Supporting Information

DIASTEREOSELECTIVE SYNTHESIS OF 2,4-SUBSTITUTED TETRAHYDROQUINOLINES VIA $Hf(OTf)_4$-CATALYZED SUBSTITUTION/CYCLIZATION OF 2-AMINOBENZYL ALCOHOLS WITH STYRENES

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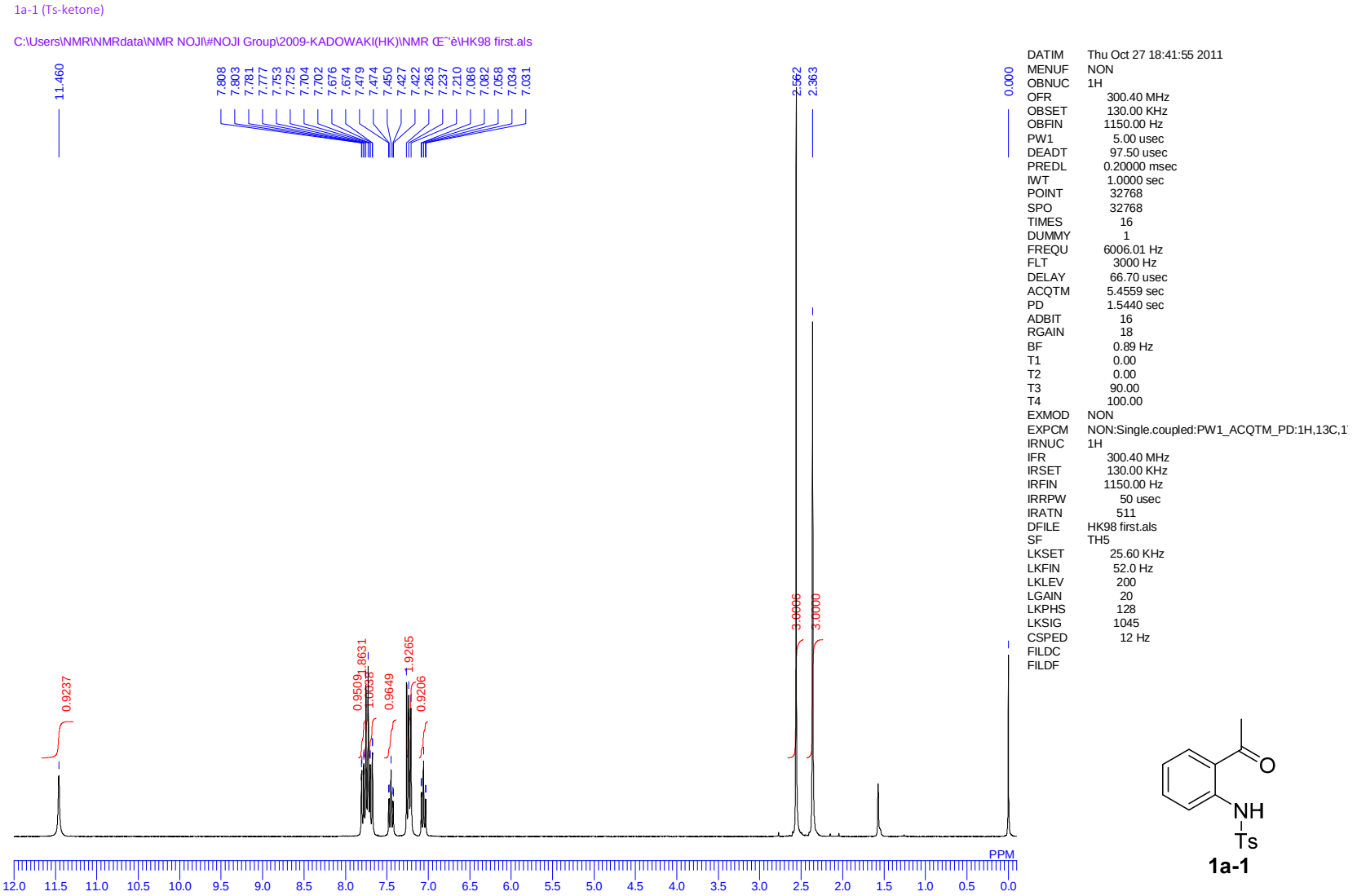
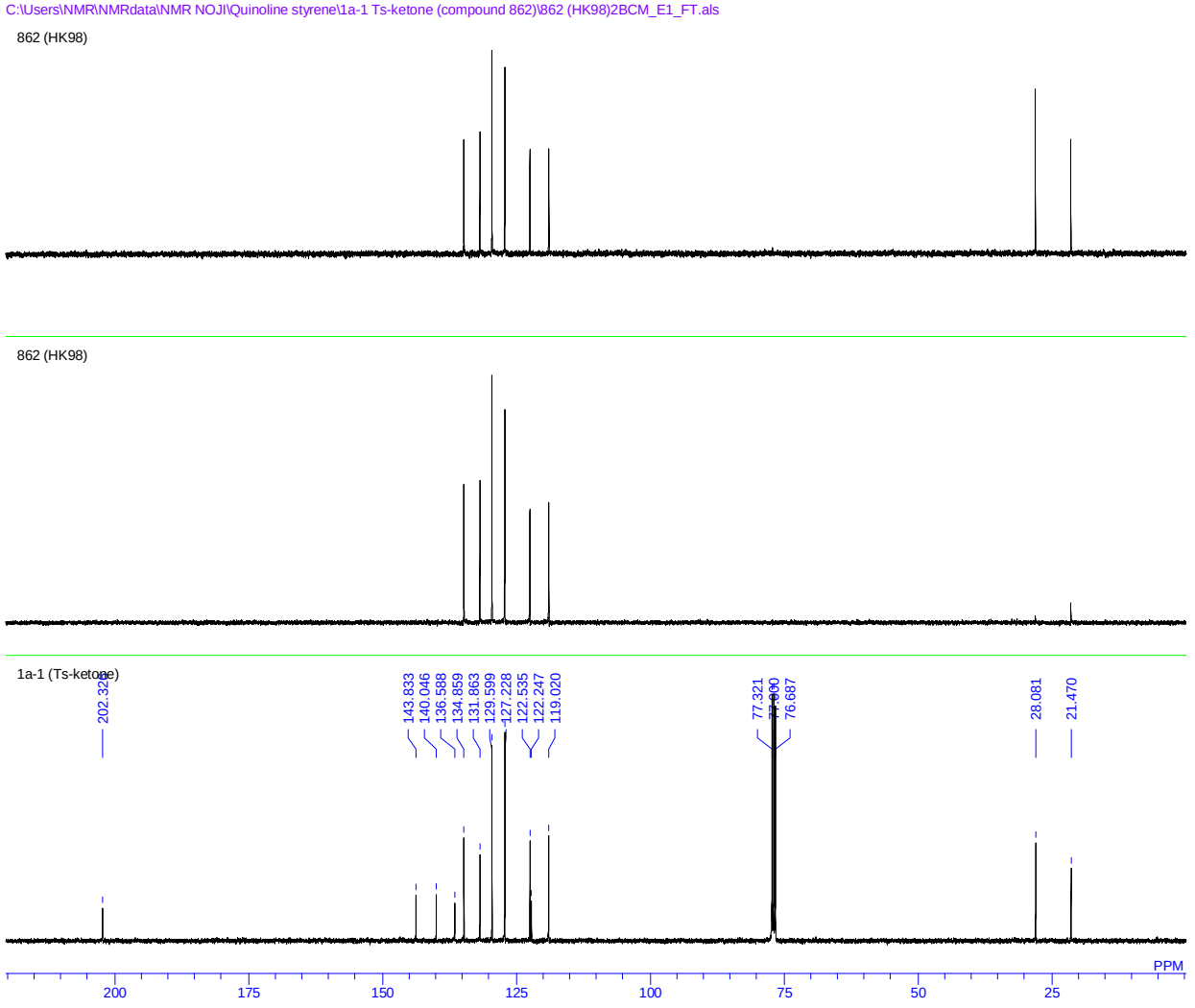
^{1}H NMR spectrum of 1a-1



