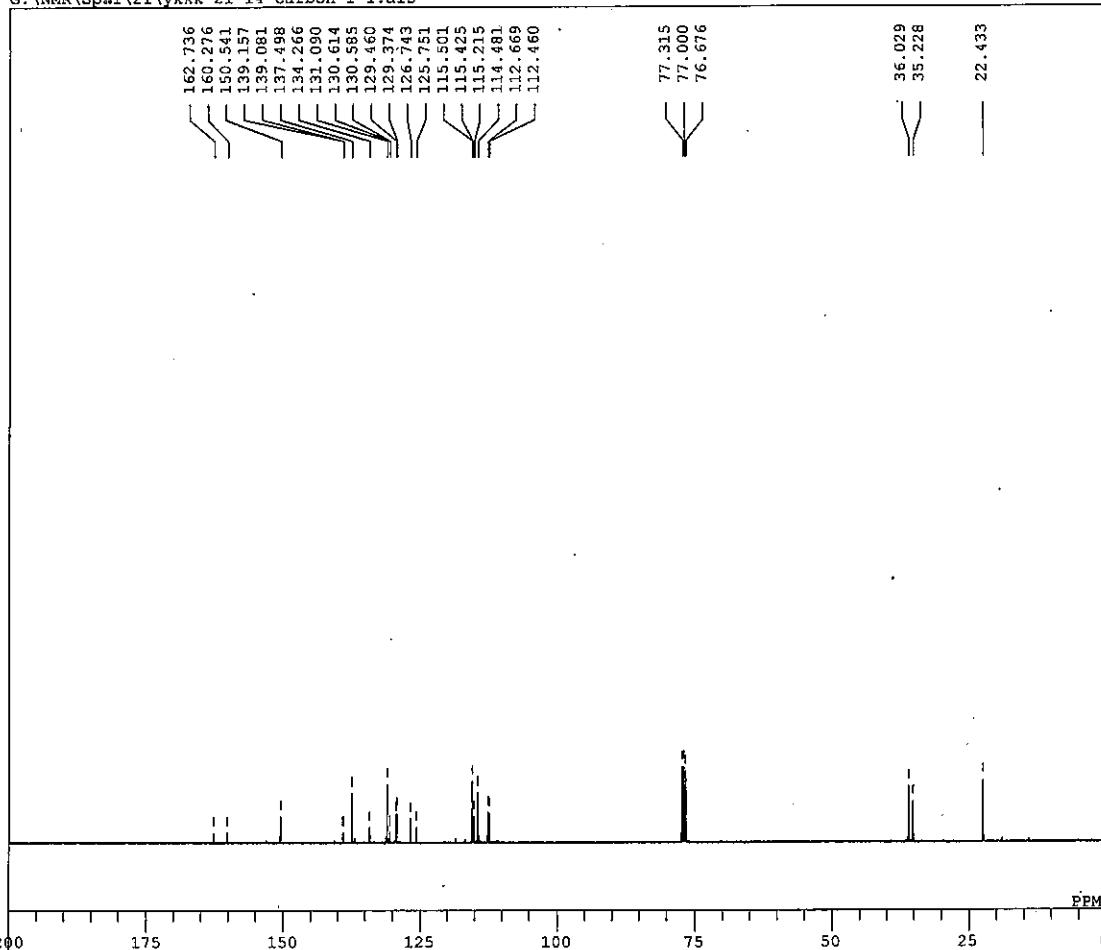
DFILE ykkk-21-14\_Proton-1-1.als  
COMNT single\_pulse  
DATIM 2012-03-10 08:07:20  
OBNUC 1H  
EXMOD proton.jxp  
OBFQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 131.07  
FREQU 6002.40 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 23.7 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 34



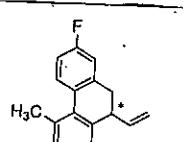
Molecular Weight: 253.2909

single pulse decoupled gated NOE

G:\NMR\Sp\ff\21\ykkk-21-14\_Carbon-1-1.als



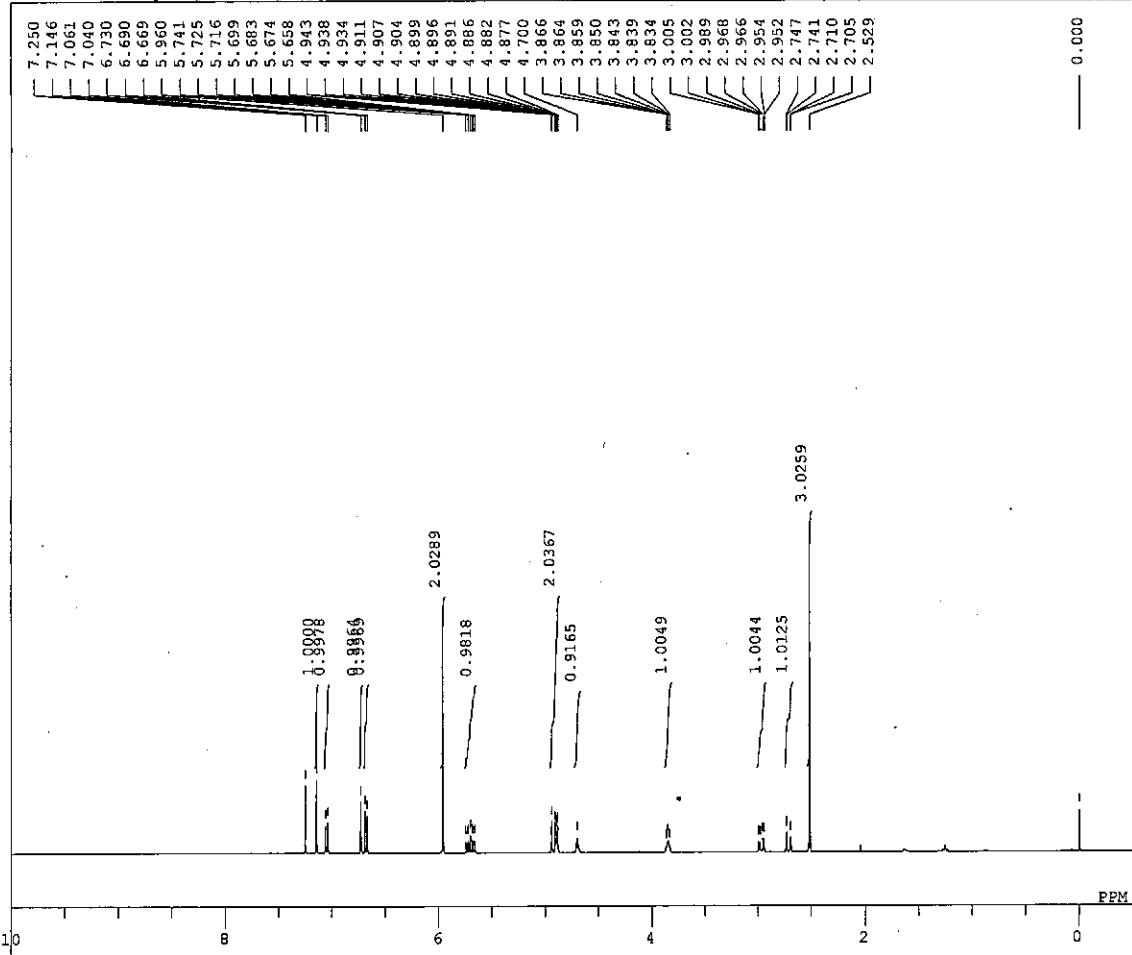
DFILE ykkk-21-14\_Carbon-1-1.als  
COMNT single pulse decoupled gated  
DATIM 2012-03-10 08:10:14  
OBNUC 13C  
EXMOD carbon.jxp  
OBFQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 2621.4  
FREQU 25125.63 Hz  
SCANS 350  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 23.9 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



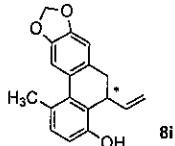
Molecular Weight: 253.2909

### single\_pulse

G:\NMR\-\e-\Biphenyl data\yk-ys-8i\_Proton-1-1.jdf

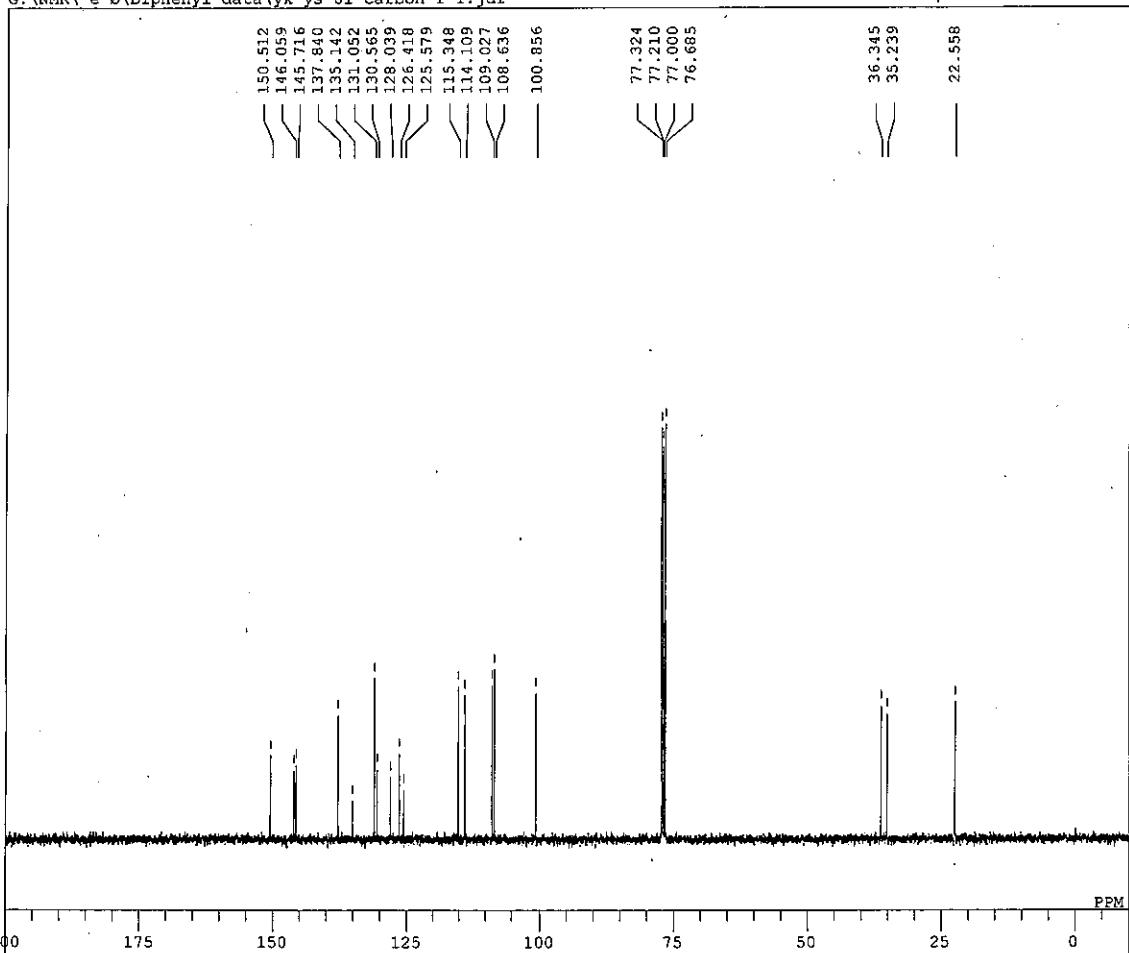


DFILE yk-ys-8i\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-02-29 22:51:45  
OBNUC 1H  
EXMOD proton.jxp  
OBFREQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 used  
IRNUC 1H  
CTEMP 21.0 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 38

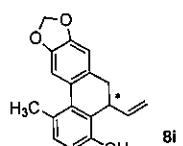


### single pulse decoupled gated NOE

G:\NMR\-\e-\Biphenyl data\yk-ys-8i\_Carbon-1-1.jdf

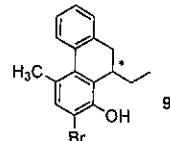
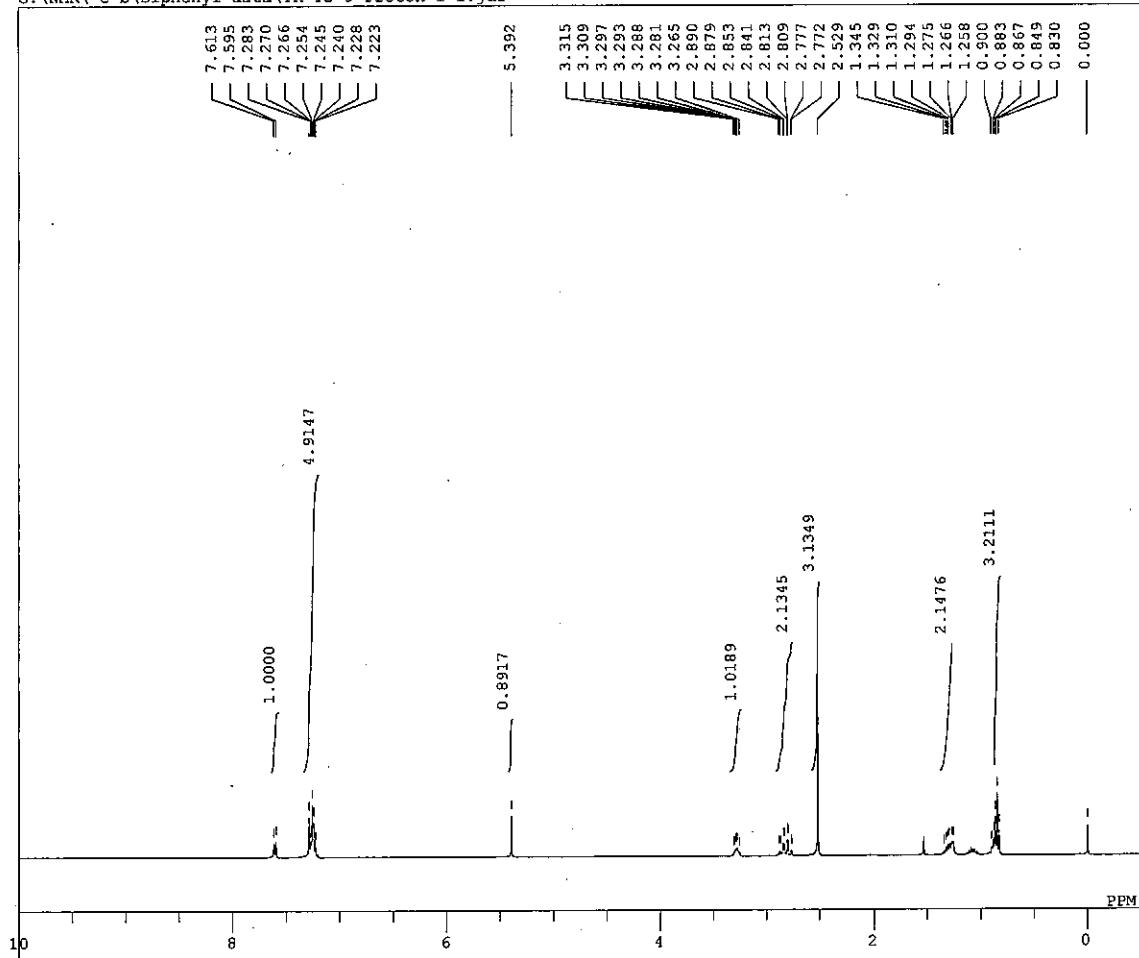


DFILE yk-ys-8i\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-02-29 22:53:06  
OBNUC 13C  
EXMOD carbon.jxp  
OBFREQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 128  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 22.0 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



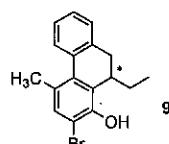
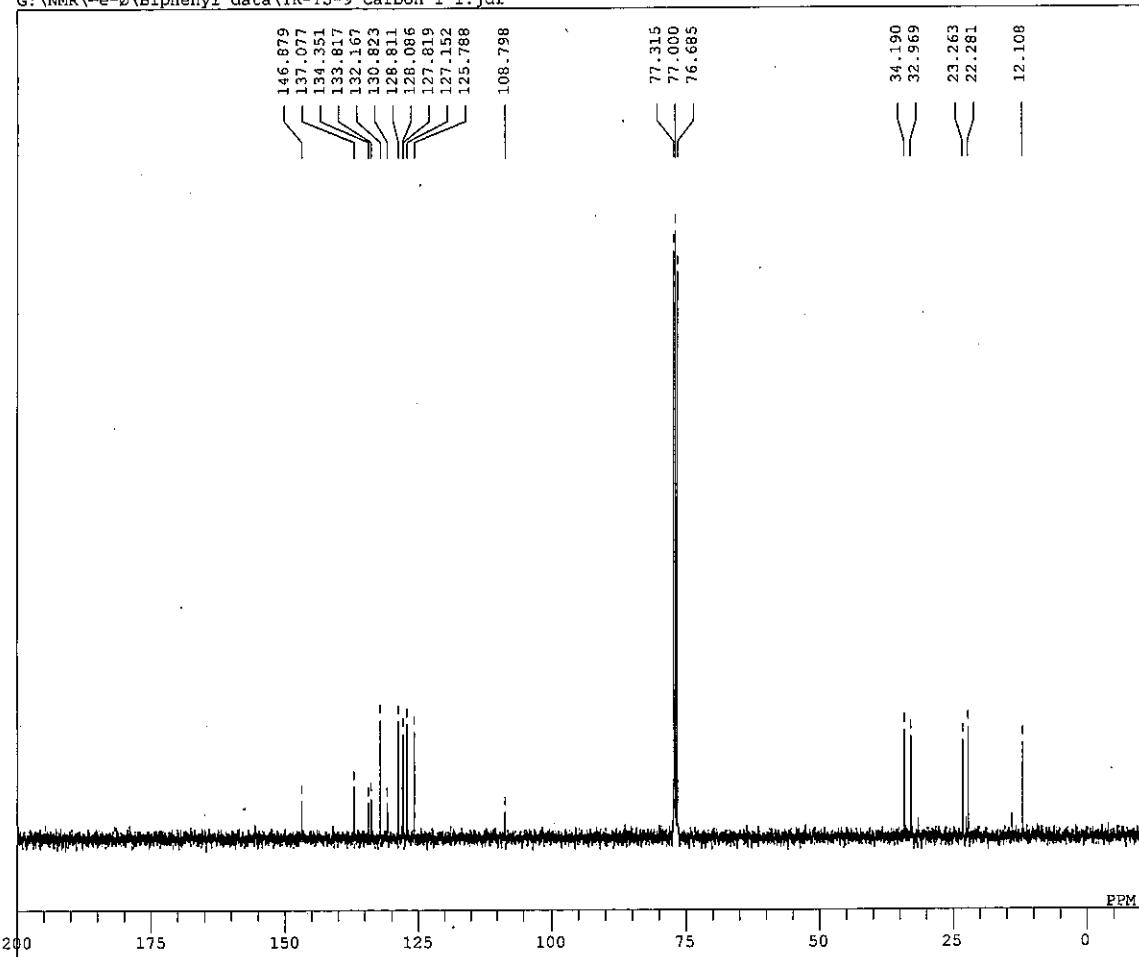
single\_pulse