^{13}C NMR spectrum of 1a-1



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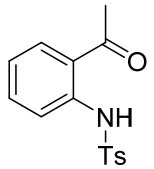
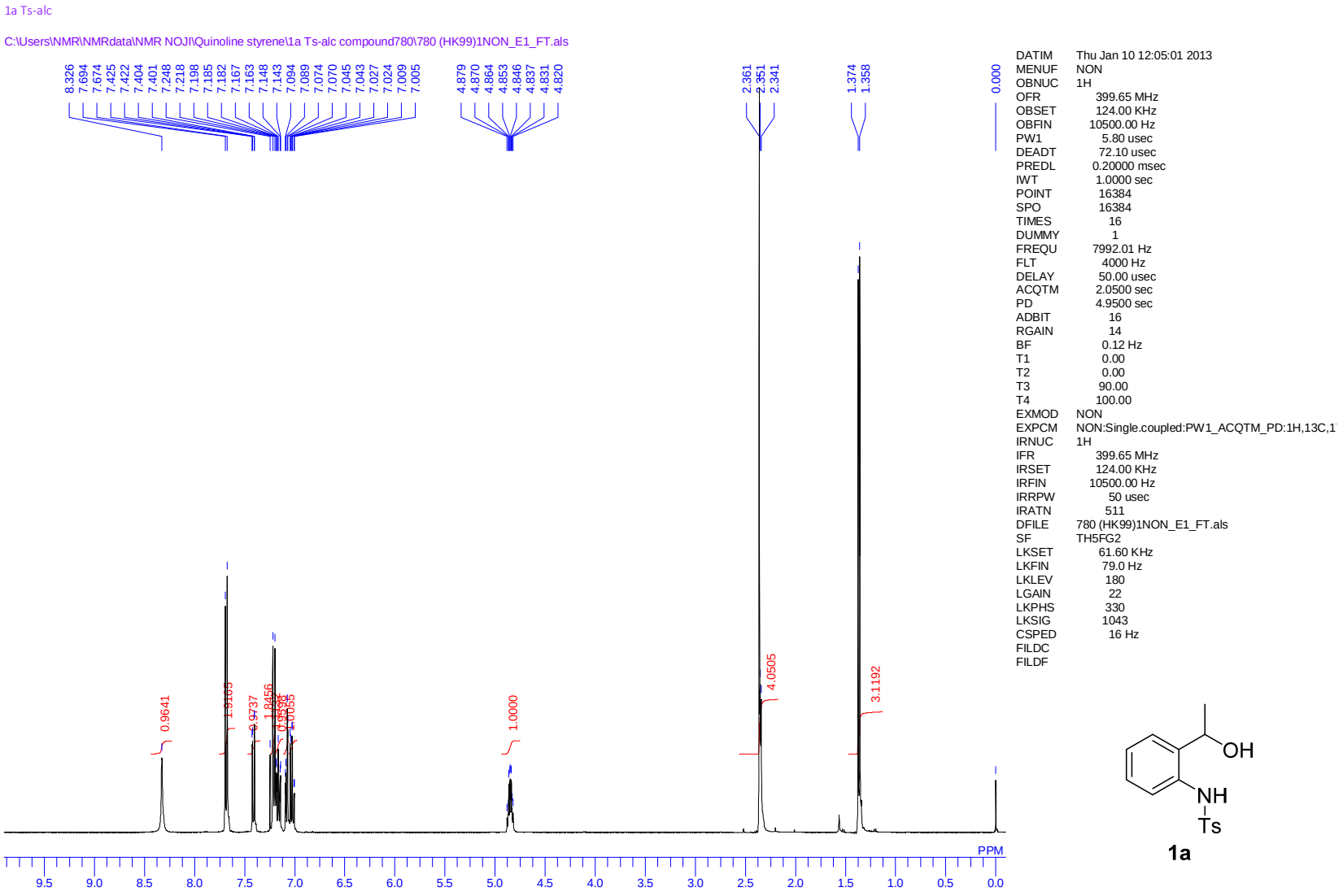
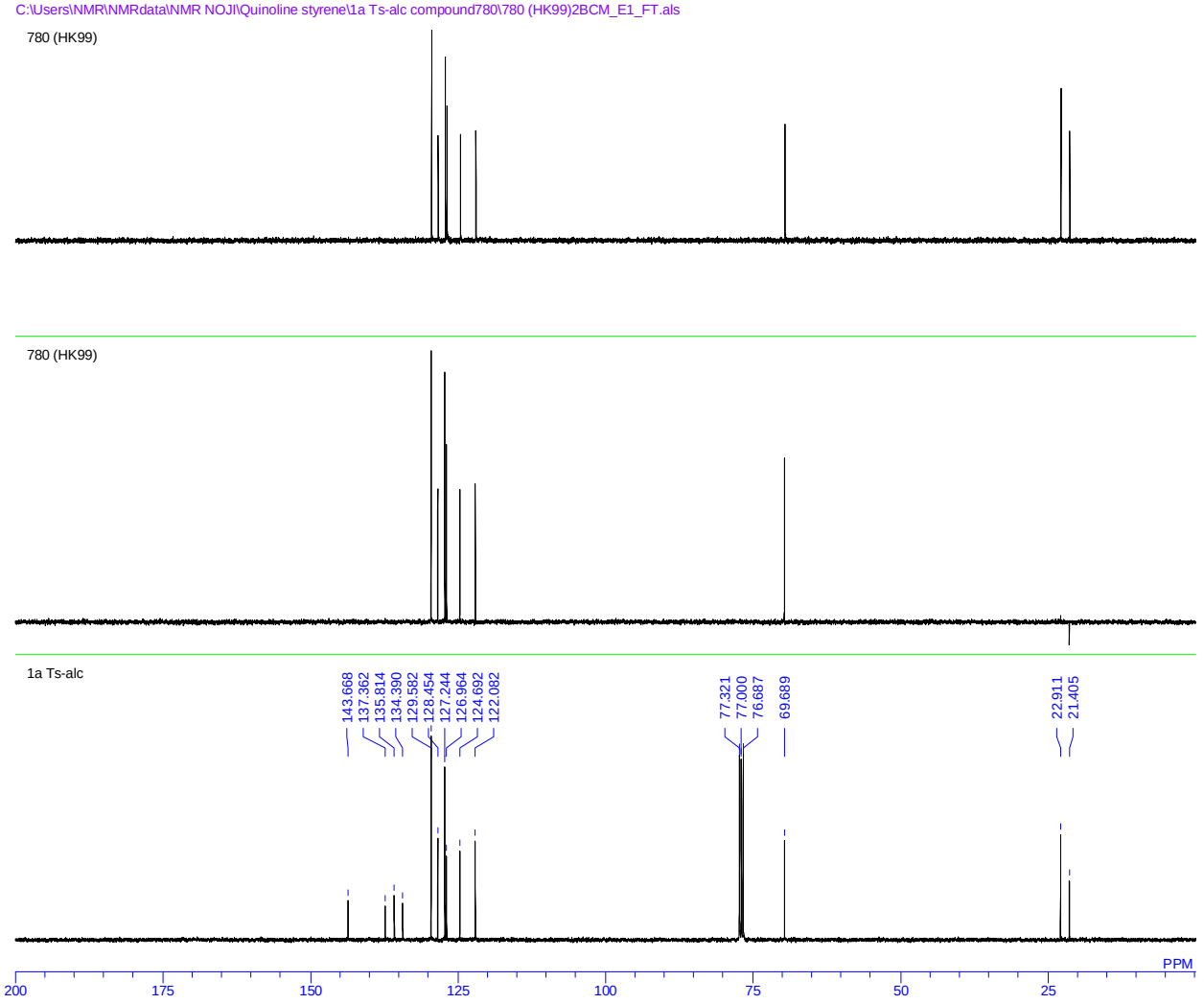


1a-1

^{1}H NMR spectrum of 1a



^{13}C NMR spectrum of 1a



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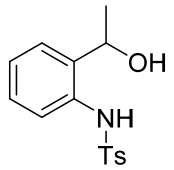
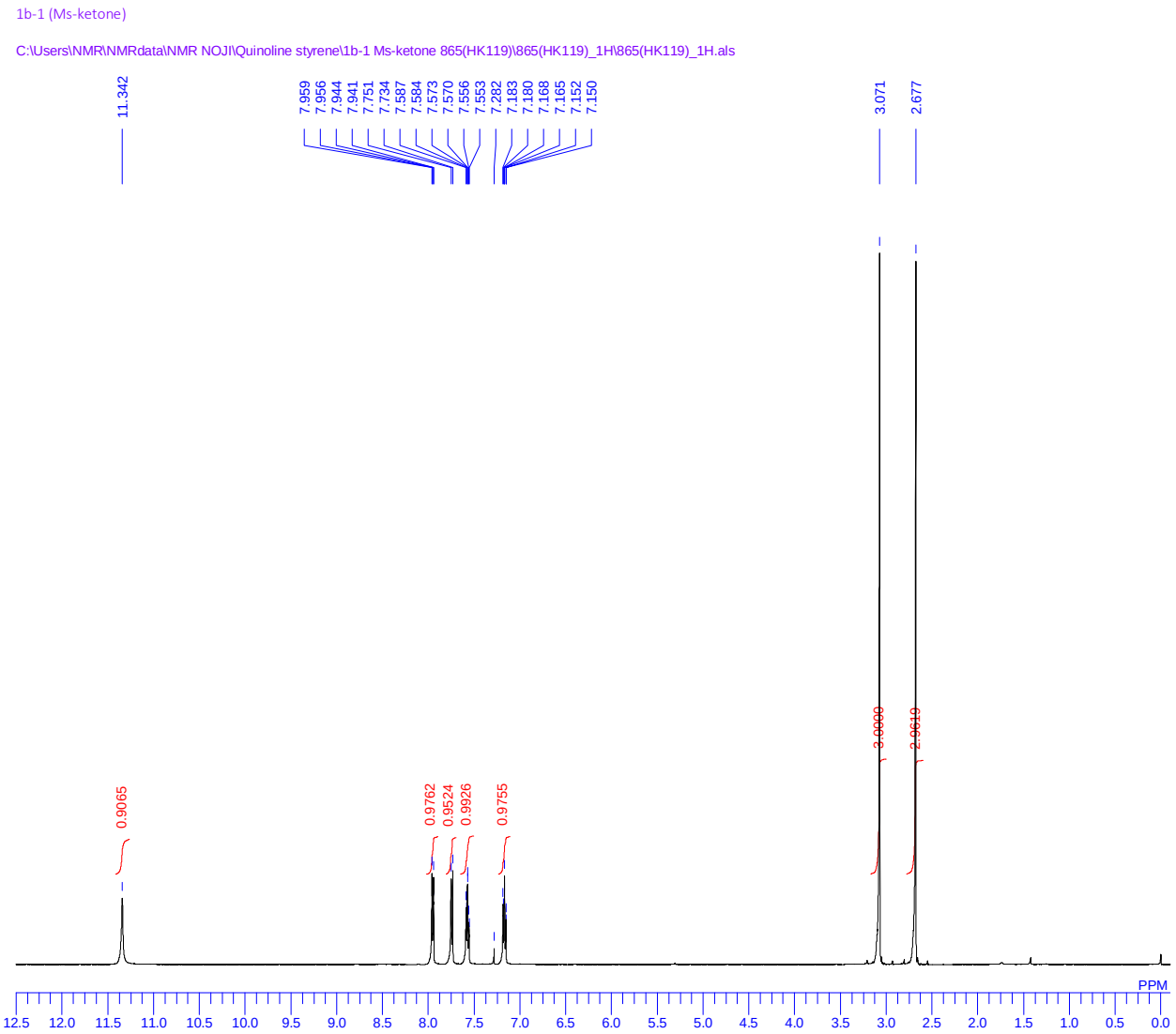


1a

^{1}H NMR spectrum of 1b-1



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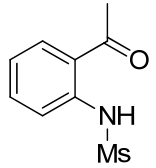
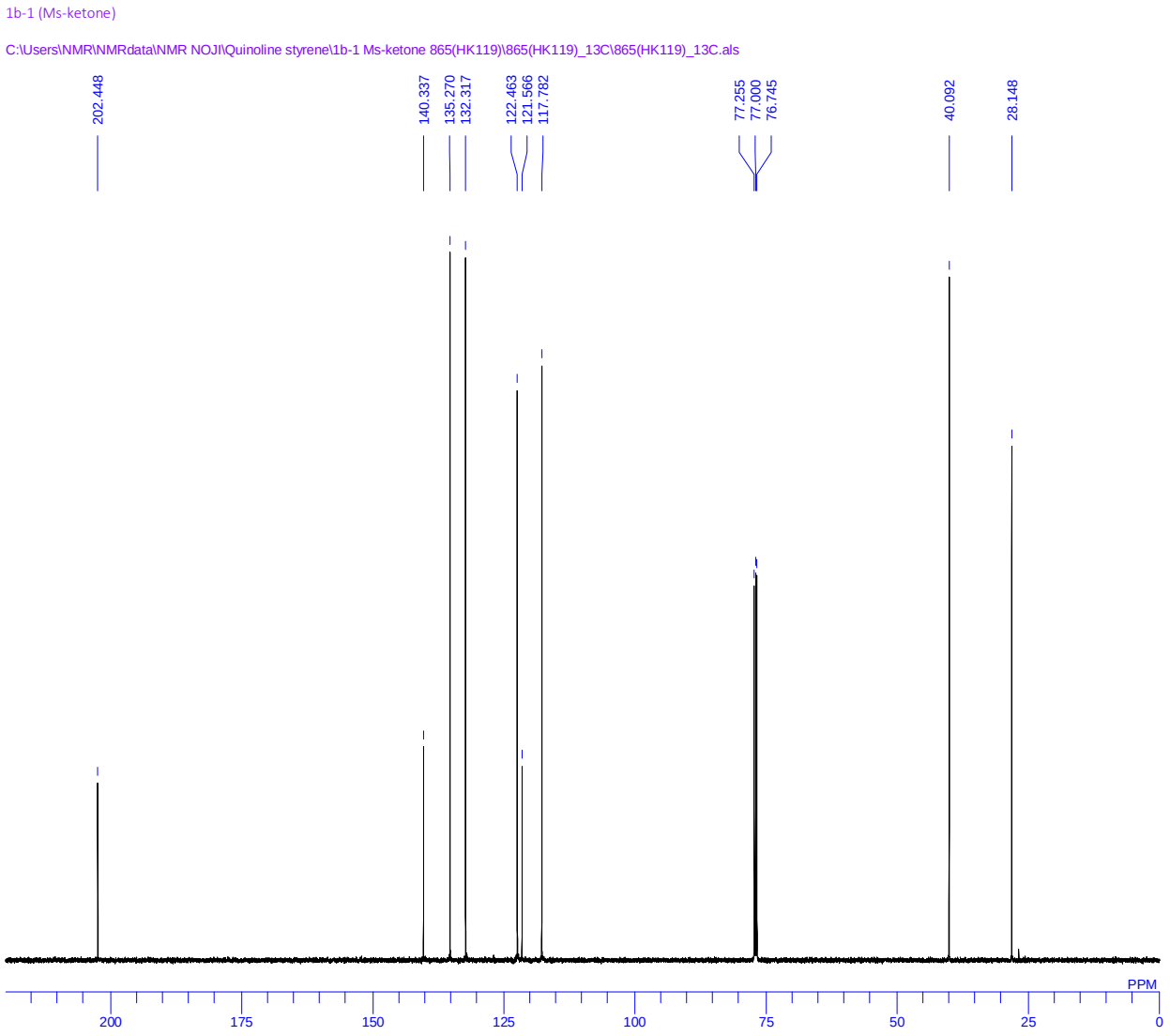


1b-1

^{13}C NMR spectrum of 1b-1



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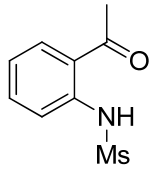
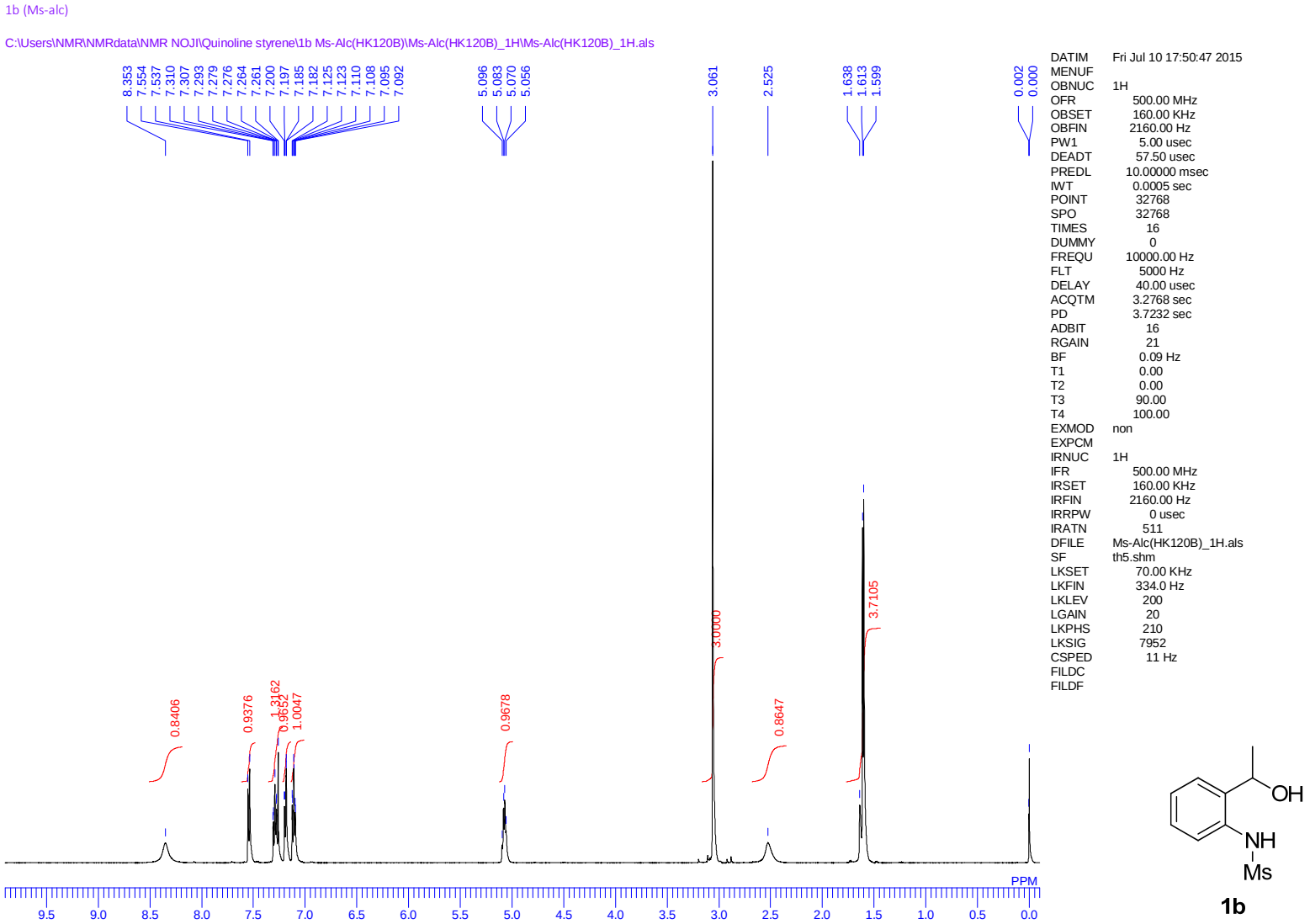
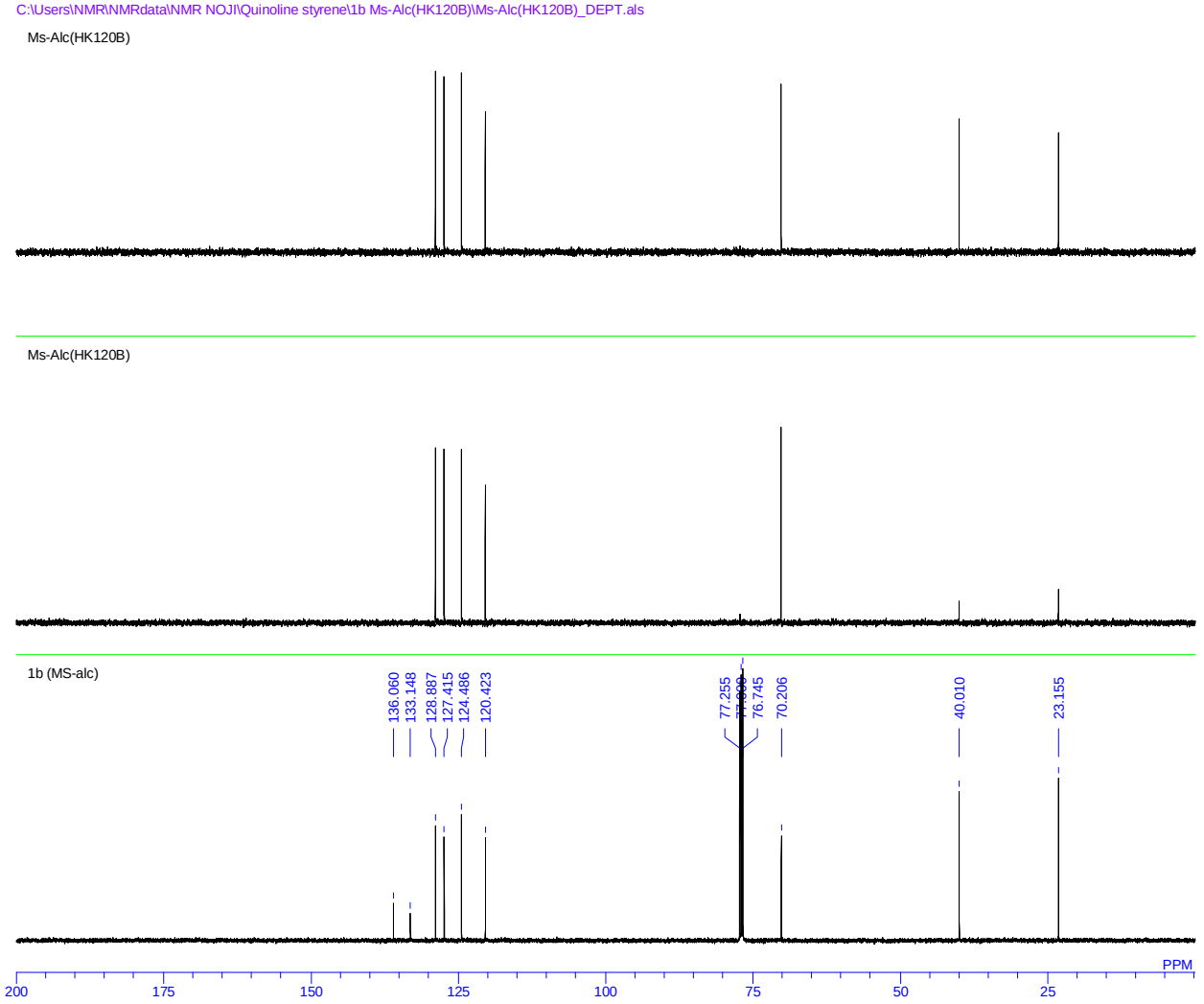