G:\NMR\-\é-\Ø\Biphenyl\_data\YK-YS-9\_Proton-1-1.jdf



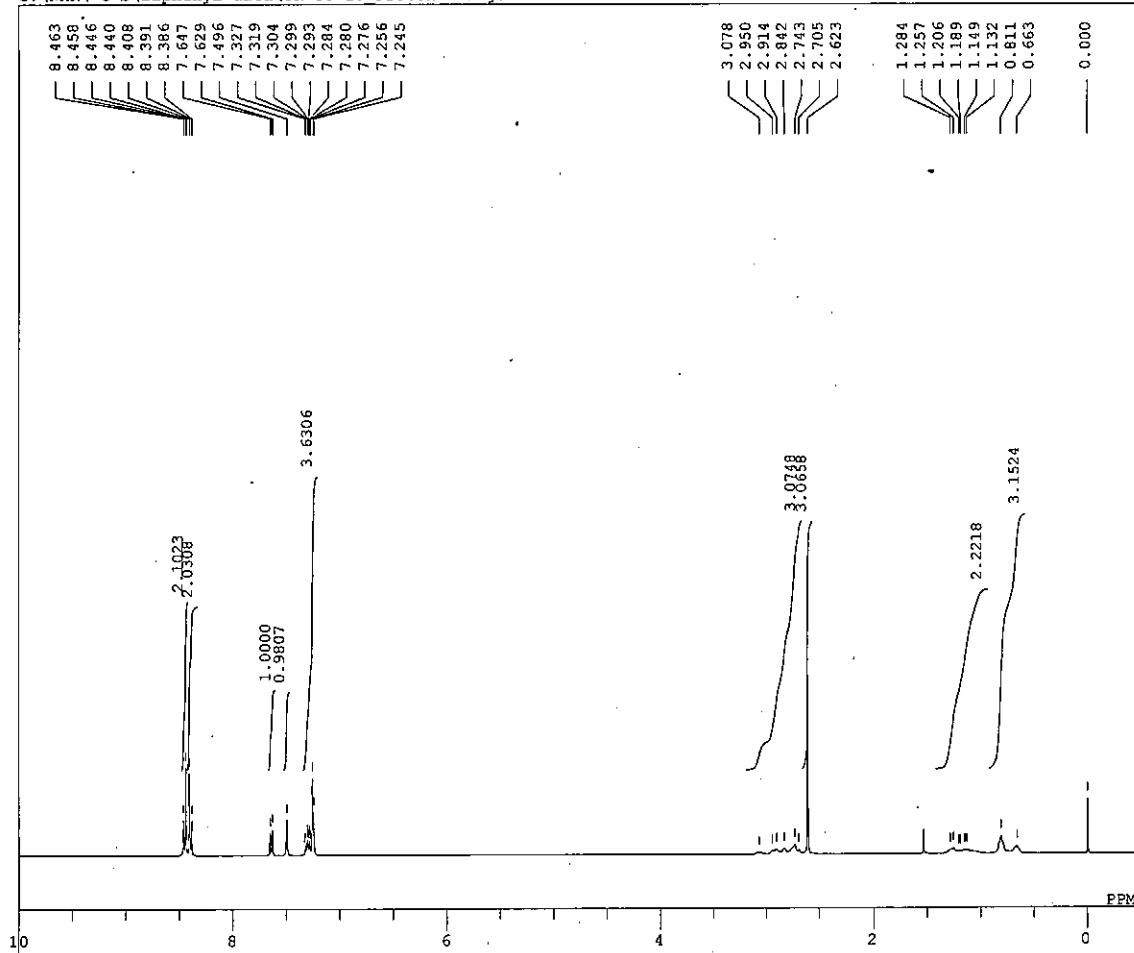
single pulse decoupled gated NOE

G:\NMR\-\é-\Ø\Biphenyl\_data\YK-YS-9\_Carbon-1-1.jdf

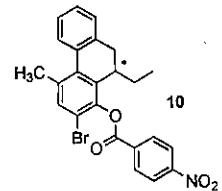


single\_pulse

G:\NMR\-\Ø\Biphenyl data\YK-YS-10\_Proton-2-1.jdf



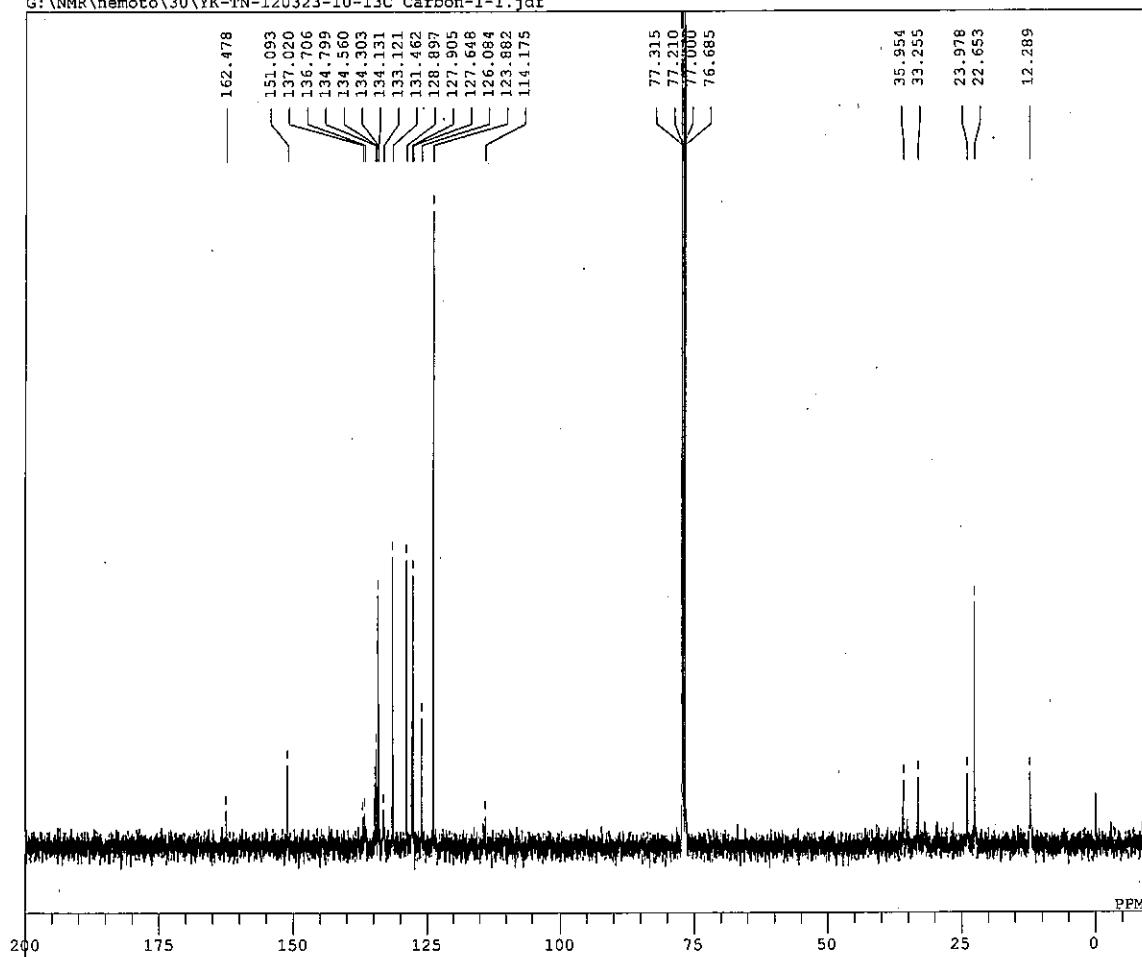
DFILE YK-YS-10\_Proton-2-1.jdf  
COMNT single\_pulse  
DATIM 2012-03-22 10:56:07  
OBNUC 1H  
EXMOD proton.jxp  
OBFREQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 26.1 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 42



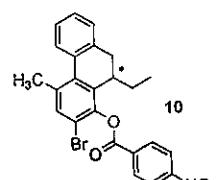
(Mixture of  
rotation isomer)

single pulse decoupled gated NOE

G:\NMR\nemoto\30\YK-TN-120323-10-13C Carbon-1-1.jdf



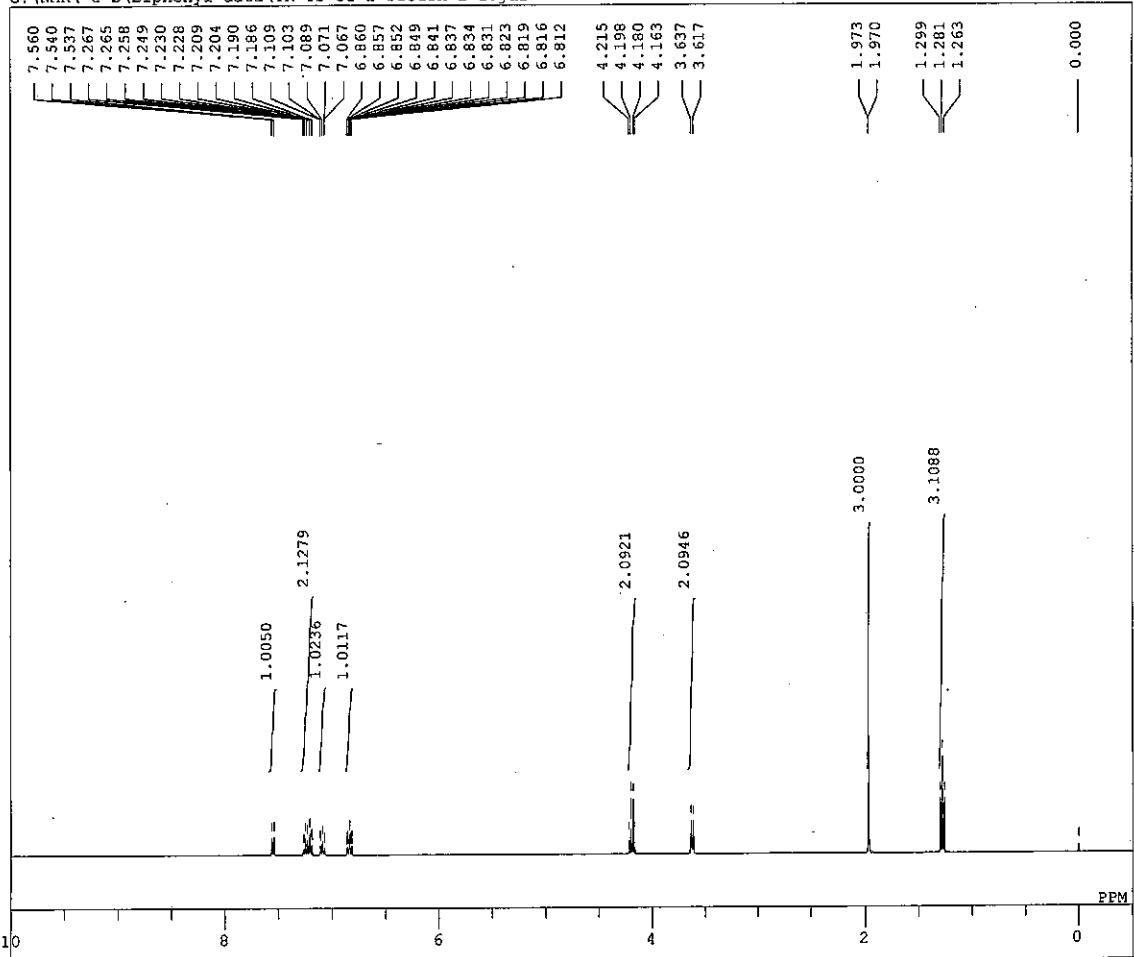
DFILE YK-TN-120323-10-13C\_Carbon-1  
COMNT single pulse decoupled gated  
DATIM 2012-03-23 16:07:41  
OBNUC 13C  
EXMOD carbon.jxp  
OBFREQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 324  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 25.8 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



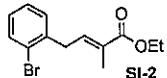
S-44

single\_pulse

G:\NMR\-\6-\0\Biphenyl data\YK-YS-SI-2\_Proton-1-1.jdf

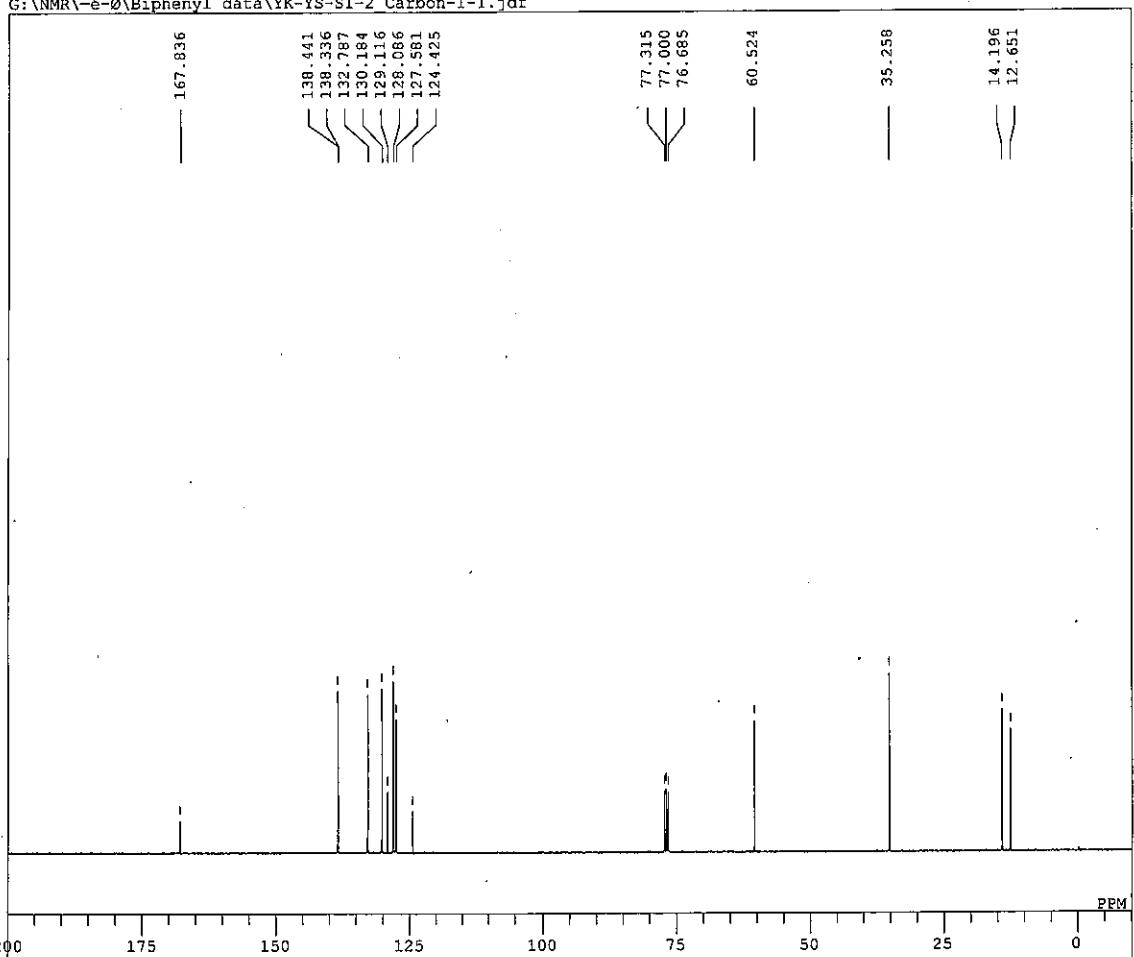


YK-YS-SI-2\_Proton-1-1.jdf  
single\_pulse  
DATIM 2012-01-26 14:53:32  
OENUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 19.8 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 26

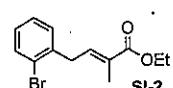


single pulse decoupled gated NOE

G:\NMR\-\6-\0\Biphenyl data\YK-YS-SI-2\_Carbon-1-1.jdf

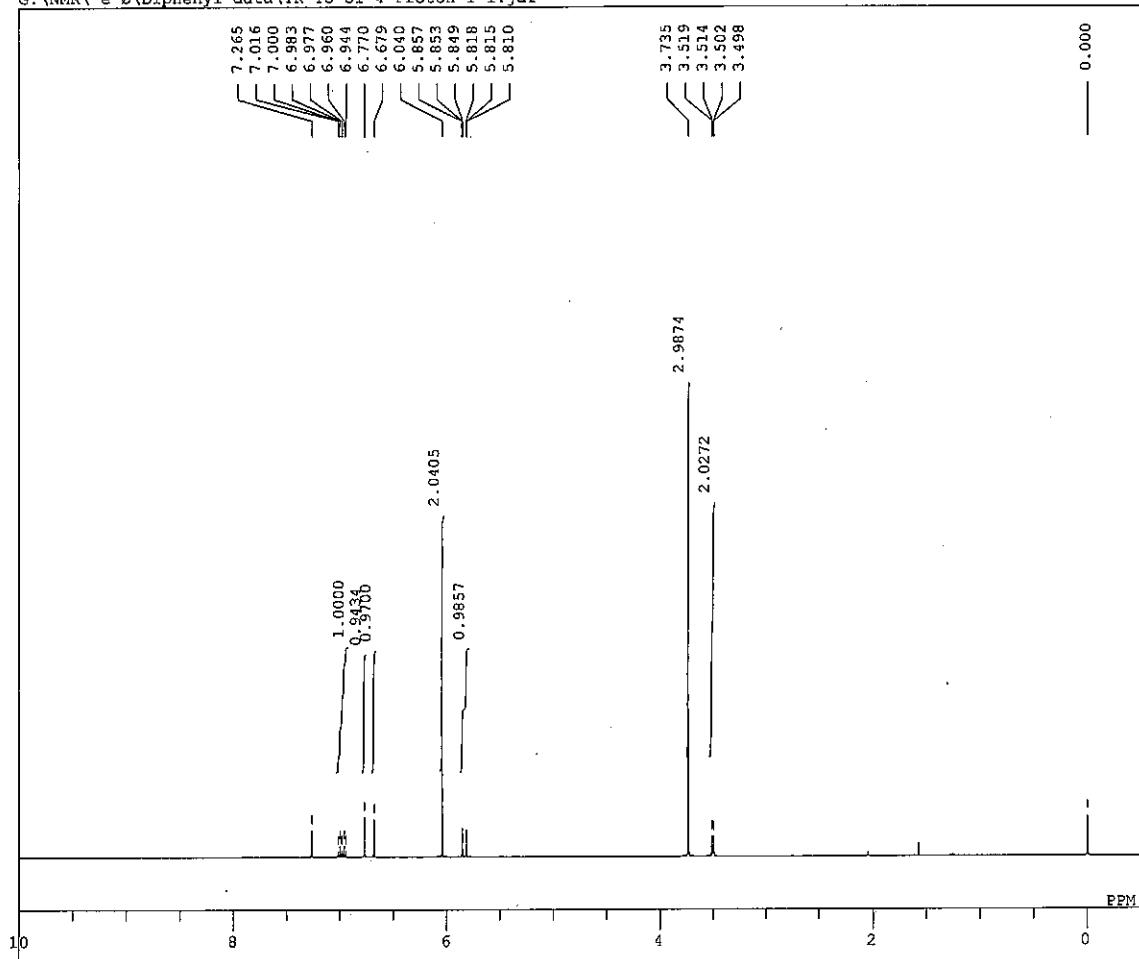


YK-YS-SI-2\_Carbon-1-1.jdf  
single pulse decoupled gated  
2012-01-26 14:54:56  
OENUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 258  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 20.1 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

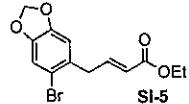


single\_pulse

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-4 Proton-1-1.jdf

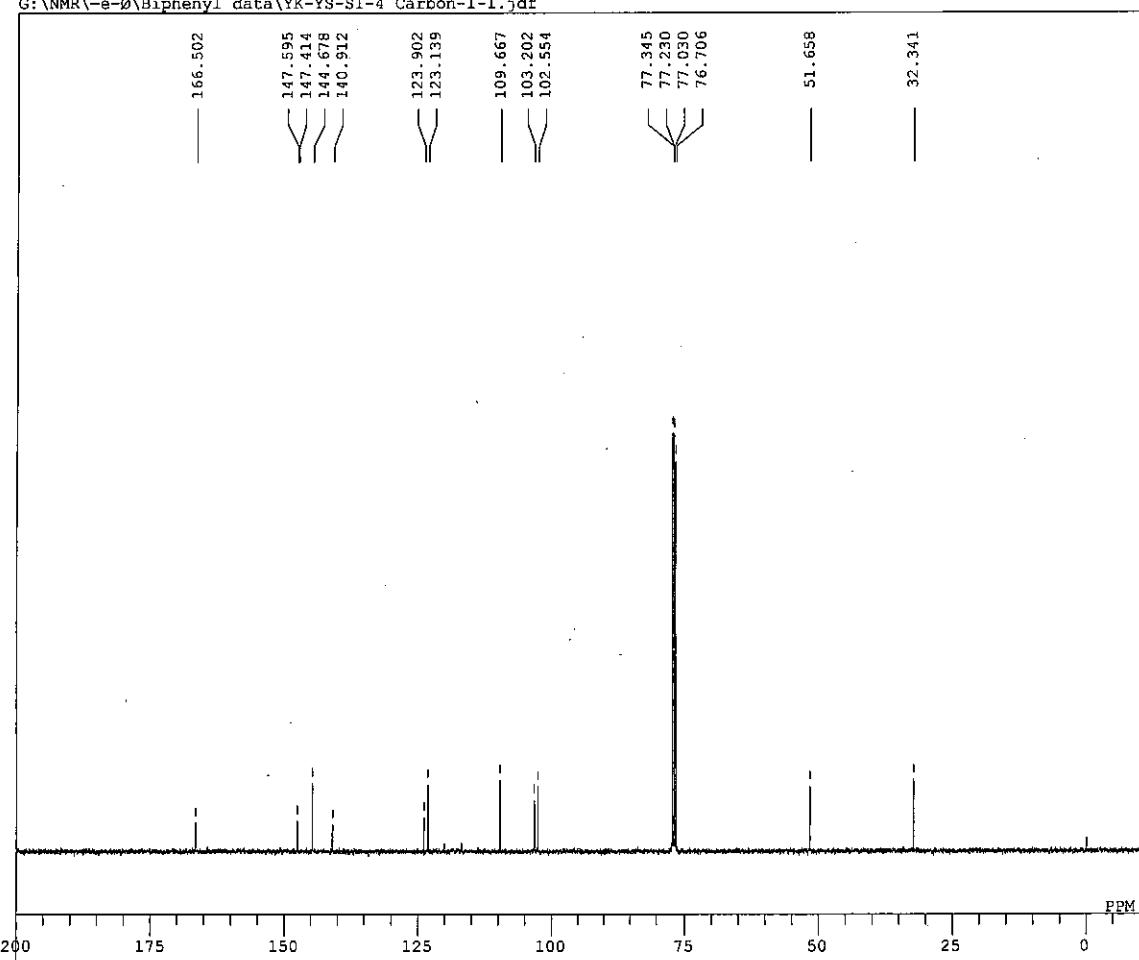


FILE YK-YS-SI-4\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-01-23 10:47:09  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 KHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 19.8 °C  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 46

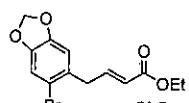


single pulse decoupled gated NOE

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-4 Carbon-1-1.jdf



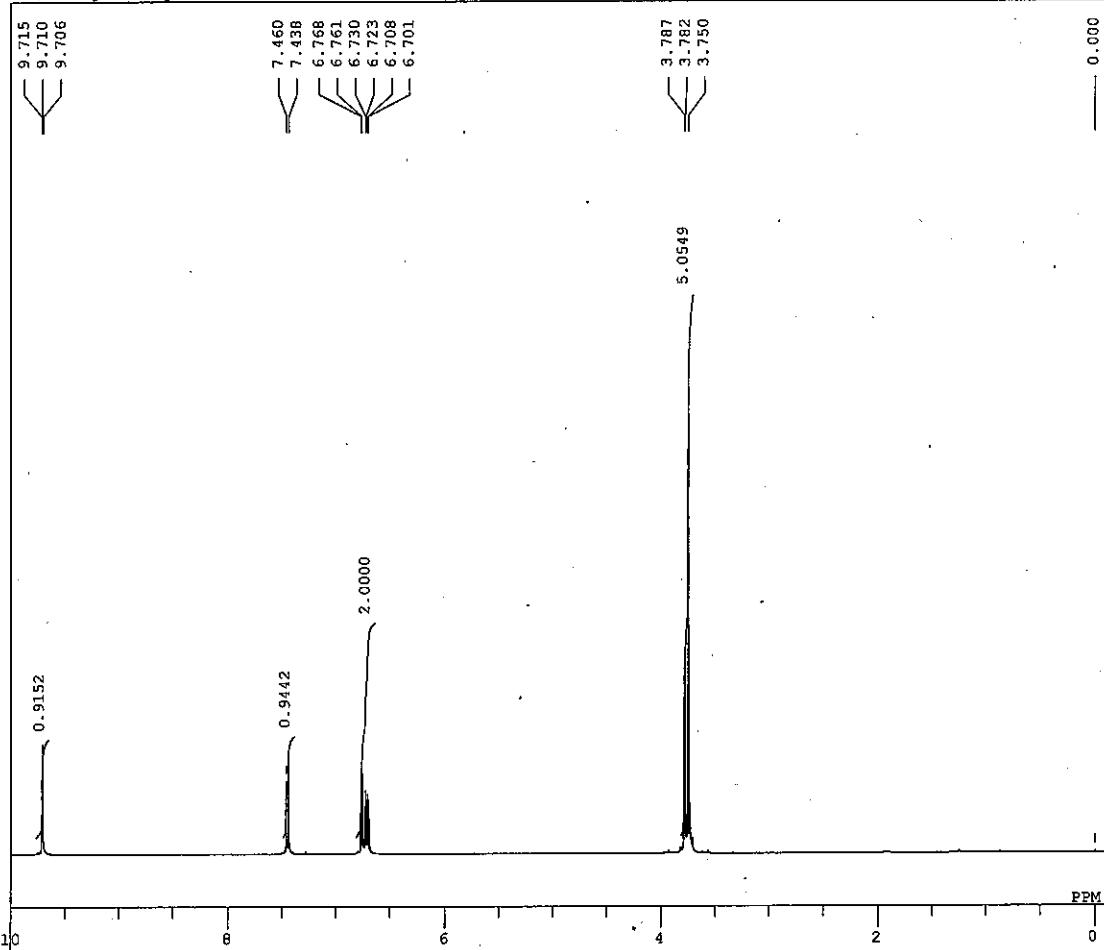
FILE YK-YS-SI-4\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-01-23 10:49:47  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 KHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 512  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 20.0 °C  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 1.20 Hz  
RGAIN 50



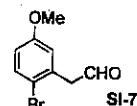
S-46

single\_pulse

G:\NMR\Špkf\20\ykkk-20-63-rt Proton-1-1.als



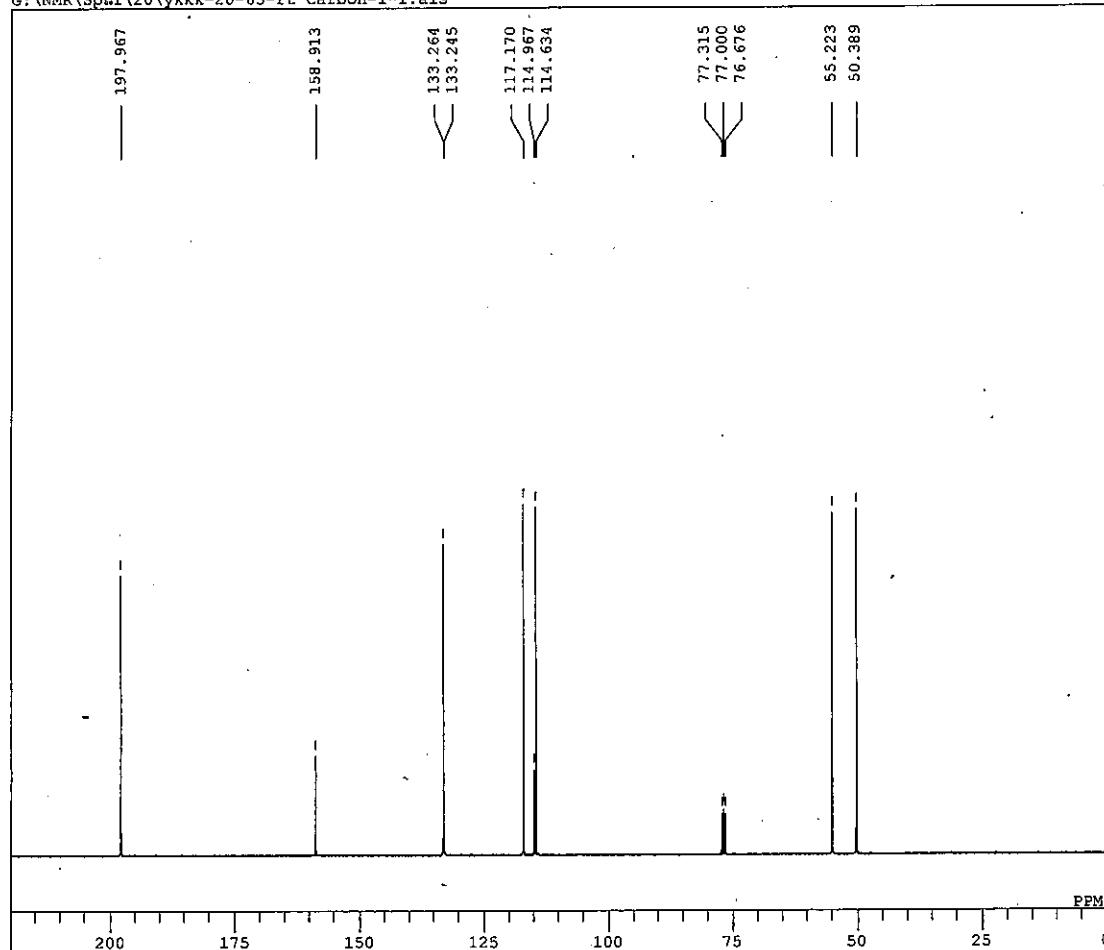
DFILE ykkk-20-63-rt\_Proton-1-1.als  
 COMNT single\_pulse  
 DATIM 2012-02-23 13:04:43  
 OENUC 1H  
 EXMOD proton.jxp  
 OBFRQ 399.78 MHz  
 OBSET 4.19 kHz  
 OBFIN 7.29 Hz  
 POINT 13107  
 FREQU 6002.40 Hz  
 SCANS 8  
 ACQTM 2.1837 sec  
 PD 5.0000 sec  
 PW1 5.00 usec  
 IRNUC 1H  
 CTEMP 22.4 c  
 SLVNT CDCL3  
 EXREF 0.00 ppm  
 BF 0.12 Hz  
 RGAIN 22



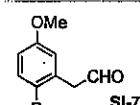
Molecular Weight: 229.0706

single pulse decoupled gated NOE

G:\NMR\Špkf\20\ykkk-20-63-rt Carbon-1-1.als



DFILE ykkk-20-63-rt\_Carbon-1-1.als  
 COMNT single\_pulse\_decoupled\_gated  
 DATIM 2012-02-23 13:07:48  
 OENUC 13C  
 EXMOD carbon.jxp  
 OBFRQ 100.53 MHz  
 OBSET 5.35 kHz  
 OBFIN 5.86 Hz  
 POINT 26214  
 FREQU 25125.63 Hz  
 SCANS 369  
 ACQTM 1.0433 sec  
 PD 2.0000 sec  
 PW1 3.07 usec  
 IRNUC 1H  
 CTEMP 22.6 c  
 SLVNT CDCL3  
 EXREF 77.00 ppm  
 BF 1.20 Hz  
 RGAIN 50