1b-1

^{1}H NMR spectrum of 1b



^{13}C NMR spectrum of 1b



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T4	100.00
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IRFIN	2160.00 Hz
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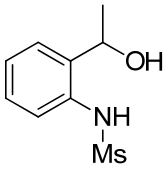
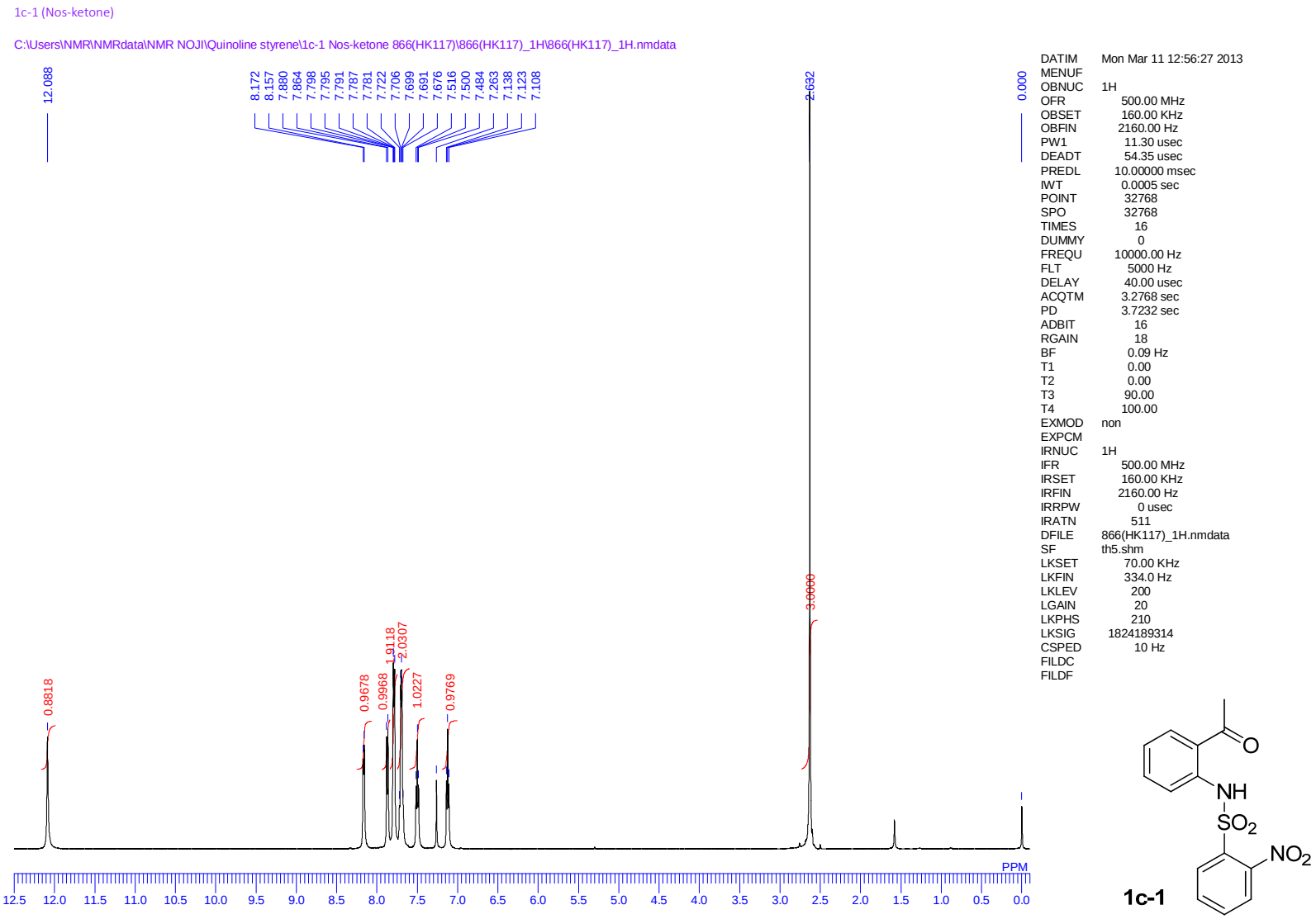
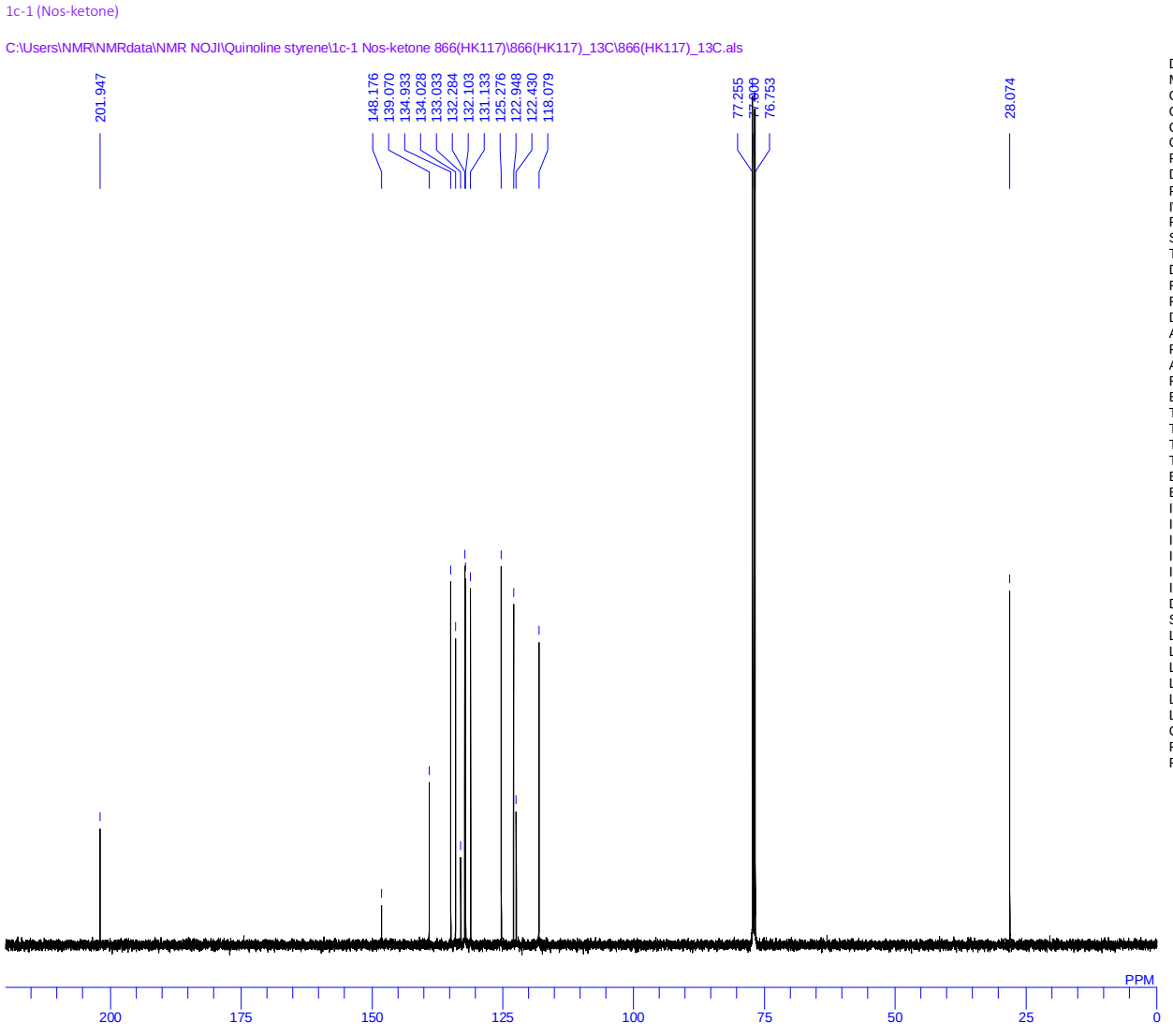


1b

^{1}H NMR spectrum of 1c-1



^{13}C NMR spectrum of 1c-1



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FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
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EXPCM	error_expcm
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IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	866(HK117)_13C.als
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LKSET	70.00 KHz
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CSPED	12 Hz
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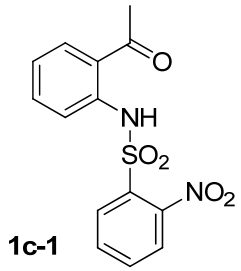
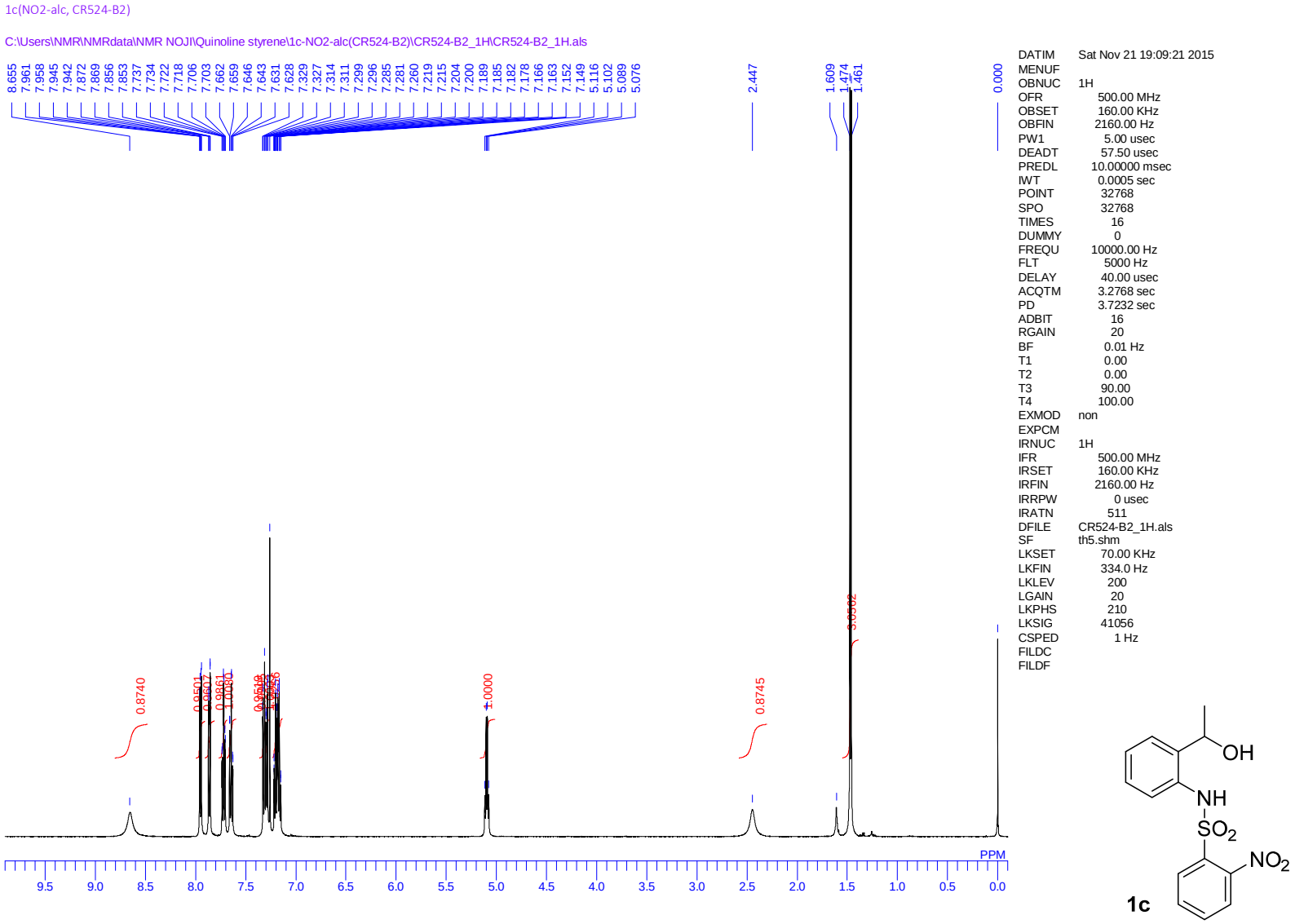
FILDF	