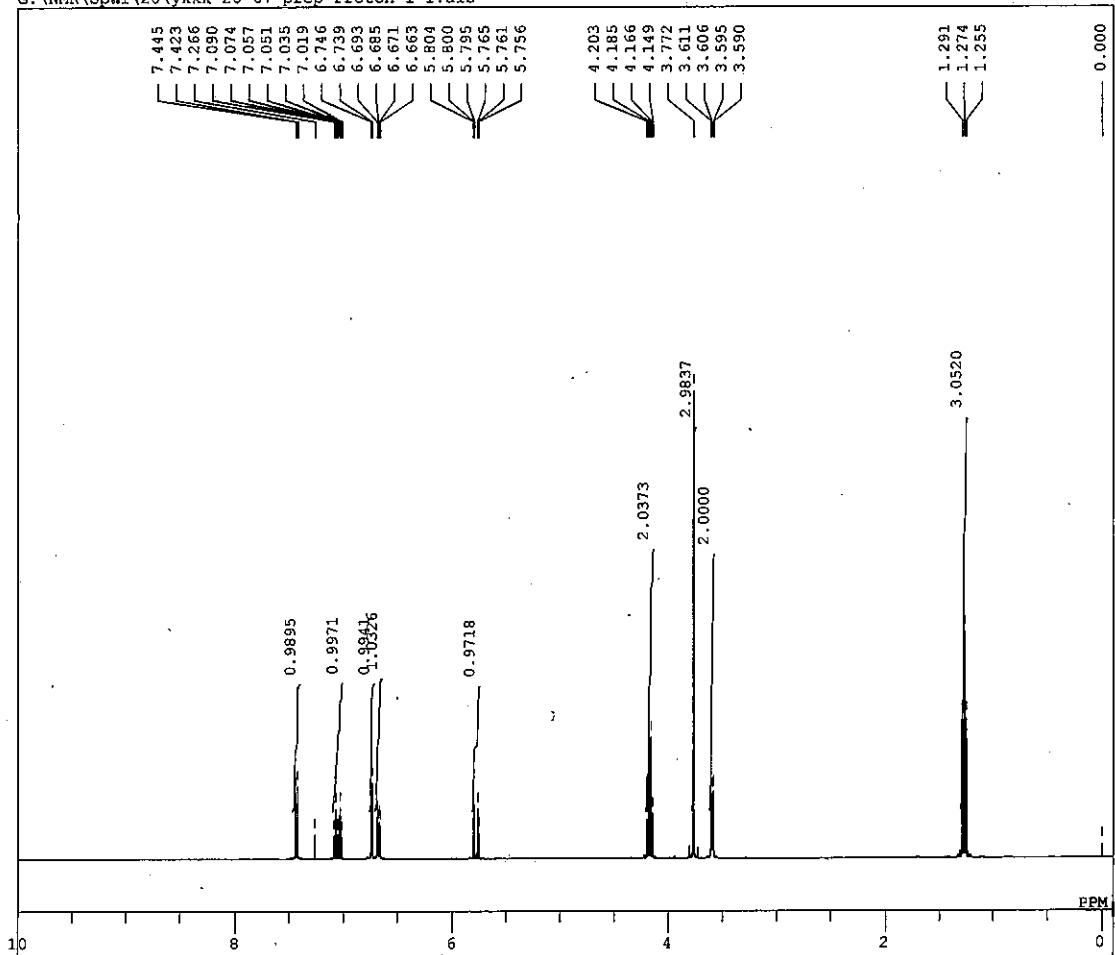


Molecular Weight: 229.0706

S-47

### single\_pulse

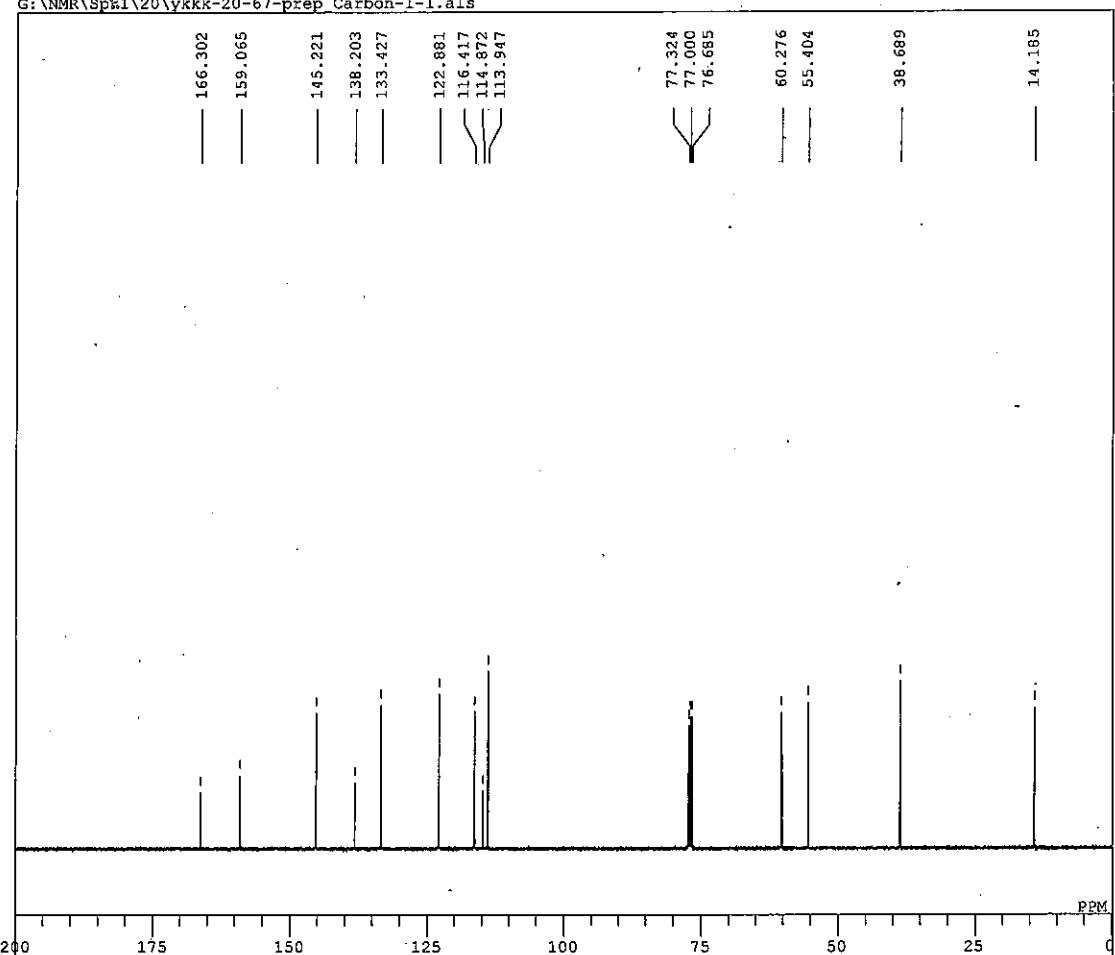
G:\NMR\Špkf\20\ykkk-20-67-prep\_Proton-1-1.als



FILE ykkk-20-67-prep\_Proton-1-1.a  
COMNT single\_pulse  
DATIM 2012-02-28 00:04:46  
OENUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 KHz  
OBFIN 7.29 Hz  
POINT 13107  
FREQU 6002.40 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 22.8 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 30

### single pulse decoupled gated NOE

G:\NMR\Špkf\20\ykkk-20-67-prep\_Carbon-1-1.als

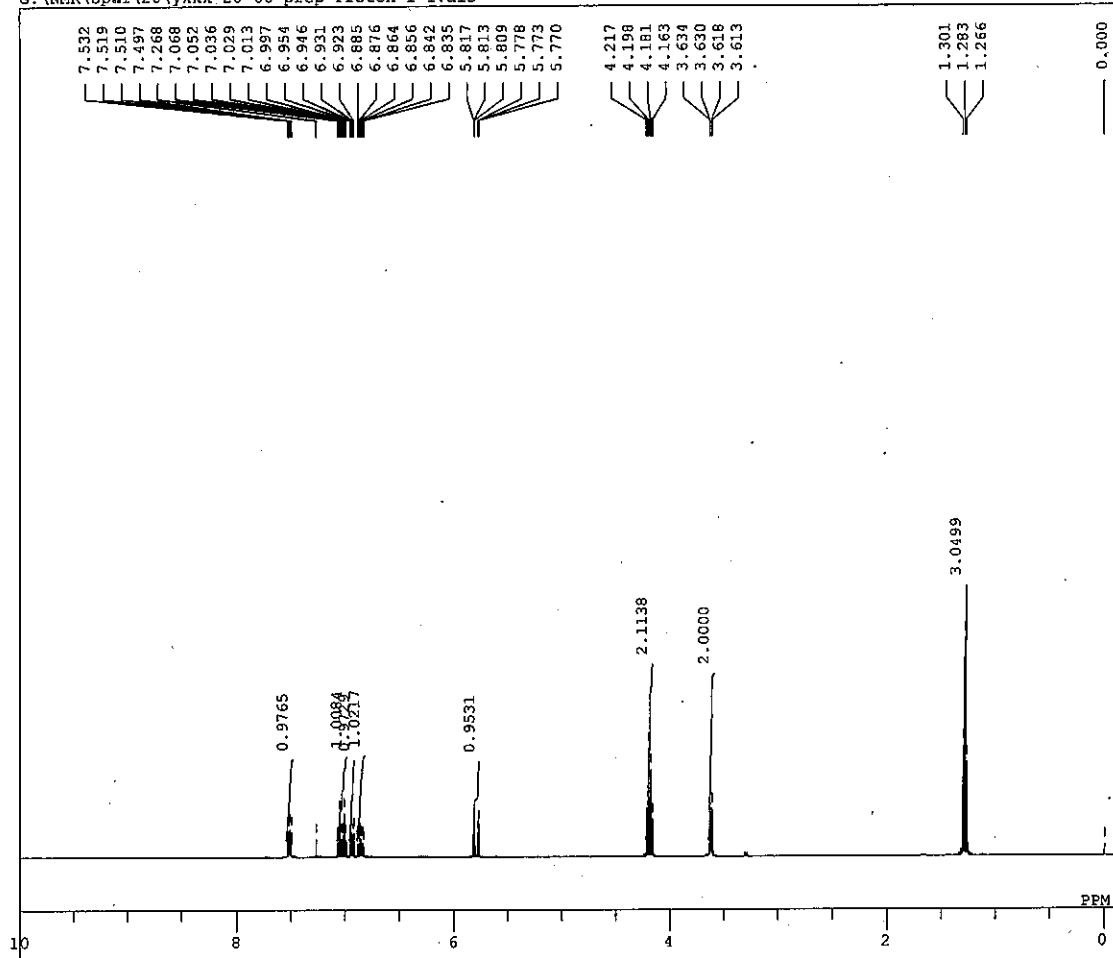


FILE ykkk-20-67-prep\_Carbon-1-1.a  
COMNT single pulse decoupled gated  
DATIM 2012-02-28 00:07:41  
OENUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 KHz  
OBFIN 5.86 Hz  
POINT 26214  
FREQU 25125.63 Hz  
SCANS 194  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 23.1 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

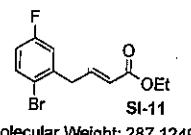
S-48

### single\_pulse

G:\NMR\Špk:\20\ykkk-20-66-prep\_Proton-1-1.als



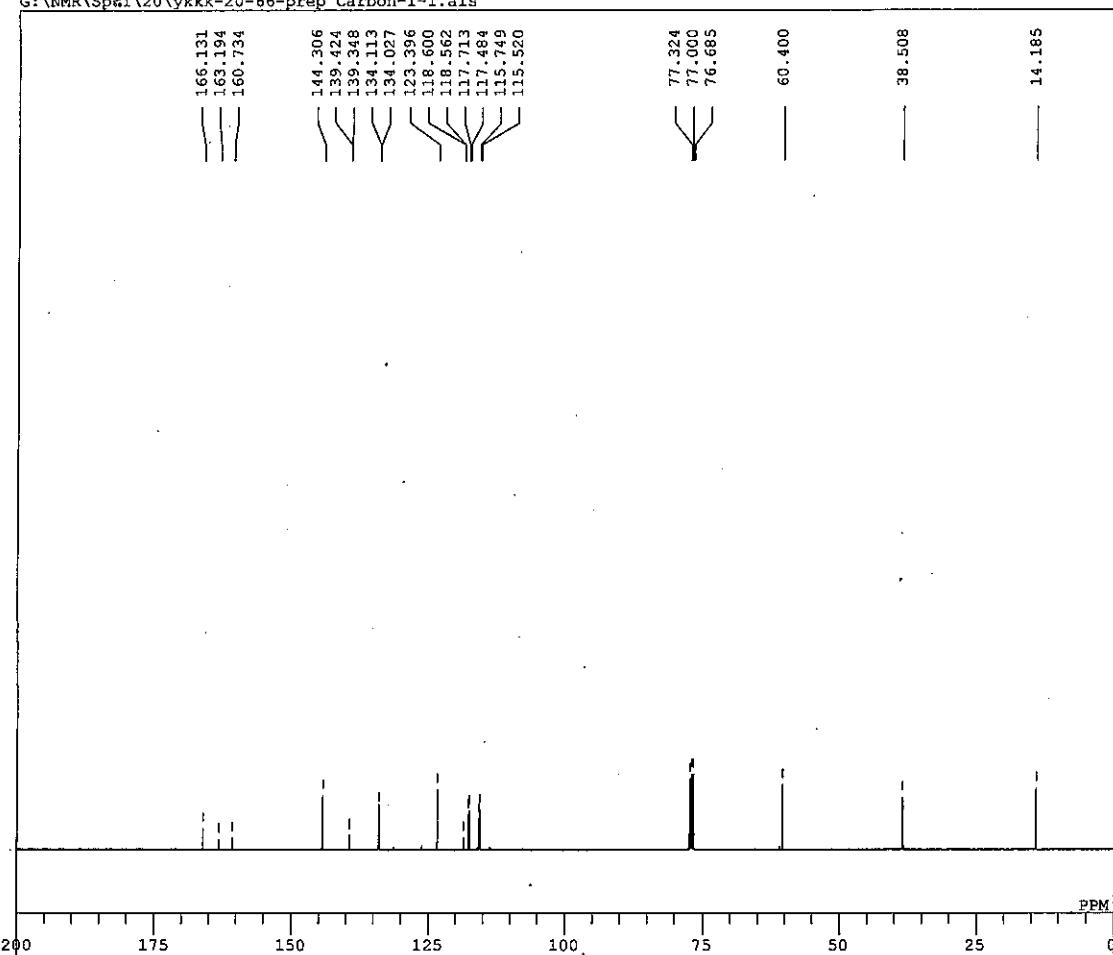
DFILE ykkk-20-66-prep\_Proton-1-1.a  
COMNT single\_pulse  
DATIM 2012-02-28 00:24:25  
OBNUC 1H  
EXMOD proton.jxp  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 13107  
FREQ 6002.40 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 22.8 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 34



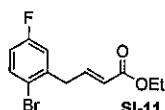
Molecular Weight: 287.1249

### single pulse decoupled gated NOE

G:\NMR\Špk:\20\ykkk-20-66-prep\_Carbon-1-1.als



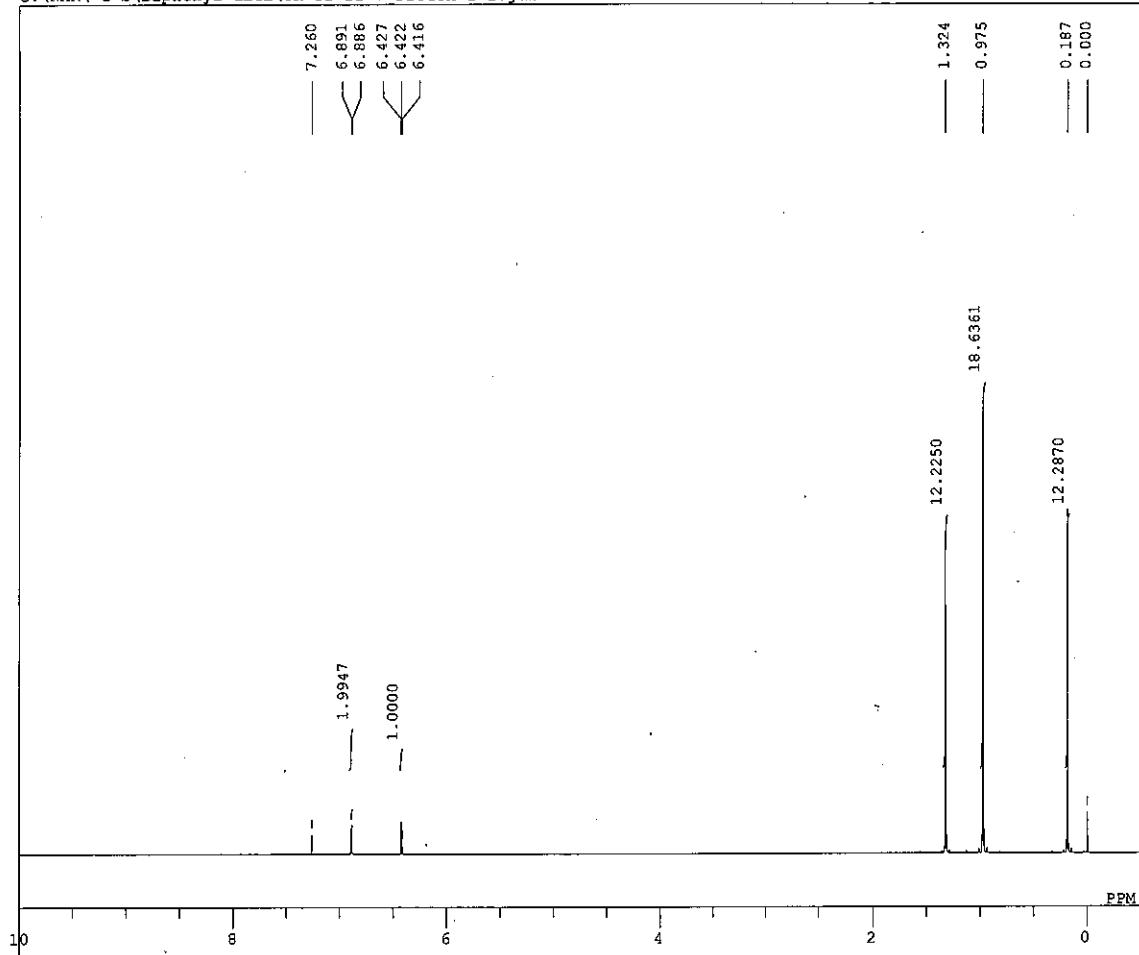
DFILE ykkk-20-66-prep\_Carbon-1-1.a  
COMNT single pulse decoupled gated  
DATIM 2012-02-28 00:27:20  
OBNUC 13C  
EXMOD carbon.jxp  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 26214  
FREQ 25125.63 Hz  
SCANS 567  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 23.1 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



Molecular Weight: 287.1249

single\_pulse

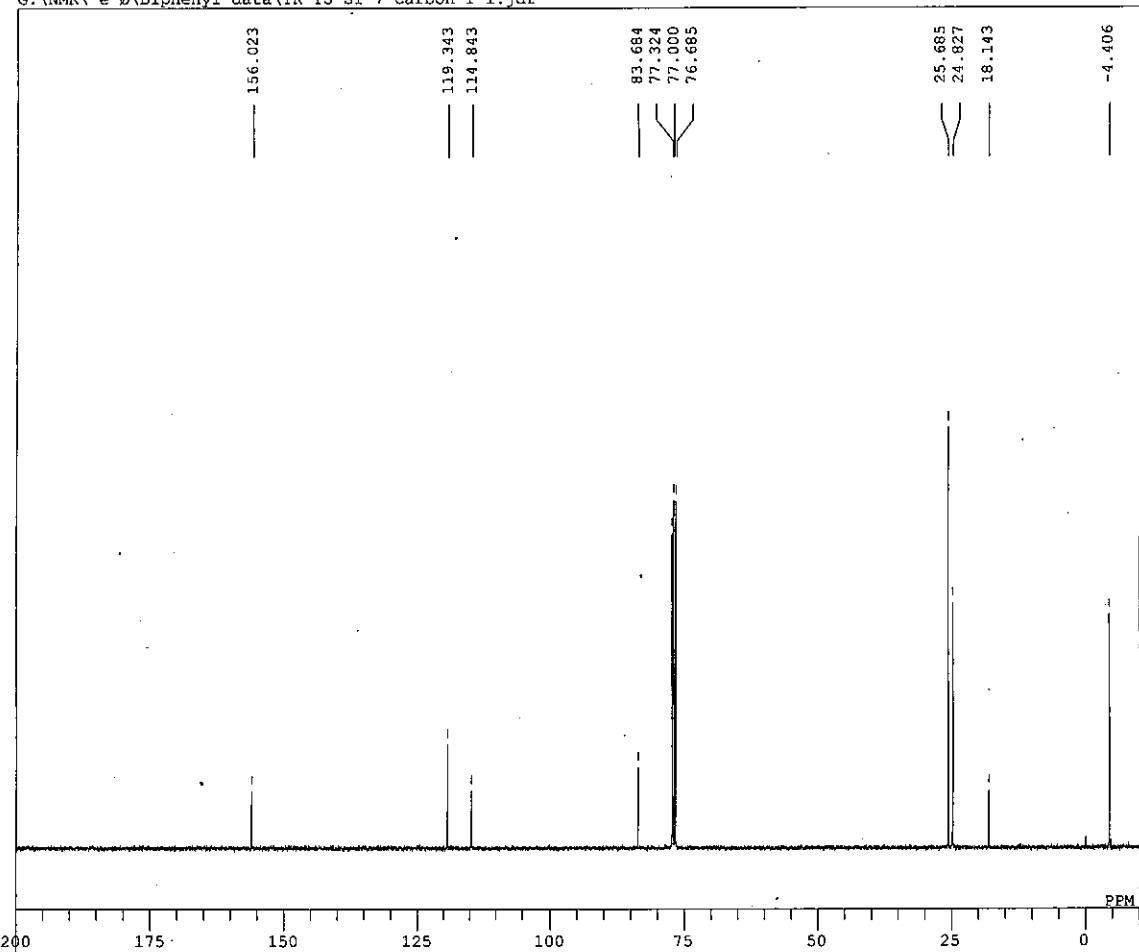
G:\NMR\~é-\Ø\Biphenyl data\YK-YS-SI-7\_Proton-1-1.jdf