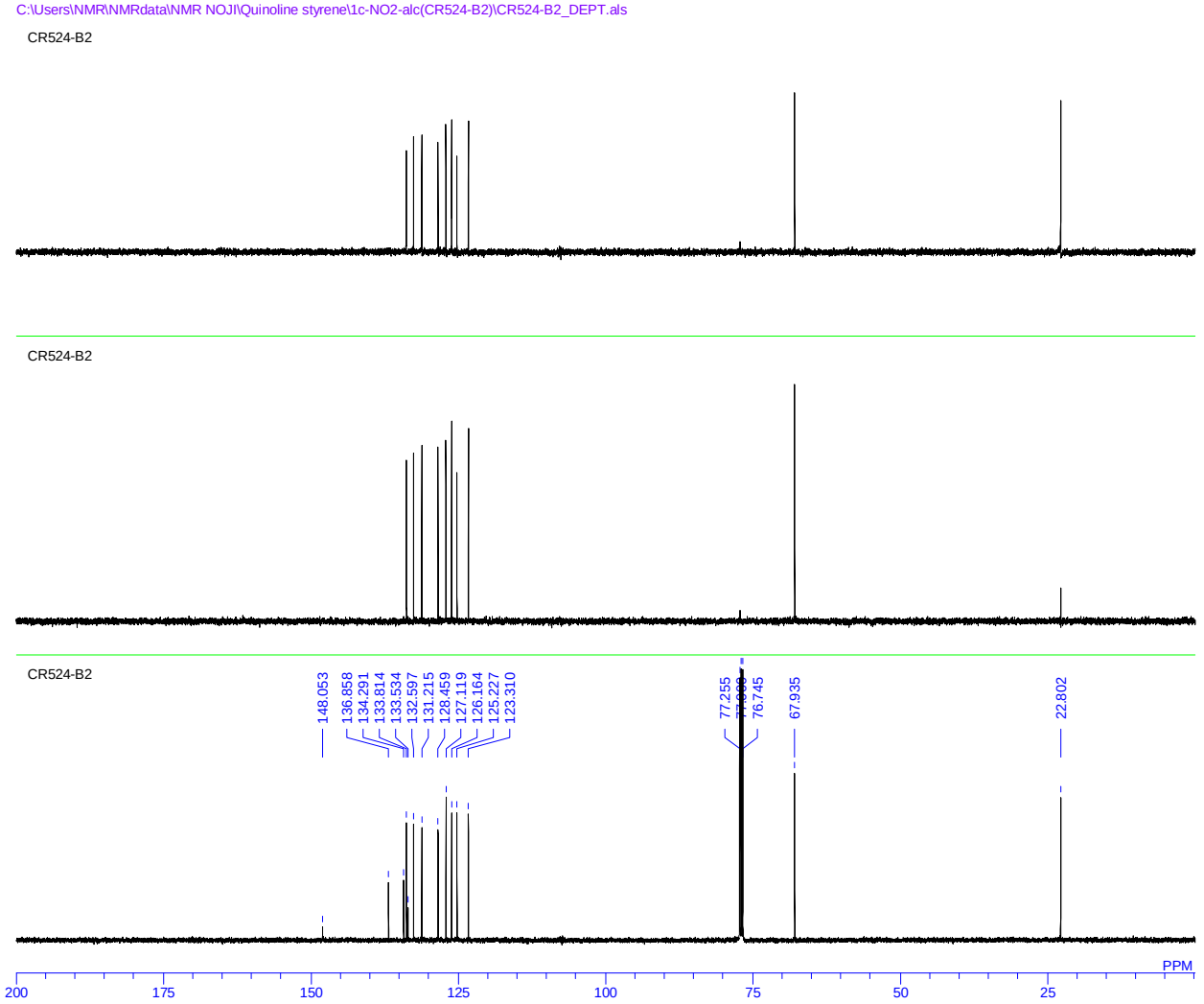


1c-1

^{1}H NMR spectrum of 1c



^{13}C NMR spectrum of 1c



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FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
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T2	0.00
T3	90.00
T4	100.00
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EXPCM	error_expcm
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IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
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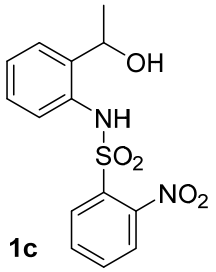
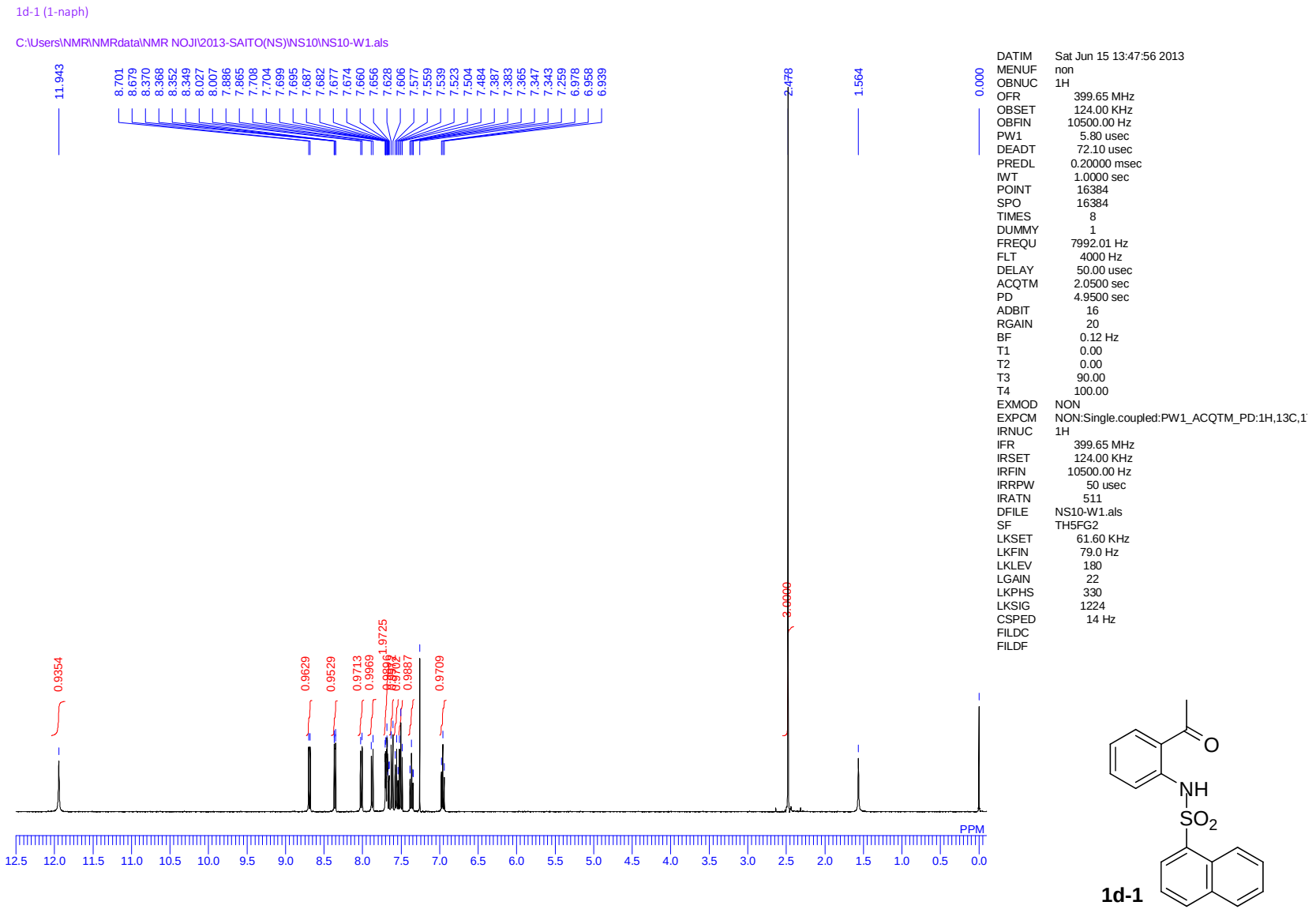
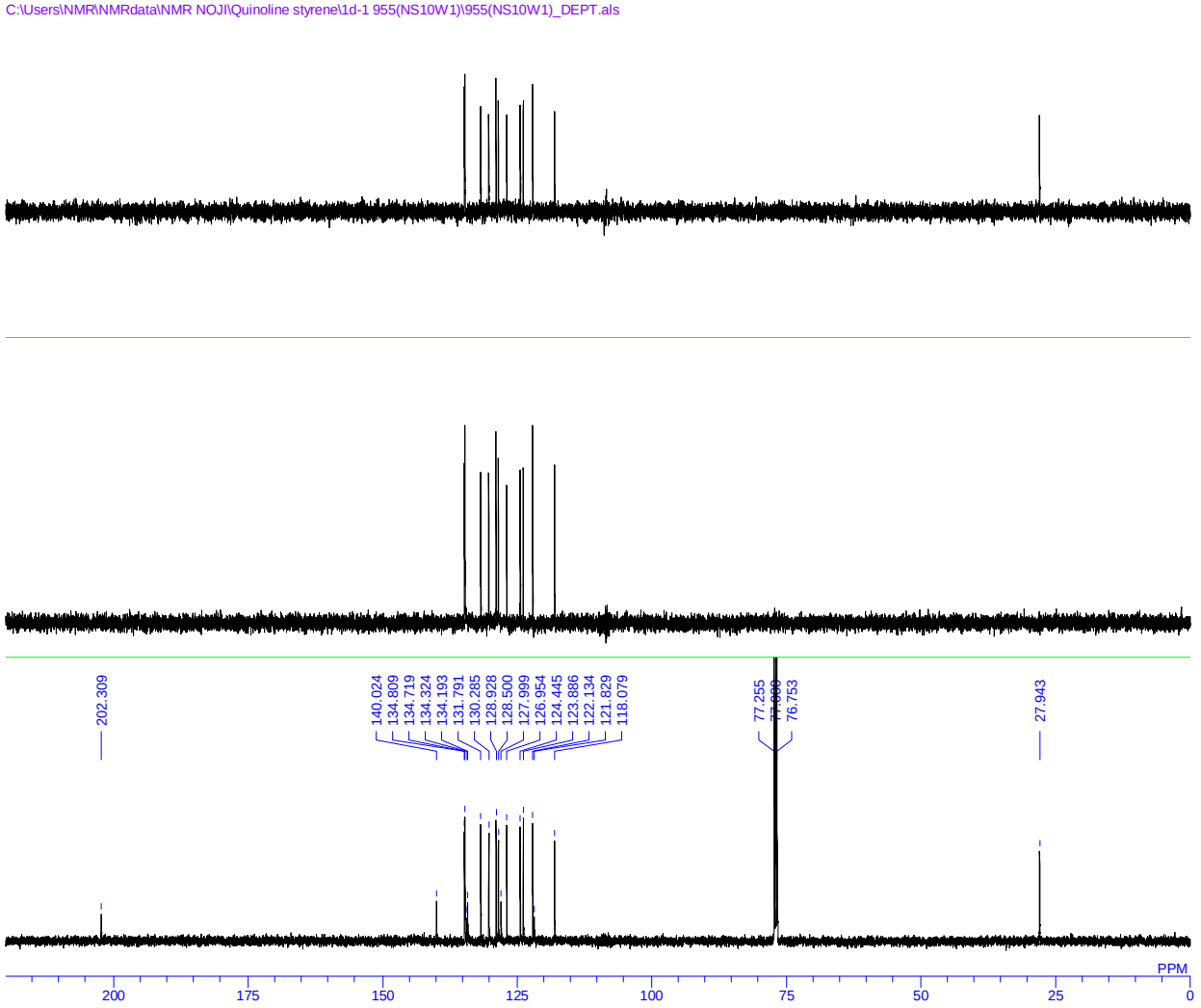