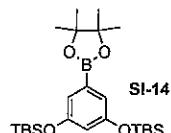
DFILE YK-YS-SI-7\_Proton-1-1.jdf  
COMNT single\_pulse  
DATIM 2012-01-25 23:51:46  
OBNUC 1H  
EXMOD proton.jxp  
OBFREQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 20.1 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 38

single pulse decoupled gated NOE

G:\NMR\~é-\Ø\Biphenyl data\YK-YS-SI-7\_Carbon-1-1.jdf

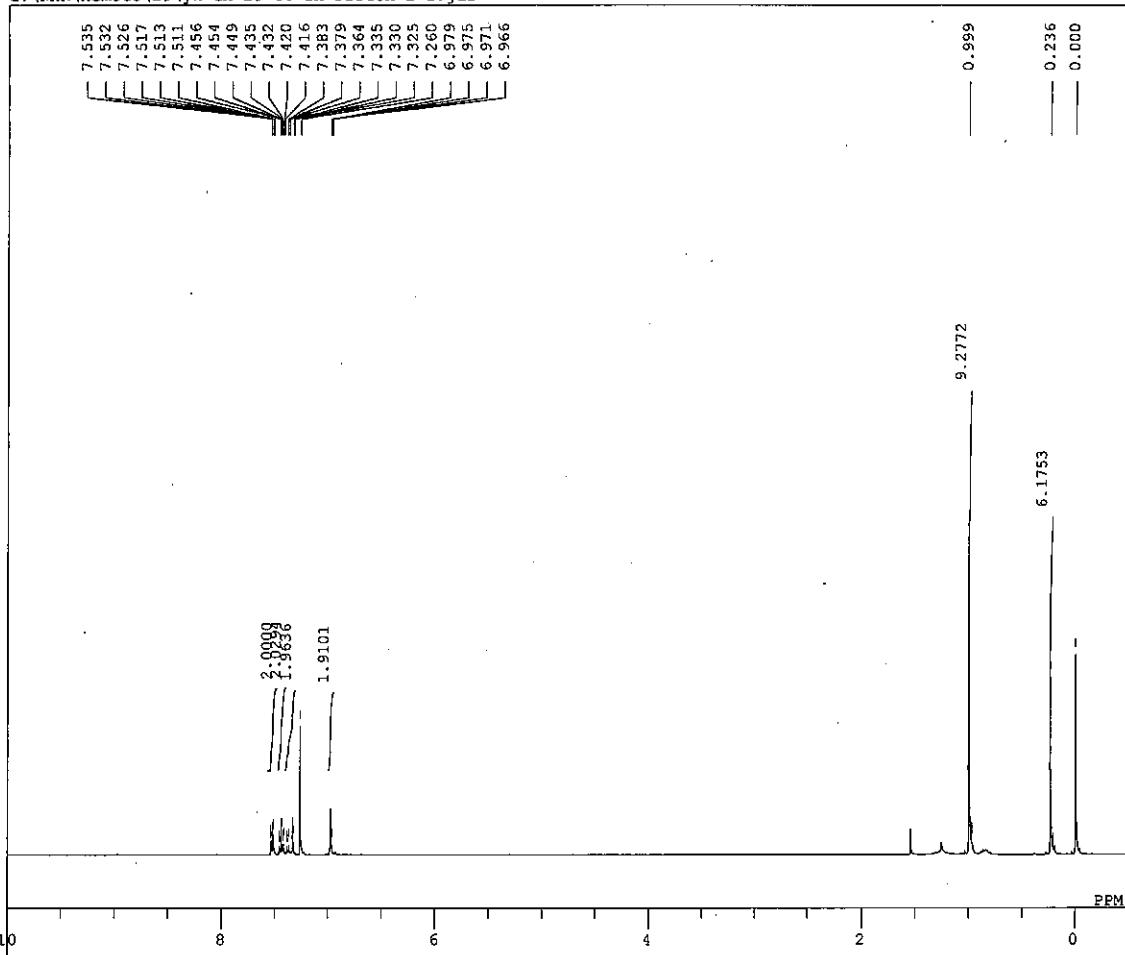


DFILE YK-YS-SI-7\_Carbon-1-1.jdf  
COMNT single pulse decoupled gated  
DATIM 2012-01-25 23:54:40  
OBNUC 13C  
EXMOD carbon.jxp  
OBFREQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 512  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 20.2 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



### single\_pulse

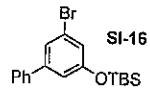
G:\NMR\nemoto\29\yk-tn-29-64-1H\_Proton-1-1.jdf



```

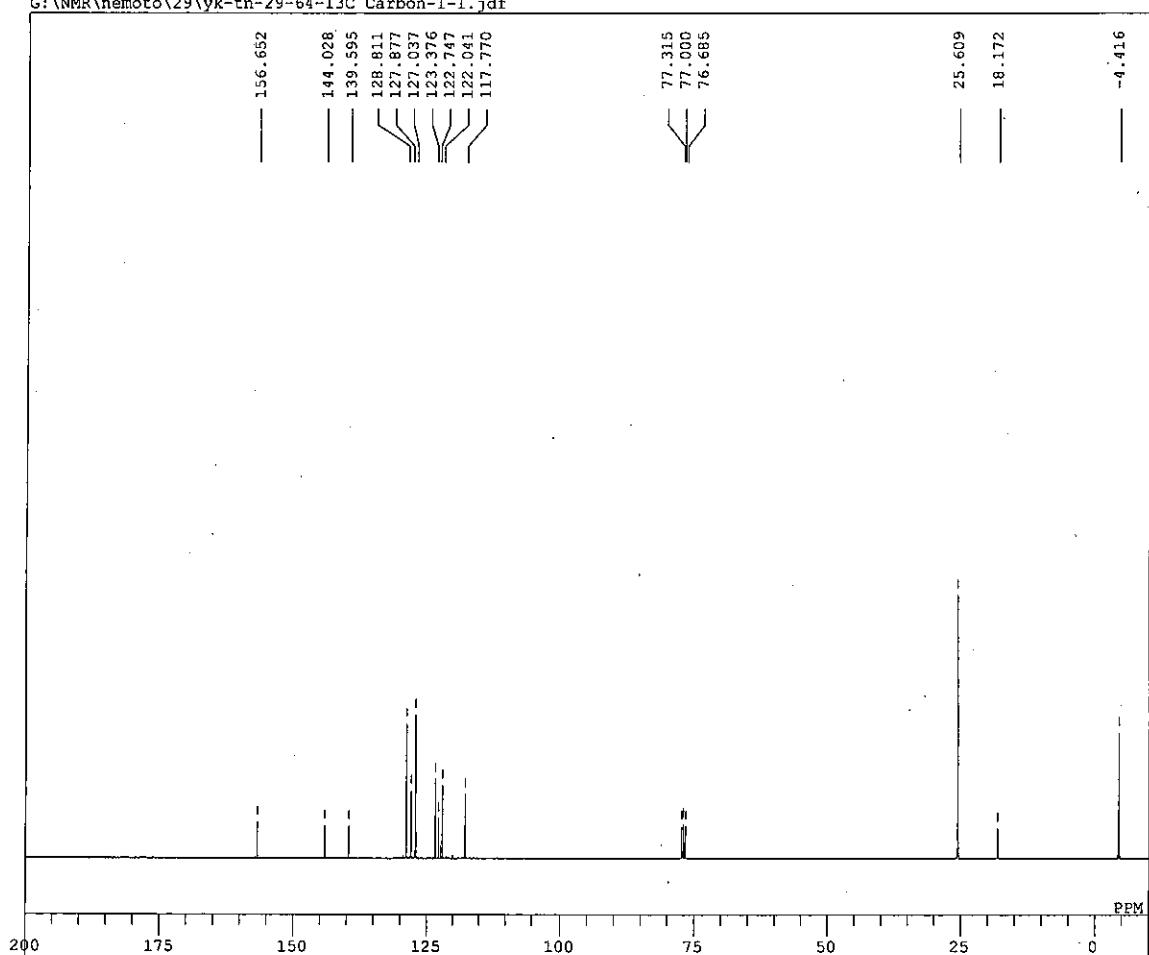
DFILE      yk-tn-29-64-1H_Proton-1-1.jdf
COMNT     single_pulse
DATIM    2012-01-28 13:05:19
OBNUC     1H
EXMOD   proton.jxp
OBFRQ    399.78 MHz
OBSET    4.19 kHz
OBFIN    7.29 Hz
POINT    16384
FREQU   7503.00 Hz
SCANS      8
ACQTM    2.1837 sec
PD       5.0000 sec
PW1      5.00 usec
IRNUC    1H
CTEMP    19.8 c
SLVNT    CDCL3
EXREF    0.00 ppm
BF       0.12 Hz
RGAIN    52

```



### single pulse decoupled gated NOE

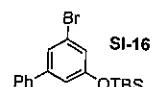
G:\NMR\nemoto\29\yk-tn-29-64-13C\_Carbon-1-1.jdf



```

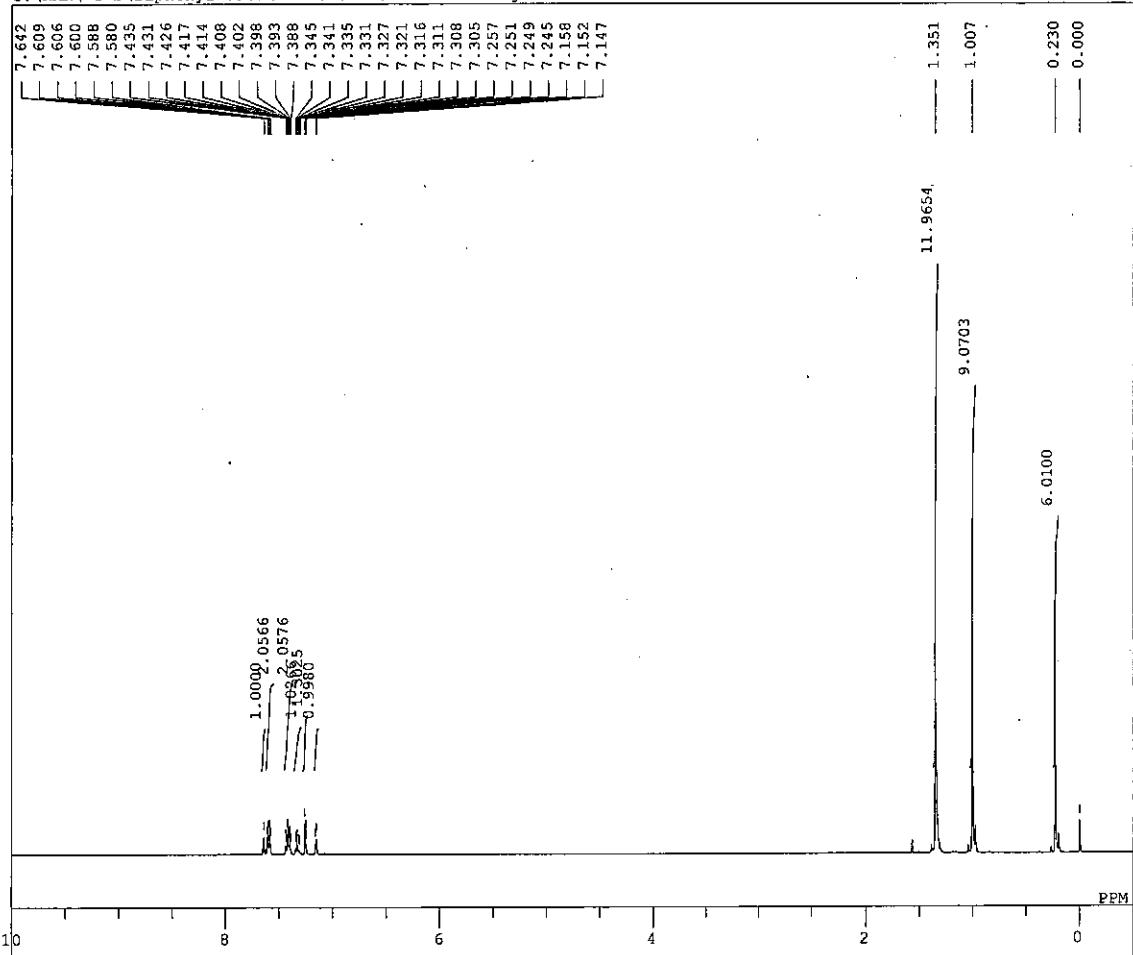
DFILE      yk-tn-29-64-13C_Carbon-1-1.jdf
COMNT     single pulse decoupled gated
DATIM    2012-01-28 13:11:36
OBNUC     13C
EXMOD   carbon.jxp
OBFRQ    100.53 MHz
OBSET    5.35 kHz
OBFIN    5.86 Hz
POINT    32767
FREQU   31407.04 Hz
SCANS      128
ACQTM    1.0433 sec
PD       2.0000 sec
PW1      3.07 usec
IRNUC    1H
CTEMP    20.0 c
SLVNT    CDCL3
EXREF    77.00 ppm
BF       1.20 Hz
RGAIN    50

```

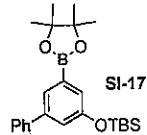


single\_pulse

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-15\_Proton-1-1.jdf

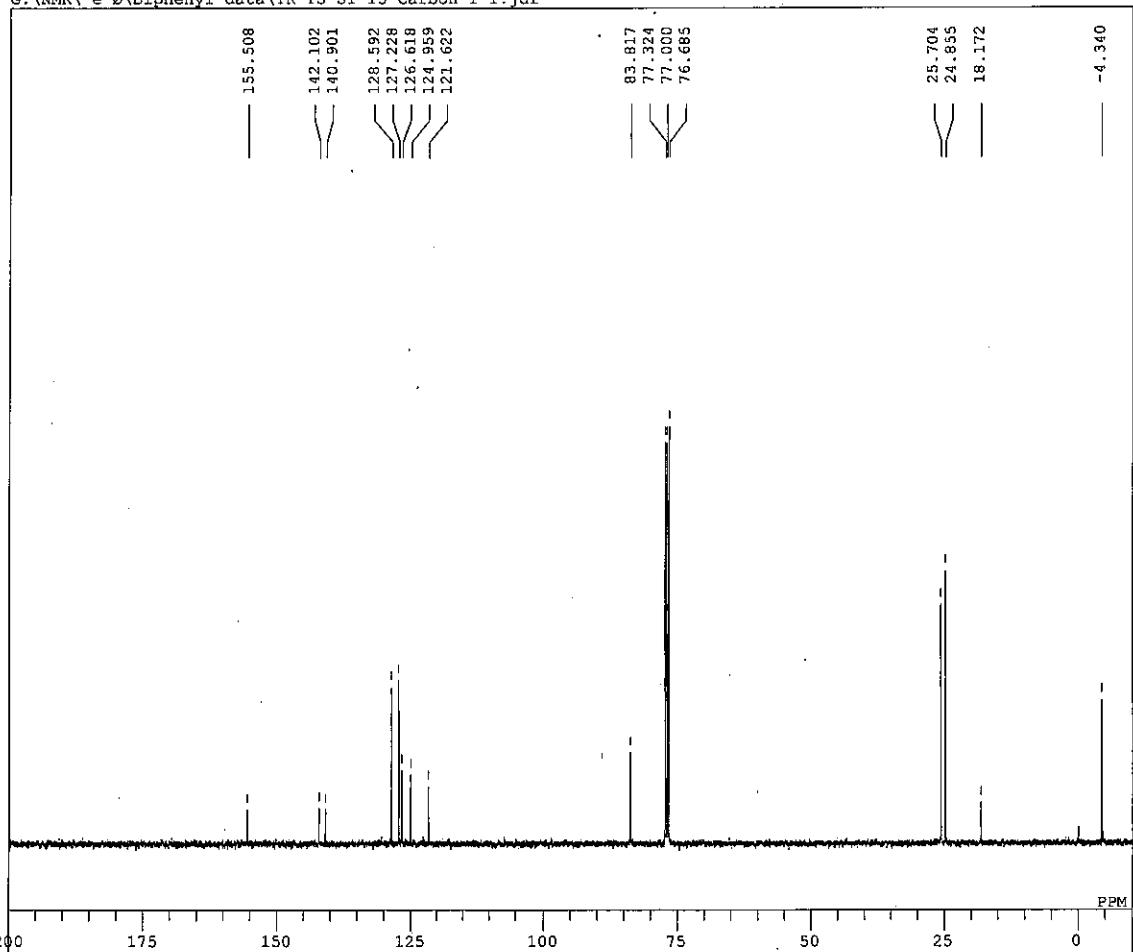


FILE YK-YS-SI-15\_Proton-1-1.jdf  
COMMENT single\_pulse  
DATE 2012-02-03 21:24:40  
1H proton.jpx  
OBFRQ 399.78 MHz  
OBSET 4.19 kHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PWI 5.00 usec  
IRNUC 1H  
CTEMP 18.3 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 36