1c

^{1}H NMR spectrum of 1d-1



^{13}C NMR spectrum of 1d-1



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FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	0.12 Hz
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T2	0.00
T3	90.00
T4	100.00
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EXPCM	error_expcm
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IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
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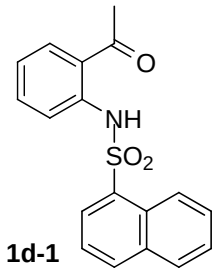
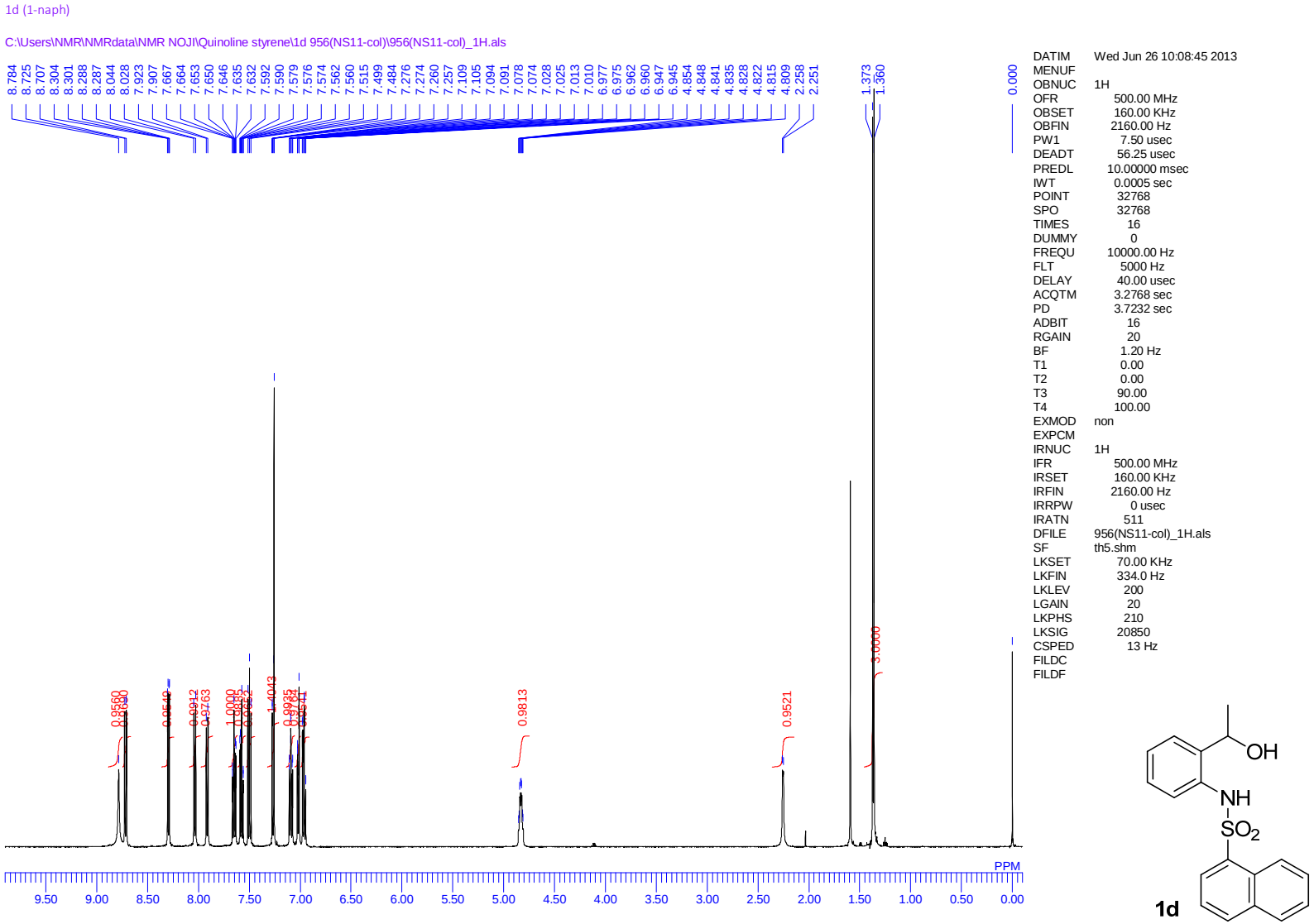
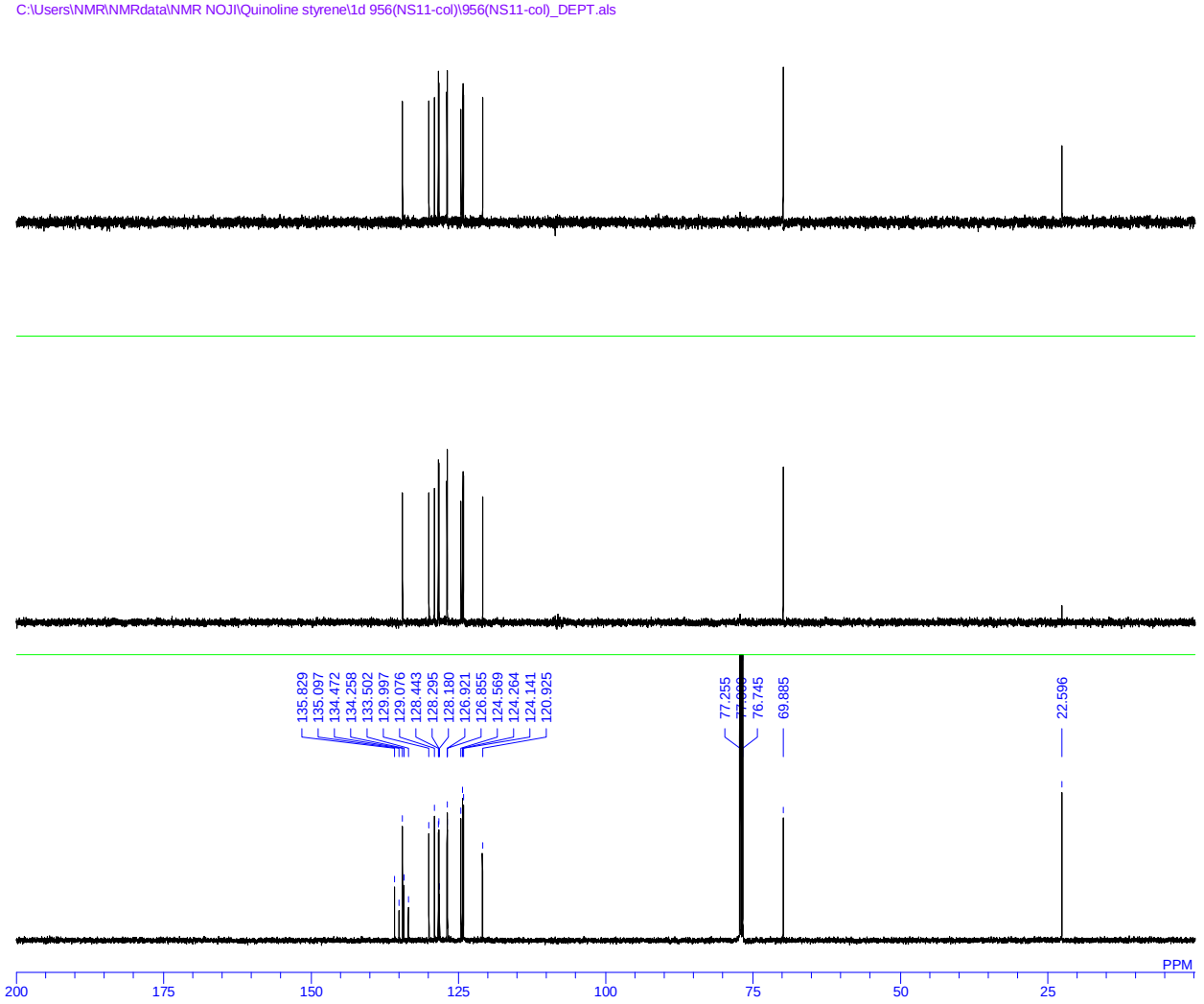