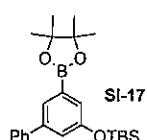


single pulse decoupled gated NOE

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-15\_Carbon-1-1.jdf

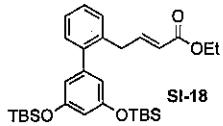
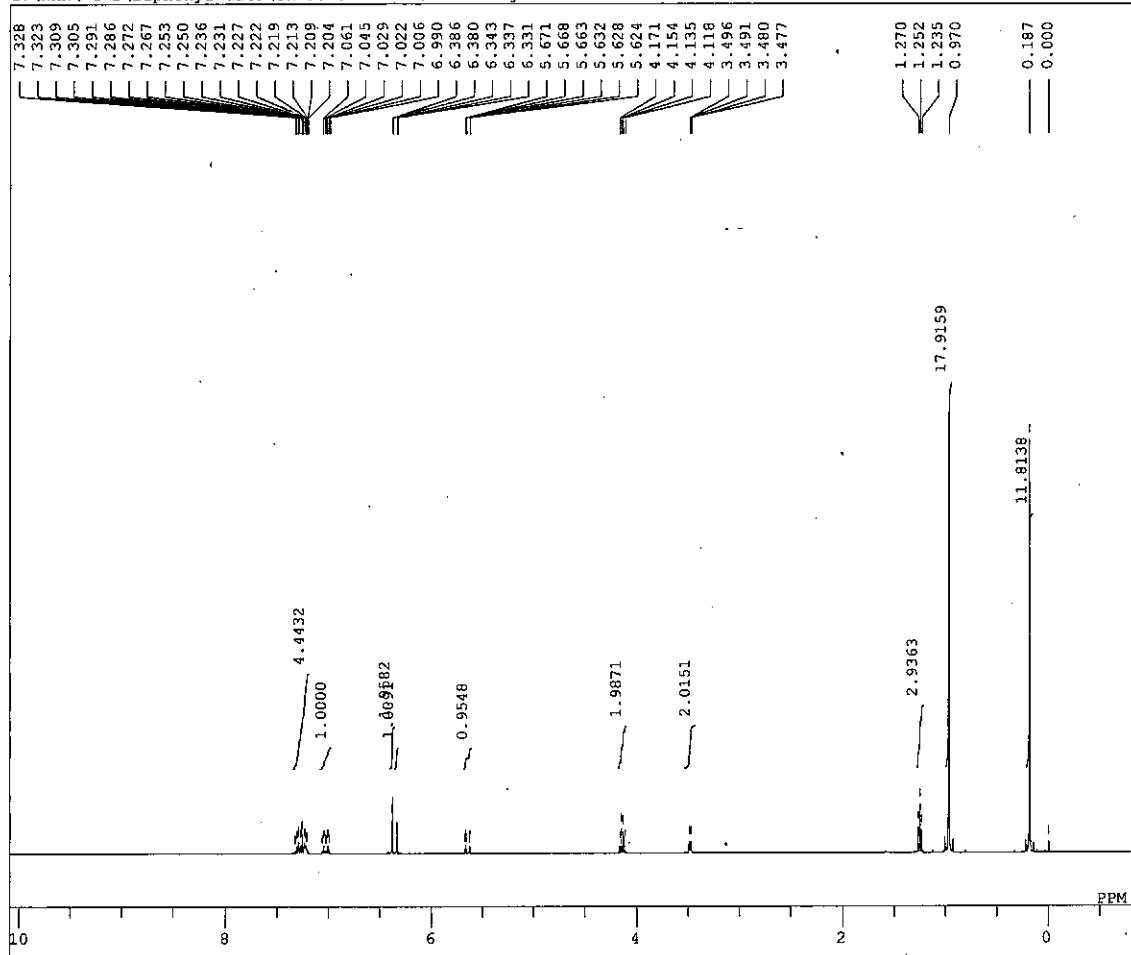


FILE YK-YS-SI-15\_Carbon-1-1.jdf  
COMMENT single pulse decoupled gated  
DATE 2012-02-03 21:26:05  
13C carbon.jpx  
OBFRQ 100.53 MHz  
OBSET 5.35 kHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 256  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PWI 3.07 usec  
IRNUC 1H  
CTEMP 18.5 c  
SLVNT CDCL<sub>3</sub>  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50



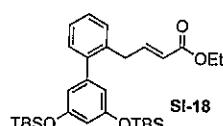
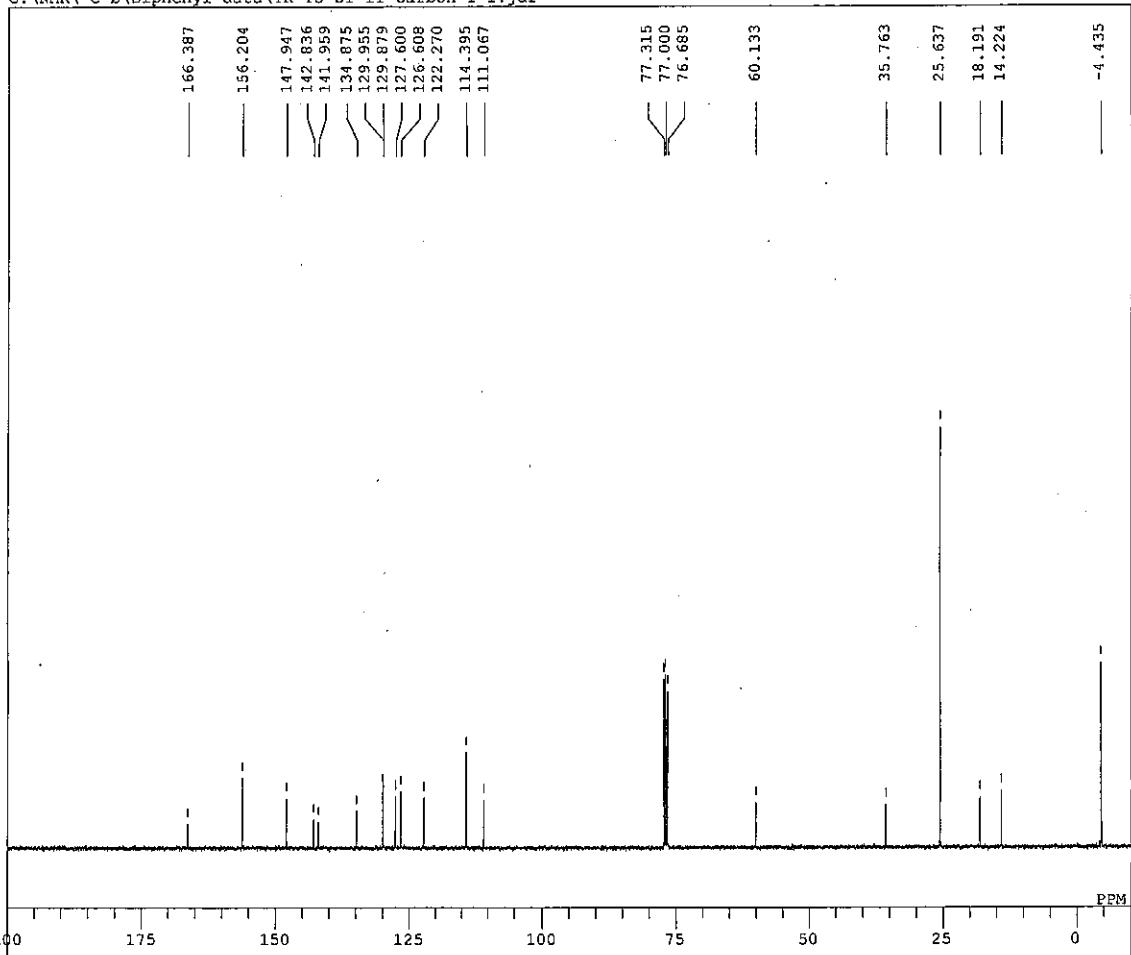
## single\_pulse

G:\NMR\é-Ø\Biphenyl data\YK-YS-SI-11\_Proton-1-1.jdf



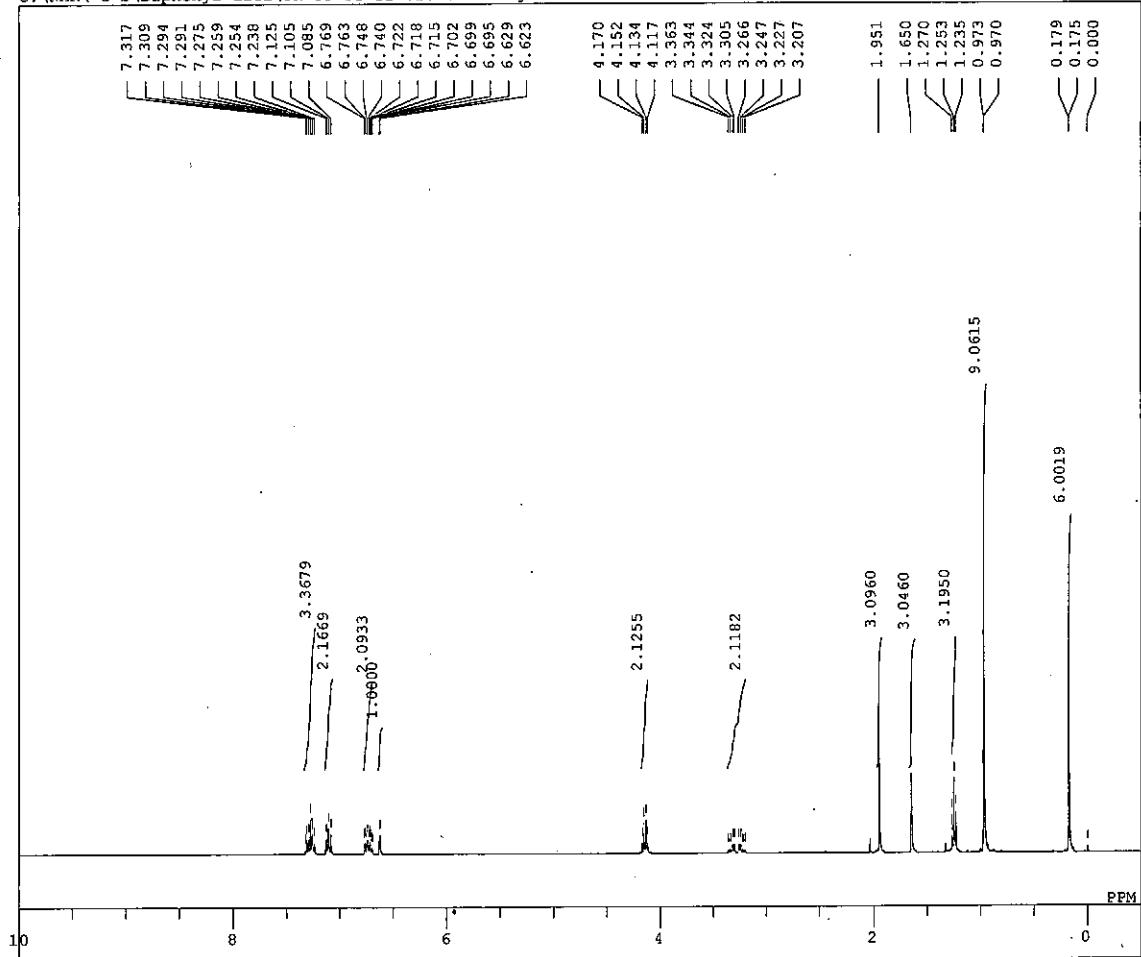
### **single pulse decoupled gated NOE**

G:\NMR\-\é-\ø\Biphenyl data\YK-YS-SI-11\_Carbon-1-1.jdf



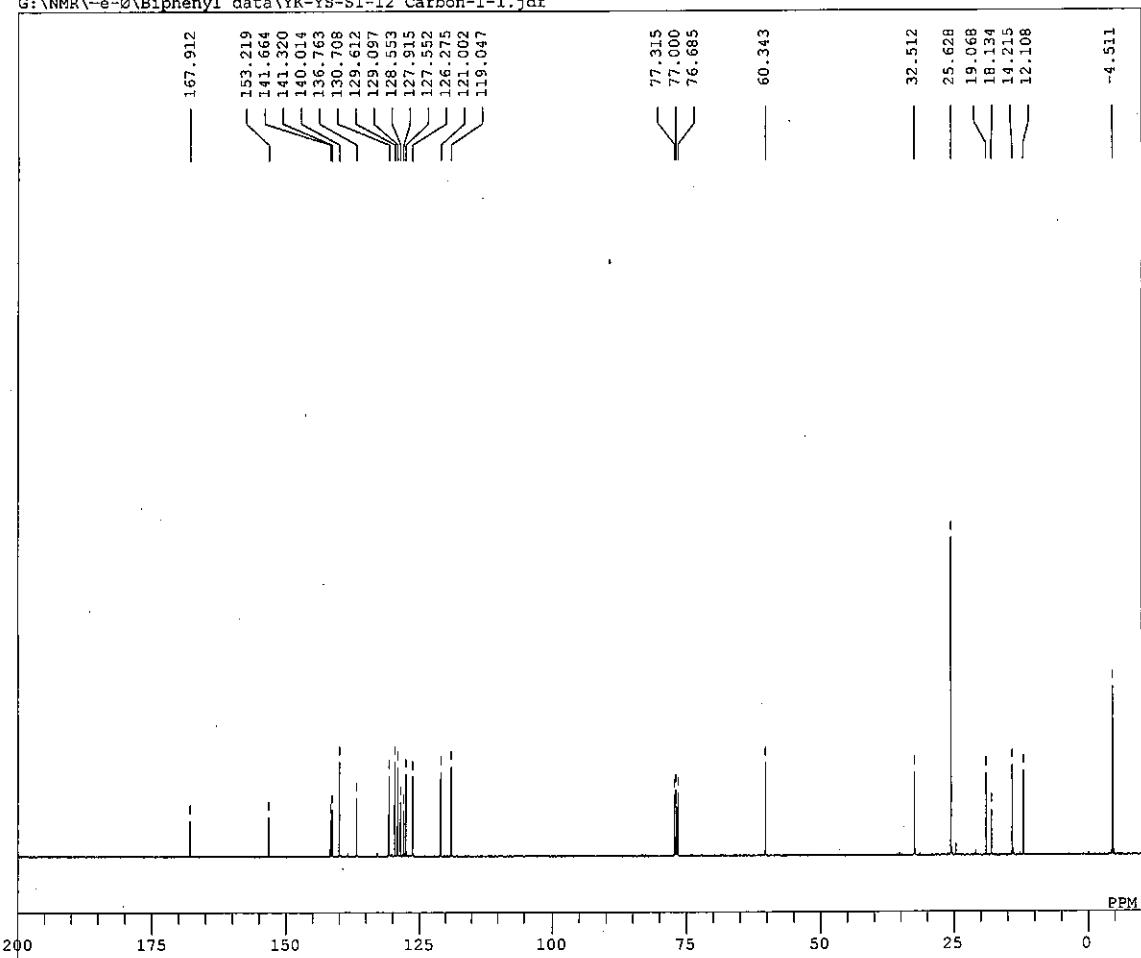
single\_pulse

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-12\_Proton-1-1.jdf



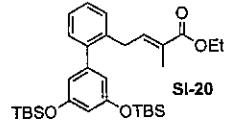
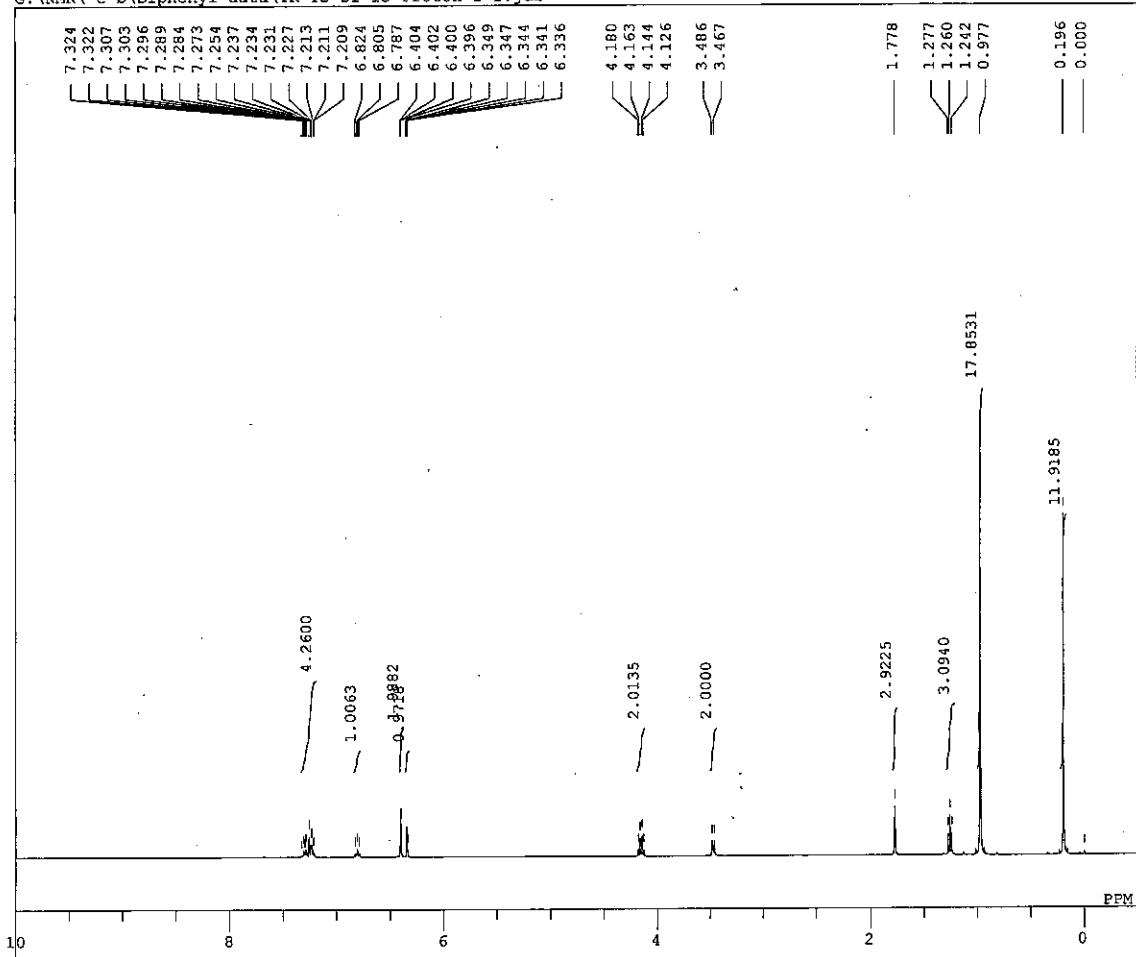
single pulse decoupled gated NOE