1d-1

^{1}H NMR spectrum of 1d



^{13}C NMR spectrum of 1d



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POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
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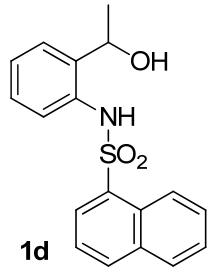
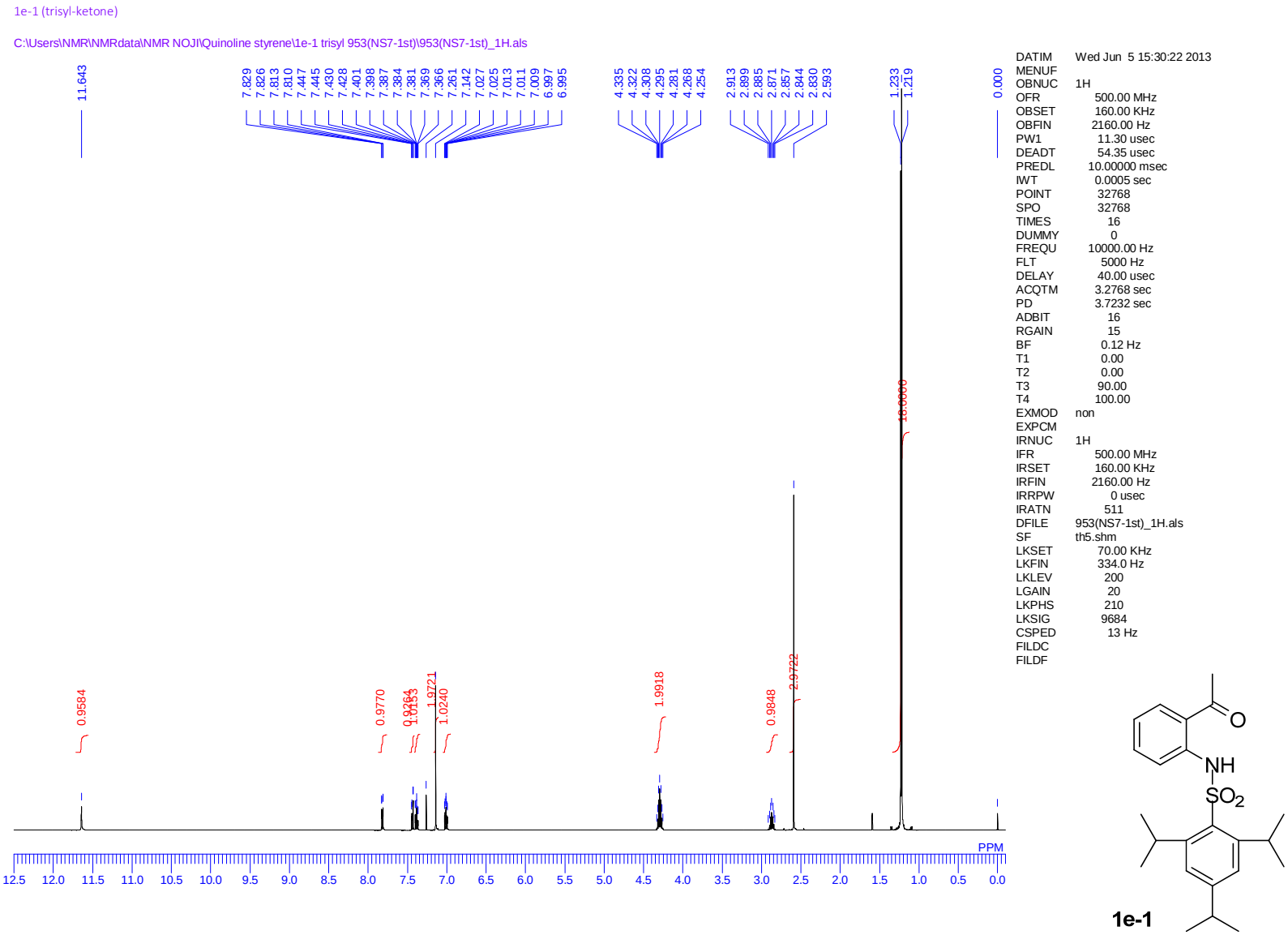
FILDF	

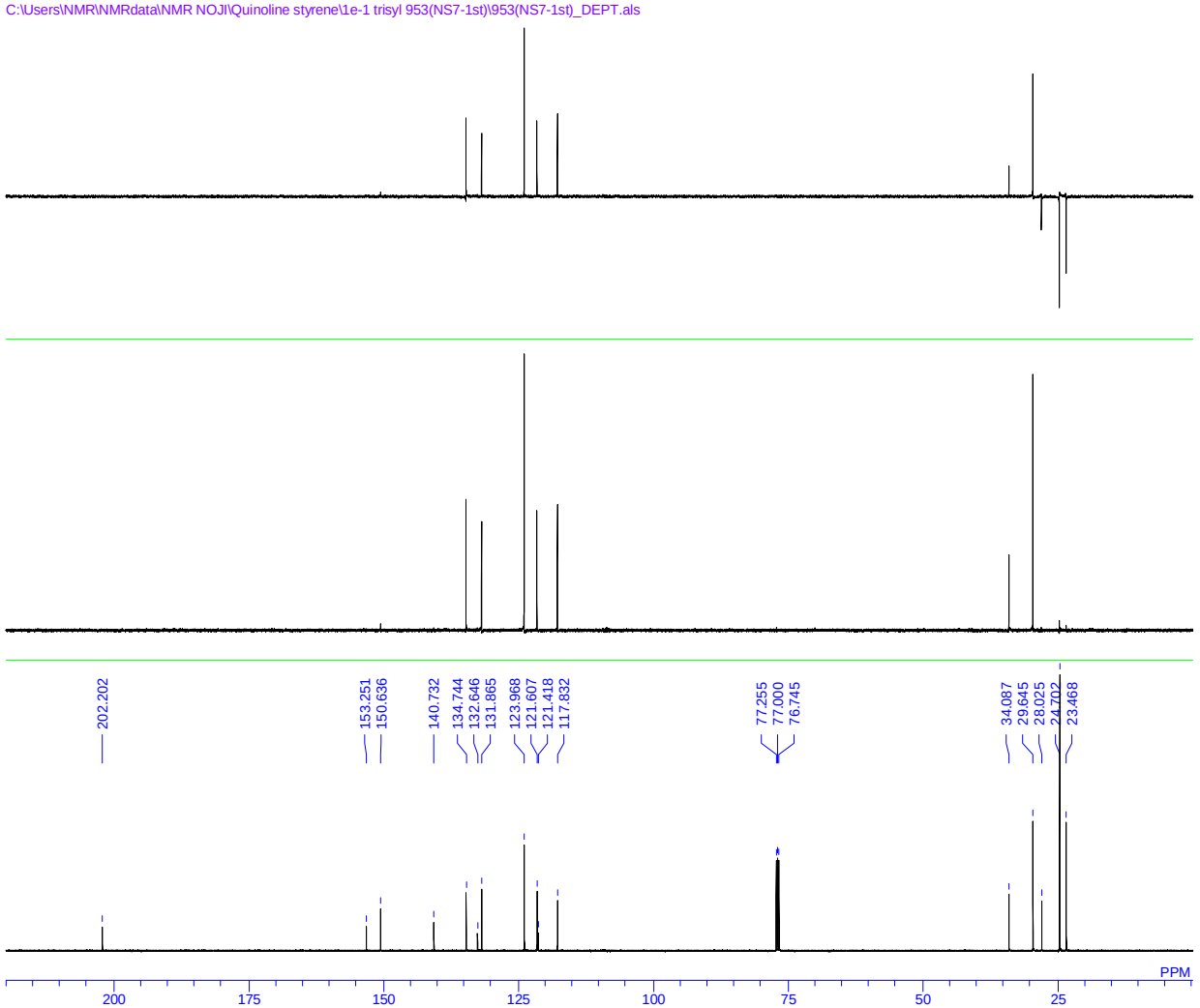


1d

^{1}H NMR spectrum of 1e-1



^{13}C NMR spectrum of 1e-1



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IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
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ADBIT	16
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EXPCM	error_expcm
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IRRPW	0 usec
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SF	th5.shm
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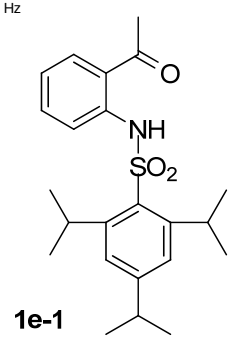
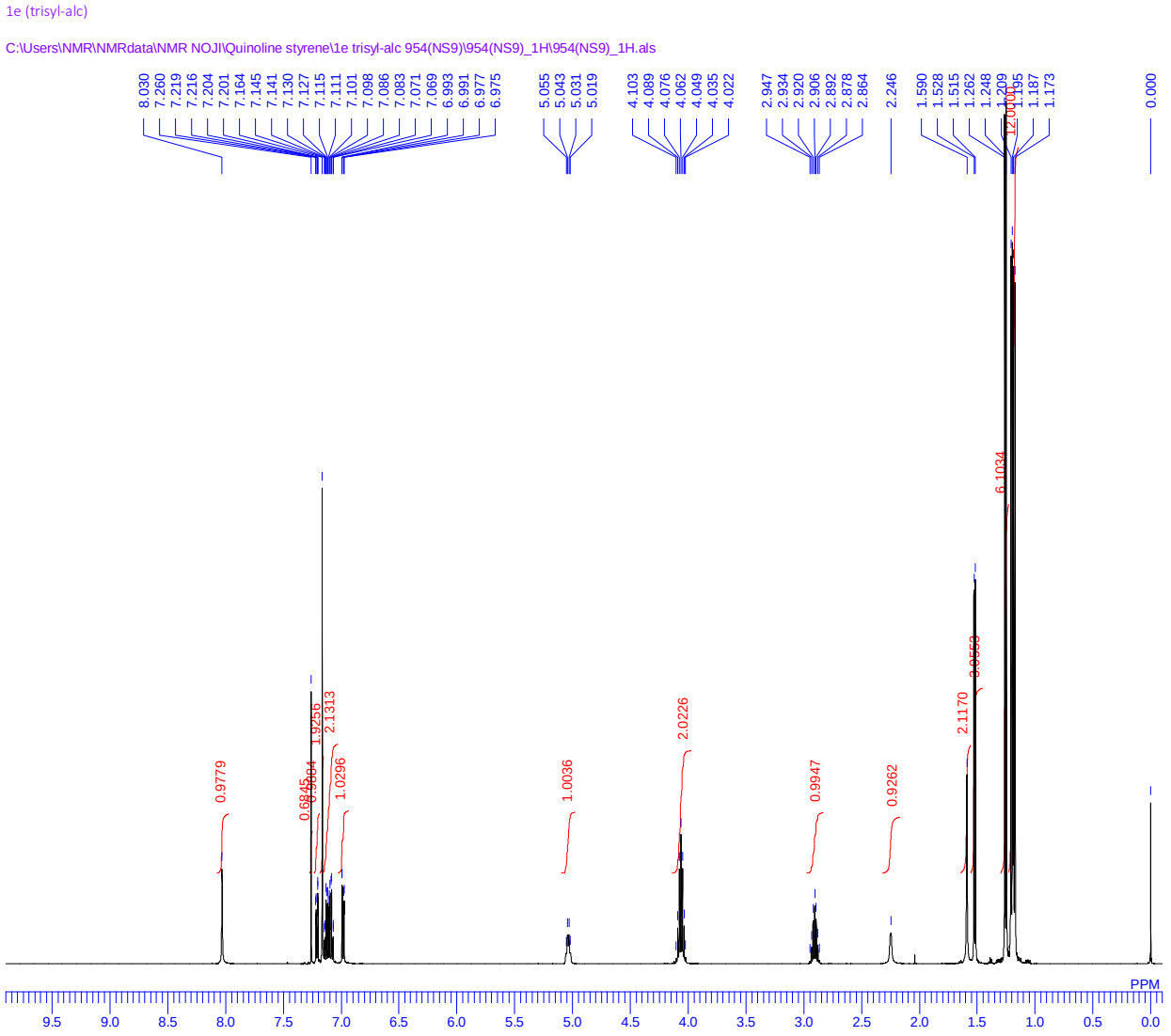