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-12\_Carbon-1-1.jdf



### single pulse

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-13\_Proton-1-1.jdf



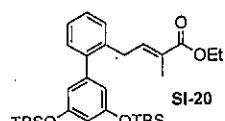
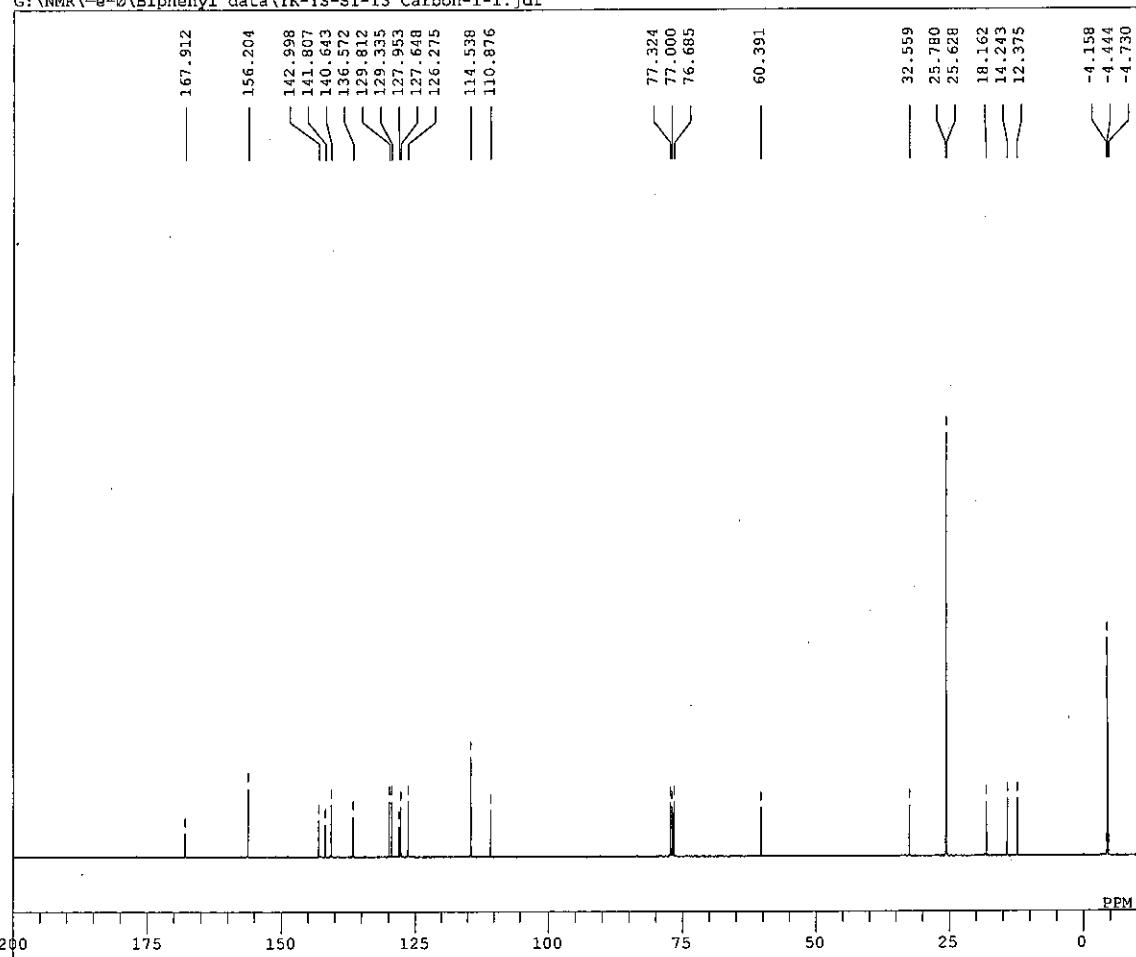
```

DFILE YK-YS-SI-13_Proton-1-1.jdf
COMNT single_pulse
DATIM 2012-01-28 22:46:05
OBNUC 1H
EXMOD proton.jxp
OBFRQ      399.78 MHz
OBSET       4.19 KHz
OBFIN       7.29 Hz
POINT        16384
FREQU       7503.00 Hz
SCANS         8
ACQTM        2.1837 sec
PD           5.0000 sec
PW1          5.00 usec
IRNUC       1H
CTEMP        19.6 c
SLVNT       CDCL3
EXREF        0.00 ppm
BF           0.12 Hz
RGAIN        20

```

#### **single pulse decoupled gated NOE**

G:\NMR\é-0\Biphenyl data\YK-YS-SI-13 Carbon-1-1.jdf



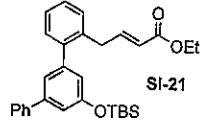
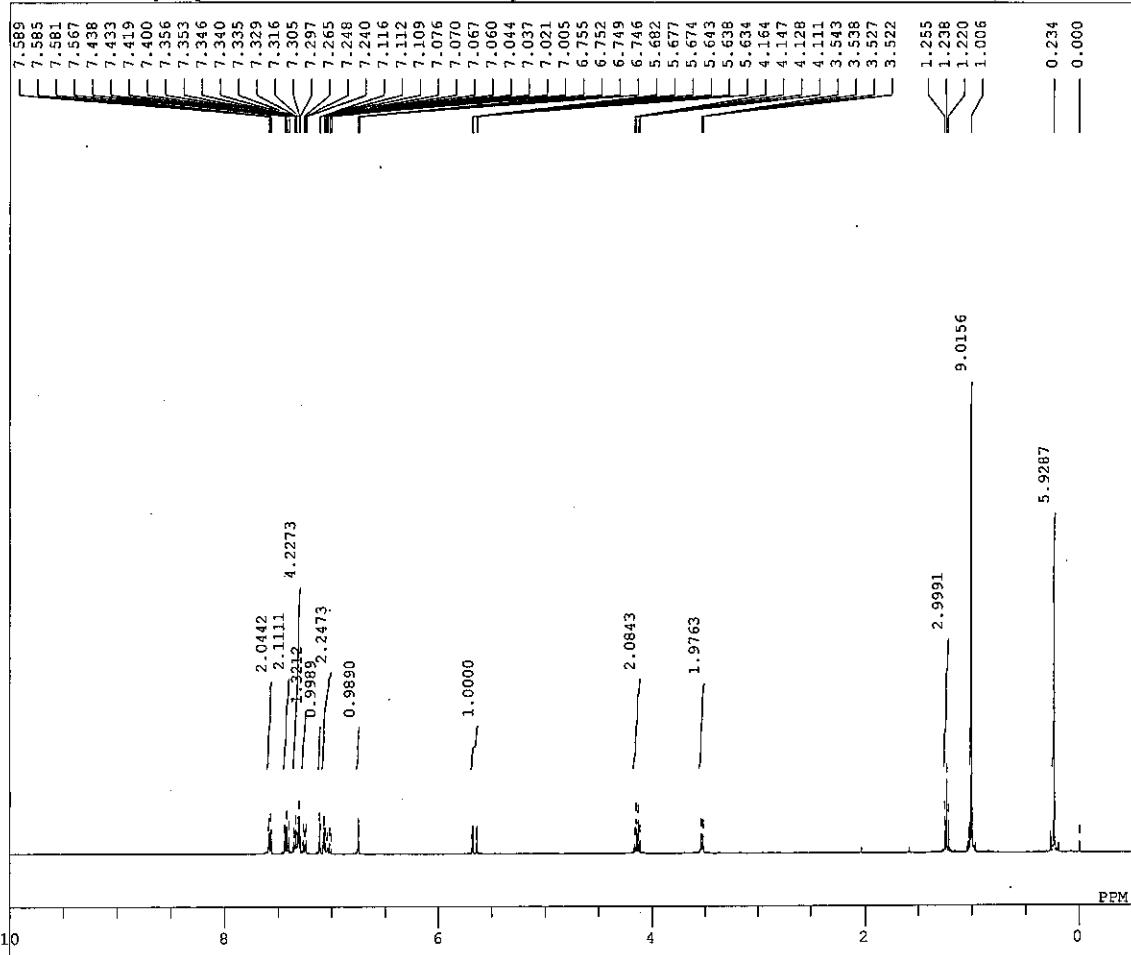
```

DFILE YK-YS-SI-13_Carbon-1-1.jdf
COMNT single pulse decoupled gated
DATIM 2012-01-28 22:47:31
OBNUC 13C
EXMOD carbon.jxp
OBFRQ      100.53 MHz
OBSET       5.35 kHz
OBFIN       5.86 Hz
POINT        32767
FREQU     31407.04 Hz
SCANS        256
ACQTM      1.0433 sec
PD          2.0000 sec
PW1         3.07 usec
IRNUC      1H
CTEMP       19.8 c
SLVNT      CDCL3
EXREF      77.00 ppm
BF          1.20 Hz
RGAIN       50

```

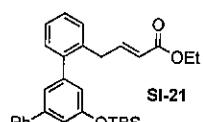
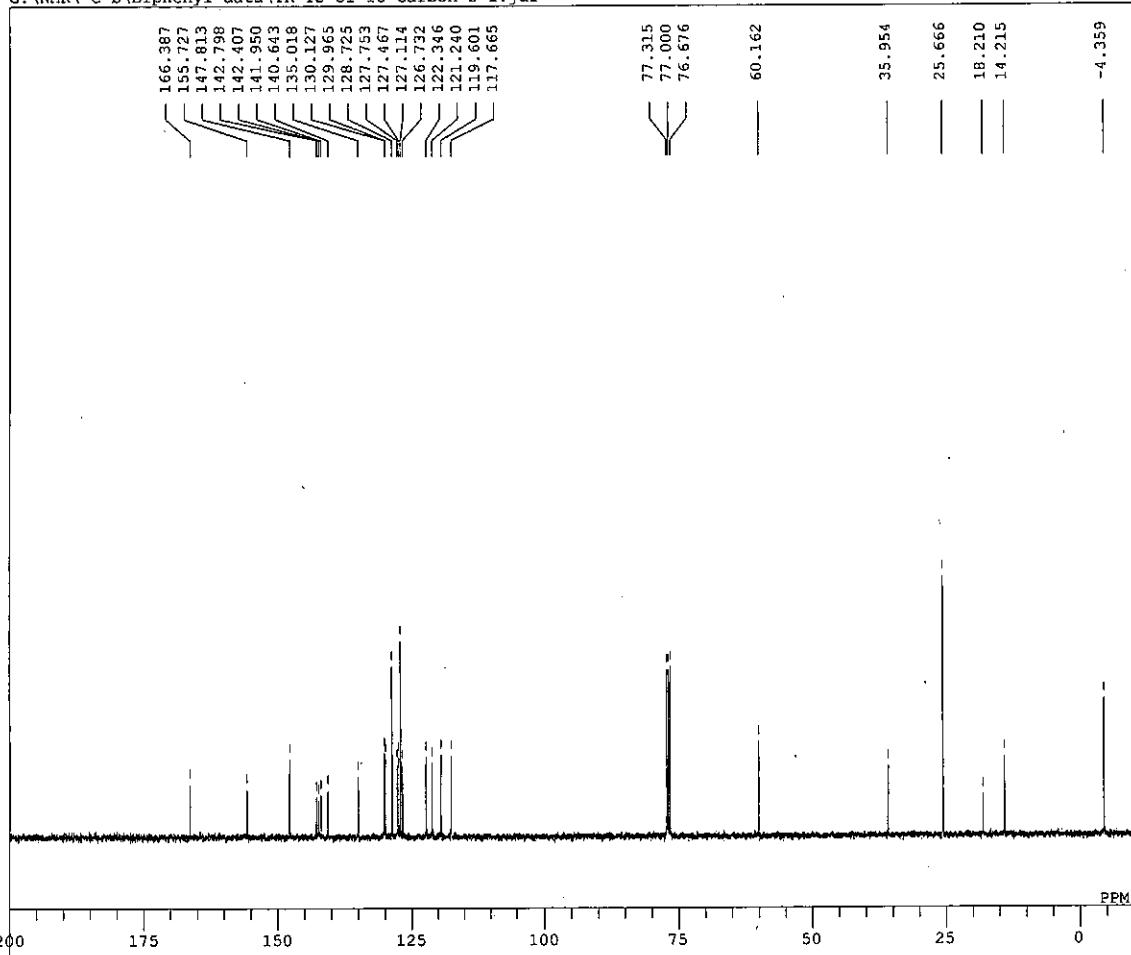
single\_pulse

G:\NMR\-\6-\0\Biphenyl data\YK-YS-SI-15\_Proton-4-1.jdf



single pulse decoupled gated NOE

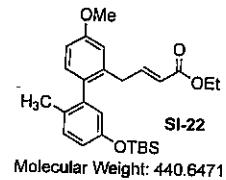
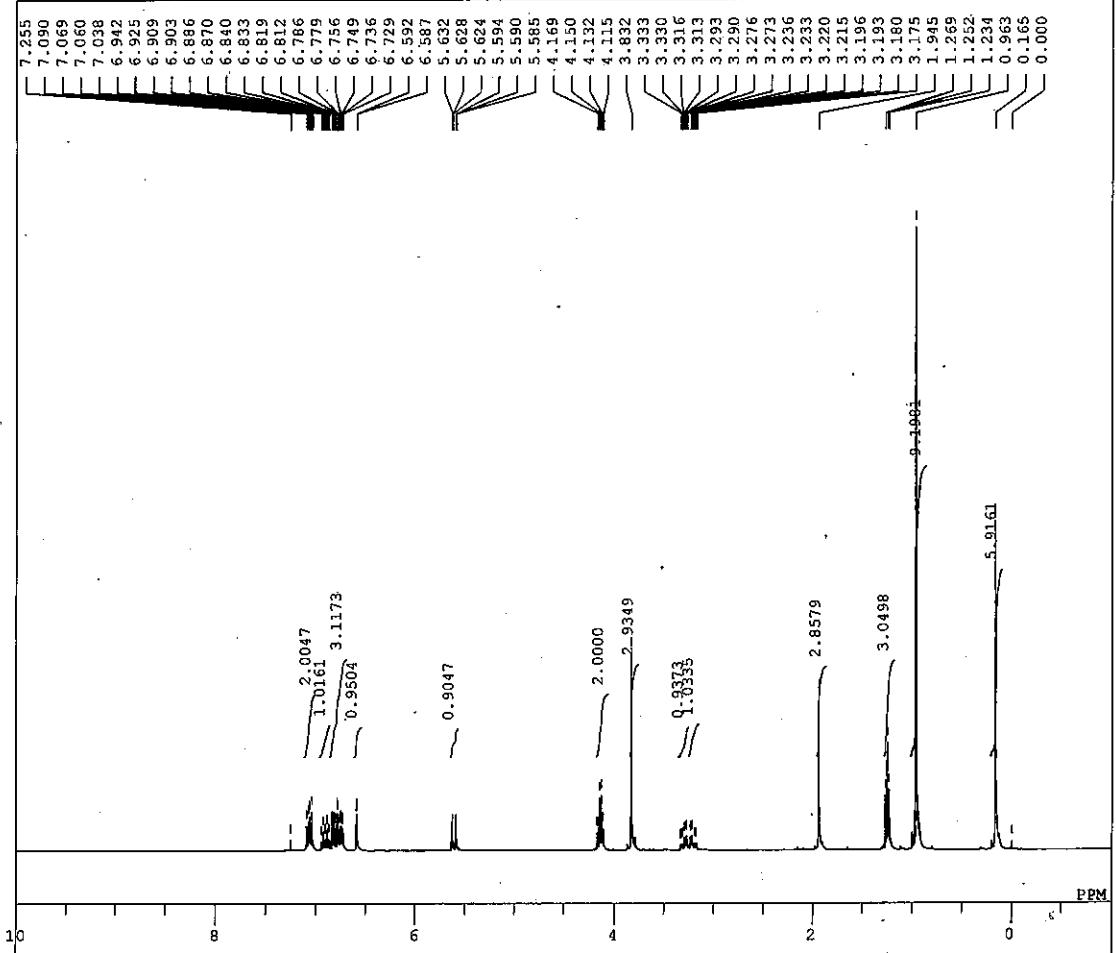
G:\NMR\-\6-\0\Biphenyl data\YK-YS-SI-15\_Carbon-2-1.jdf



S-56

### single\_pulse

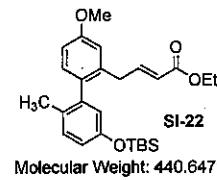
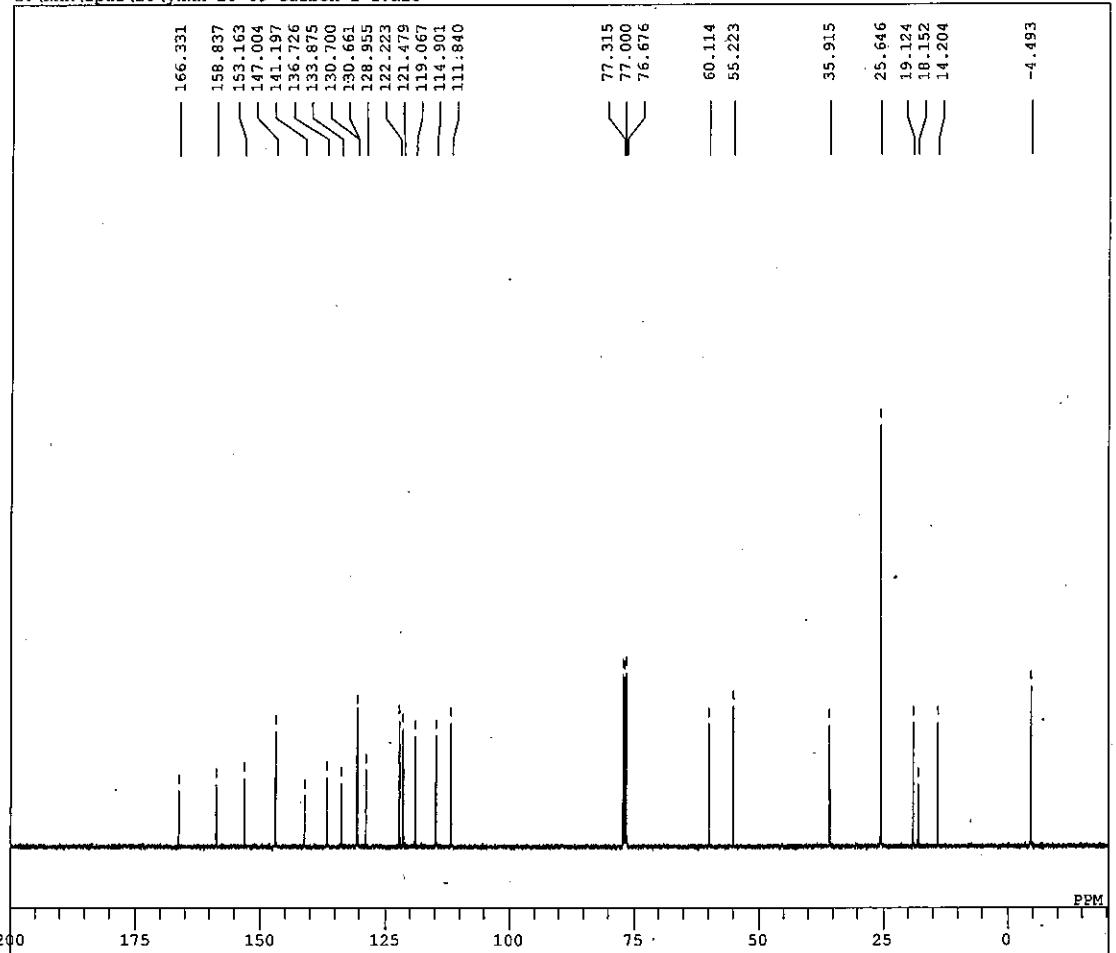
G:\NMR\Sp\ff\20\ykkk-20-69\_Proton-1-1.als



Molecular Weight: 440.6471

### single pulse decoupled gated NOE

G:\NMR\špf\20\ykkk-20-69 Carbon-1-1.als



Molecular Weight: 440.6471

```

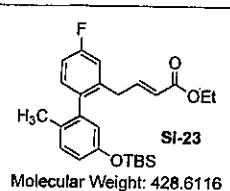
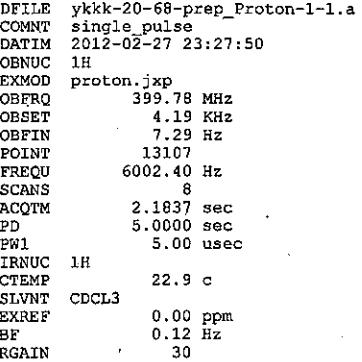
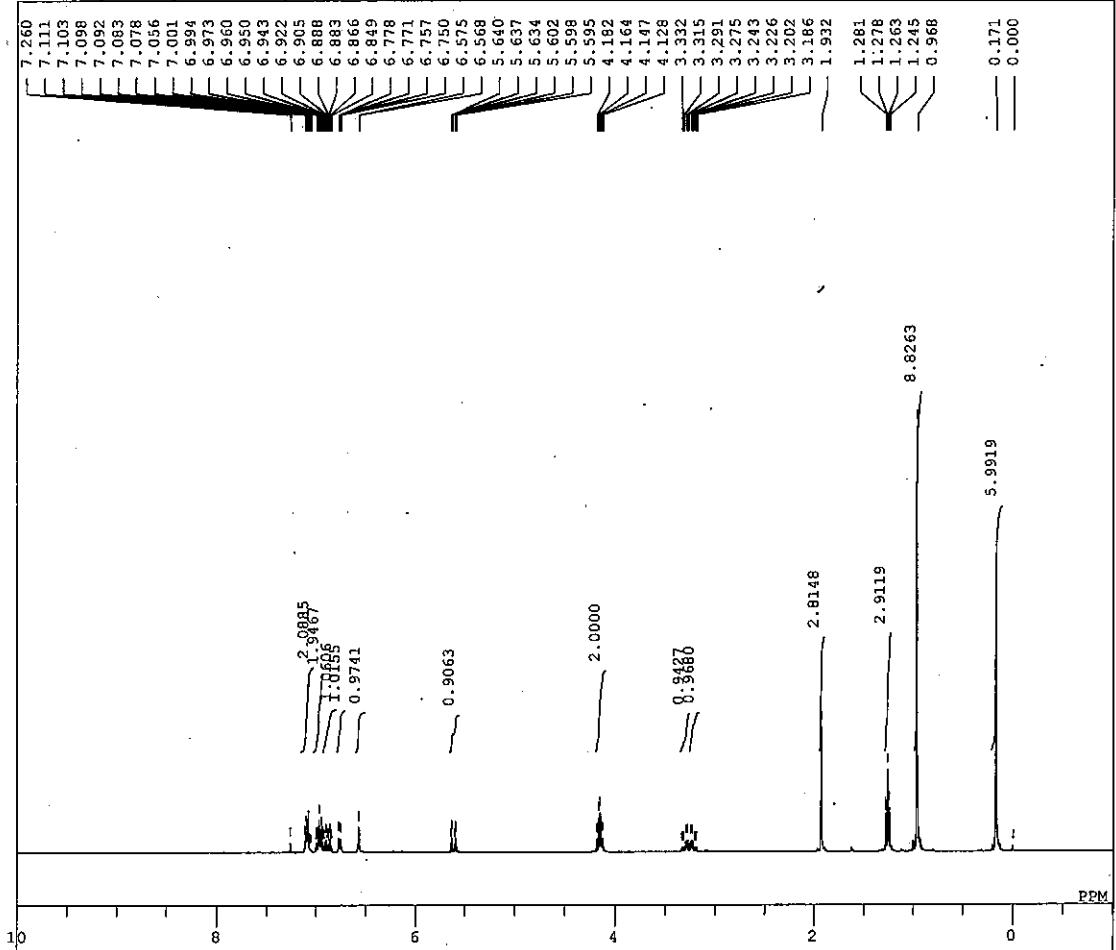
DFILE ykkk-20-69_Proton-1-1.als
COMNT single_pulse
DATIM 2012-02-27 23:05:46
OBNUC 1H
EXMOD proton.jxp
OSFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.40 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 28

```

S-57.

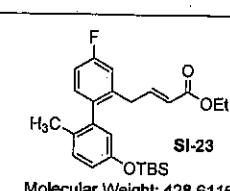
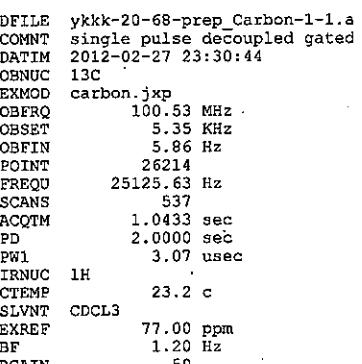
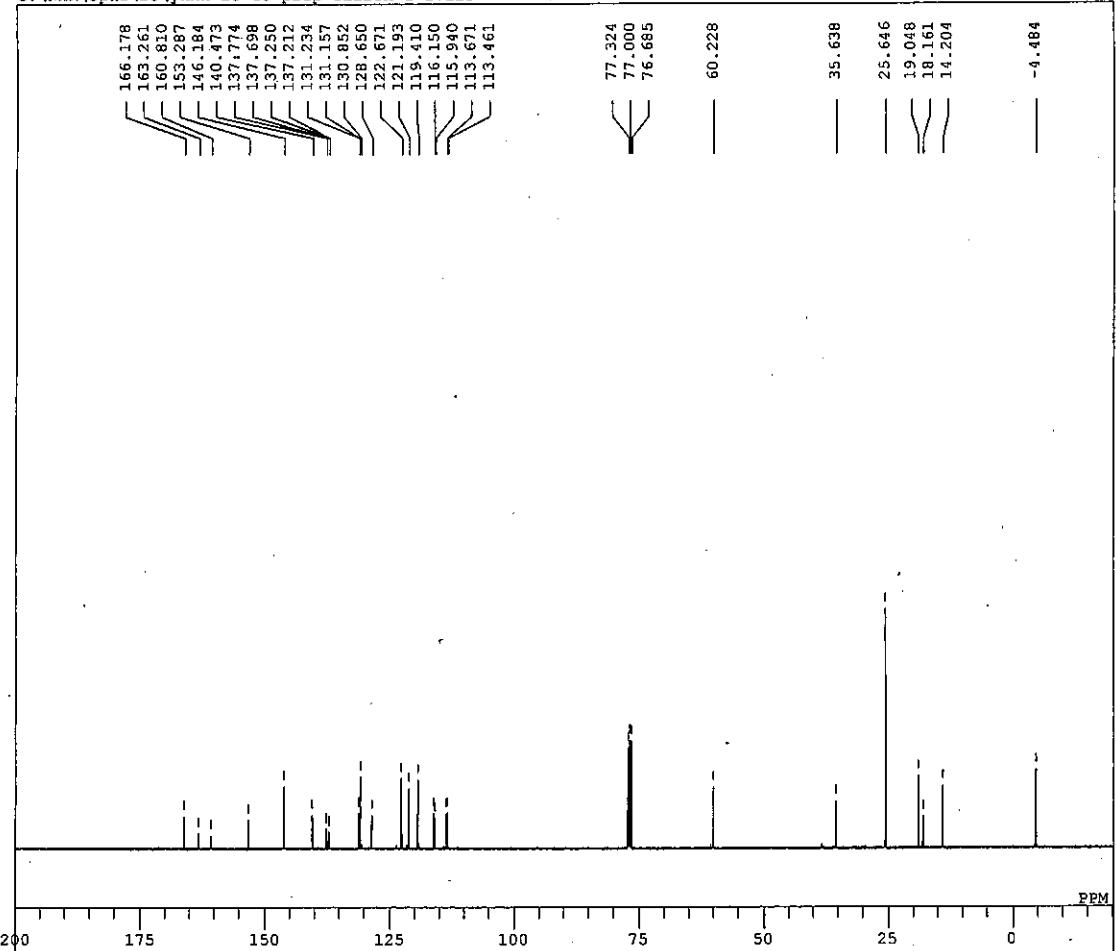
### single\_pulse

G:\NMR\Špšf\20\ykkk-20-68-prep\_Proton-1-1.als



single pulse decoupled gated NOE

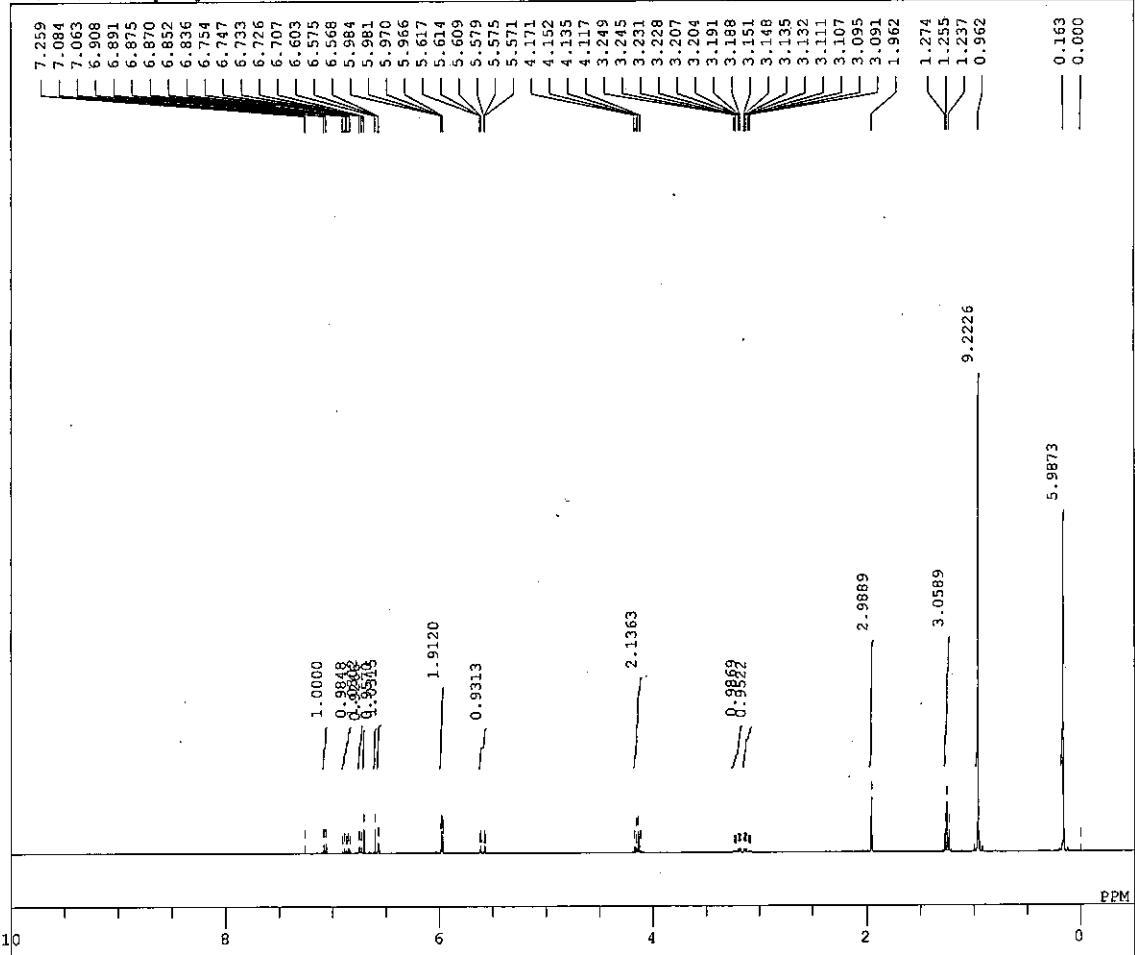
G:\NMR\Špkf\20\ykkk-20-68-prep Carbon-1-1.als



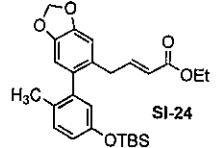
S-~~5~~

### single\_pulse

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-14\_Proton-1-1.jdf

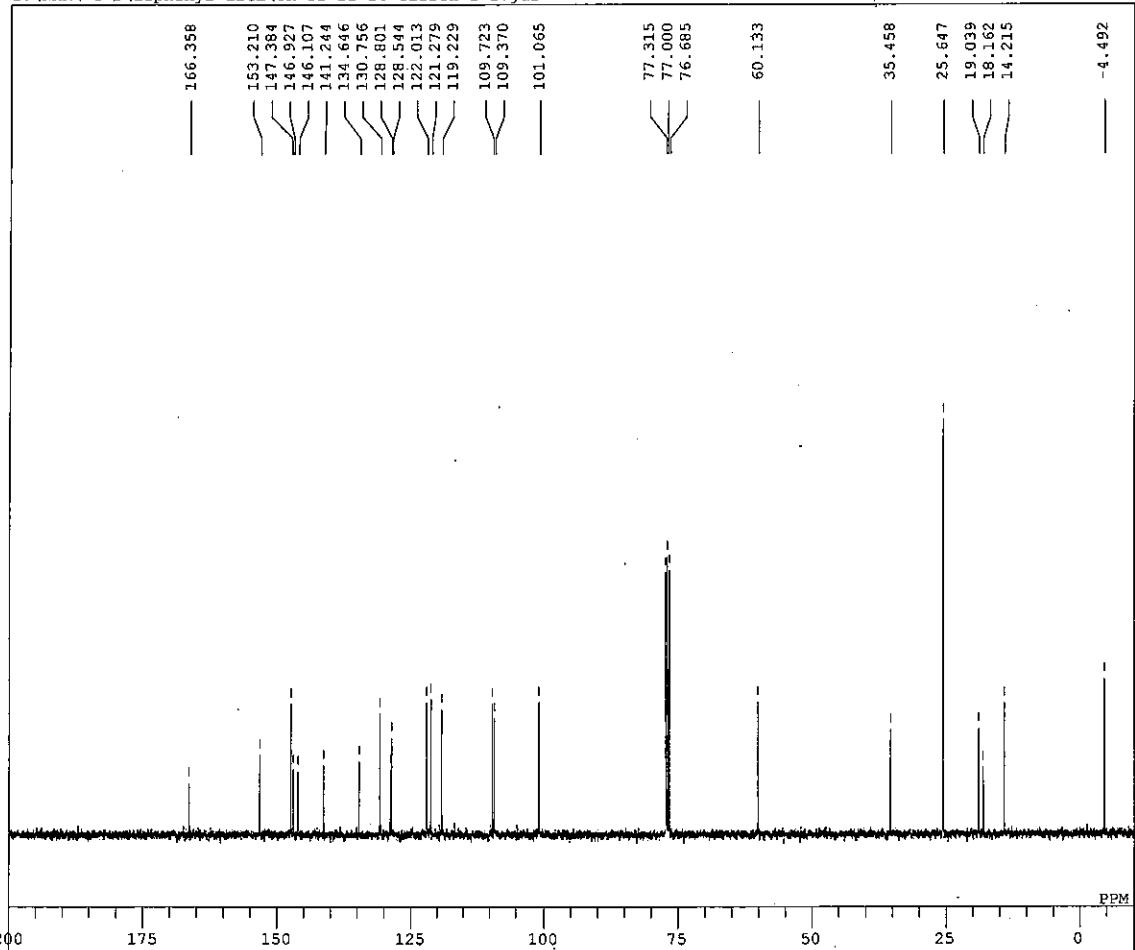


FILE YK-YS-SI-14\_Proton-1-1.jdf  
COMMENT single\_pulse  
DATE 2012-02-11 16:34:43  
OBNUC 1H  
EXMOD proton.jxp  
OBERQ 399.78 MHz  
OBSET 4.19 KHz  
OBFIN 7.29 Hz  
POINT 16384  
FREQU 7503.00 Hz  
SCANS 8  
ACQTM 2.1837 sec  
PD 5.0000 sec  
PW1 5.00 usec  
IRNUC 1H  
CTEMP 22.5 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
BF 0.12 Hz  
RGAIN 30



### single pulse decoupled gated NOE

G:\NMR\-\é-\Ø\Biphenyl data\YK-YS-SI-14\_Carbon-1-1.jdf



FILE YK-YS-SI-14\_Carbon-1-1.jdf  
COMMENT single pulse decoupled gated  
DATE 2012-02-11 16:36:07  
OBNUC 13C  
EXMOD carbon.jxp  
OBERQ 100.53 MHz  
OBSET 5.35 KHz  
OBFIN 5.86 Hz  
POINT 32767  
FREQU 31407.04 Hz  
SCANS 65  
ACQTM 1.0433 sec  
PD 2.0000 sec  
PW1 3.07 usec  
IRNUC 1H  
CTEMP 22.7 c  
SLVNT CDCL3  
EXREF 77.00 ppm  
BF 1.20 Hz  
RGAIN 50