1e-1

^{1}H NMR spectrum of 1e



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IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	18
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	954(NS9)_1H.als
SF	th5.shm
LKSET	70.00 KHz
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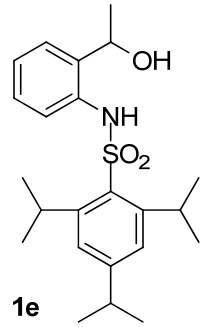
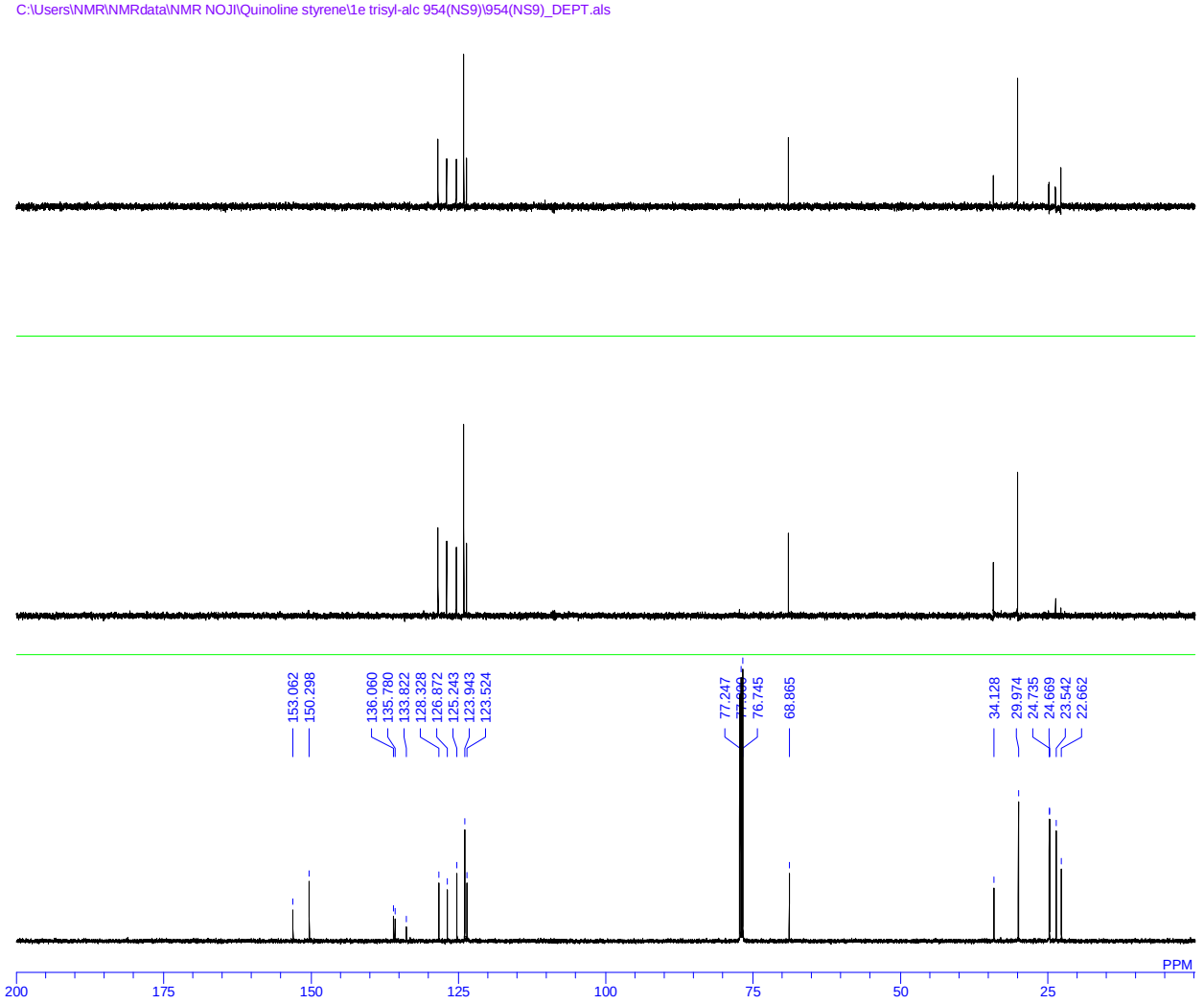
LKPHS	210
LKSIG	58664
CSPED	13 Hz
FILDC	
FILDF	



1e

^{13}C NMR spectrum of 1e



DATIM	Sat Jun 15 12:24:28 2013
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	8.50 usec
DEADT	10.00 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
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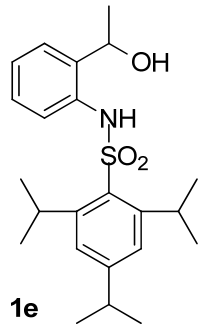
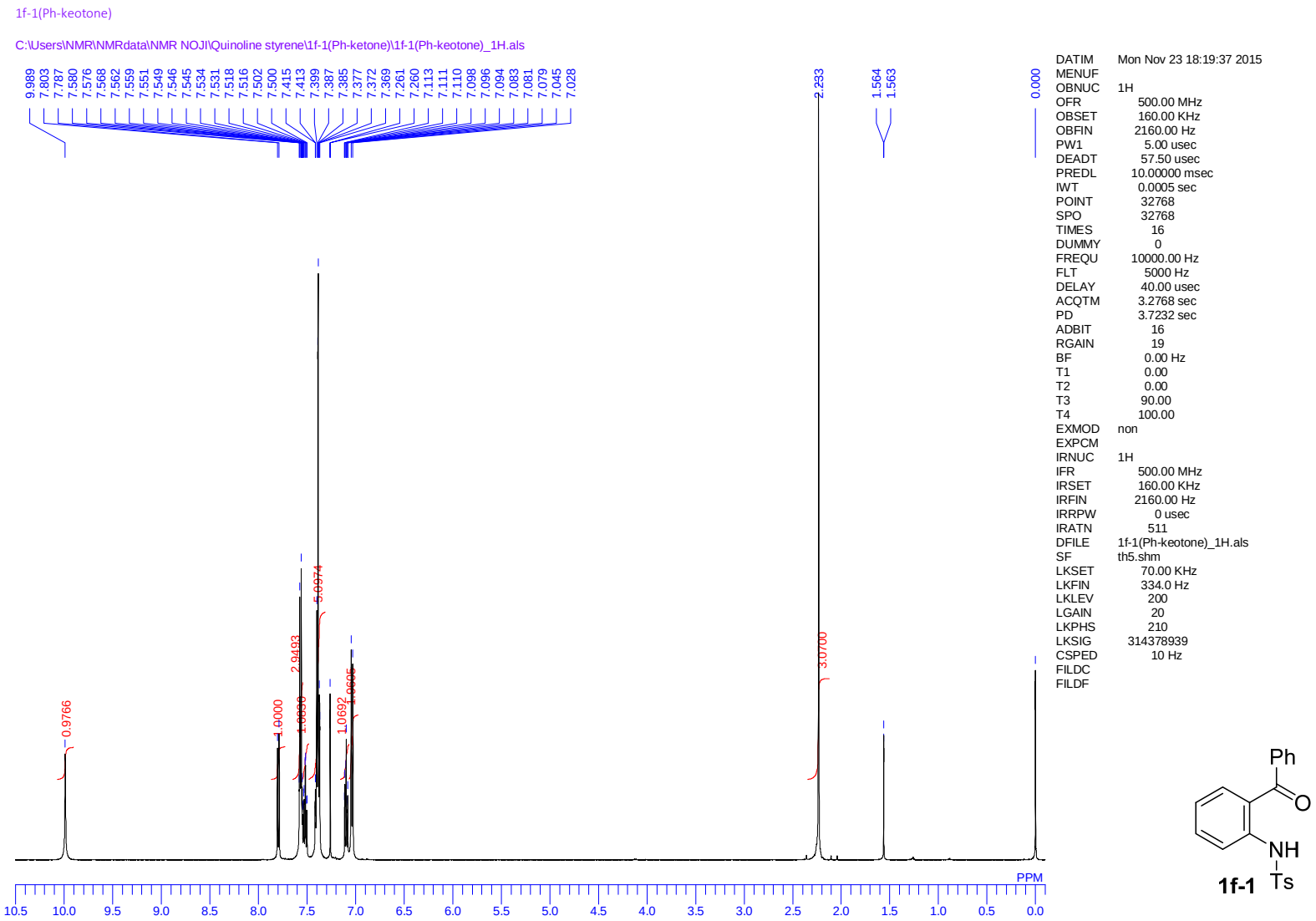
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	25292
CSPED	12 Hz
FILDC	
FILDF	

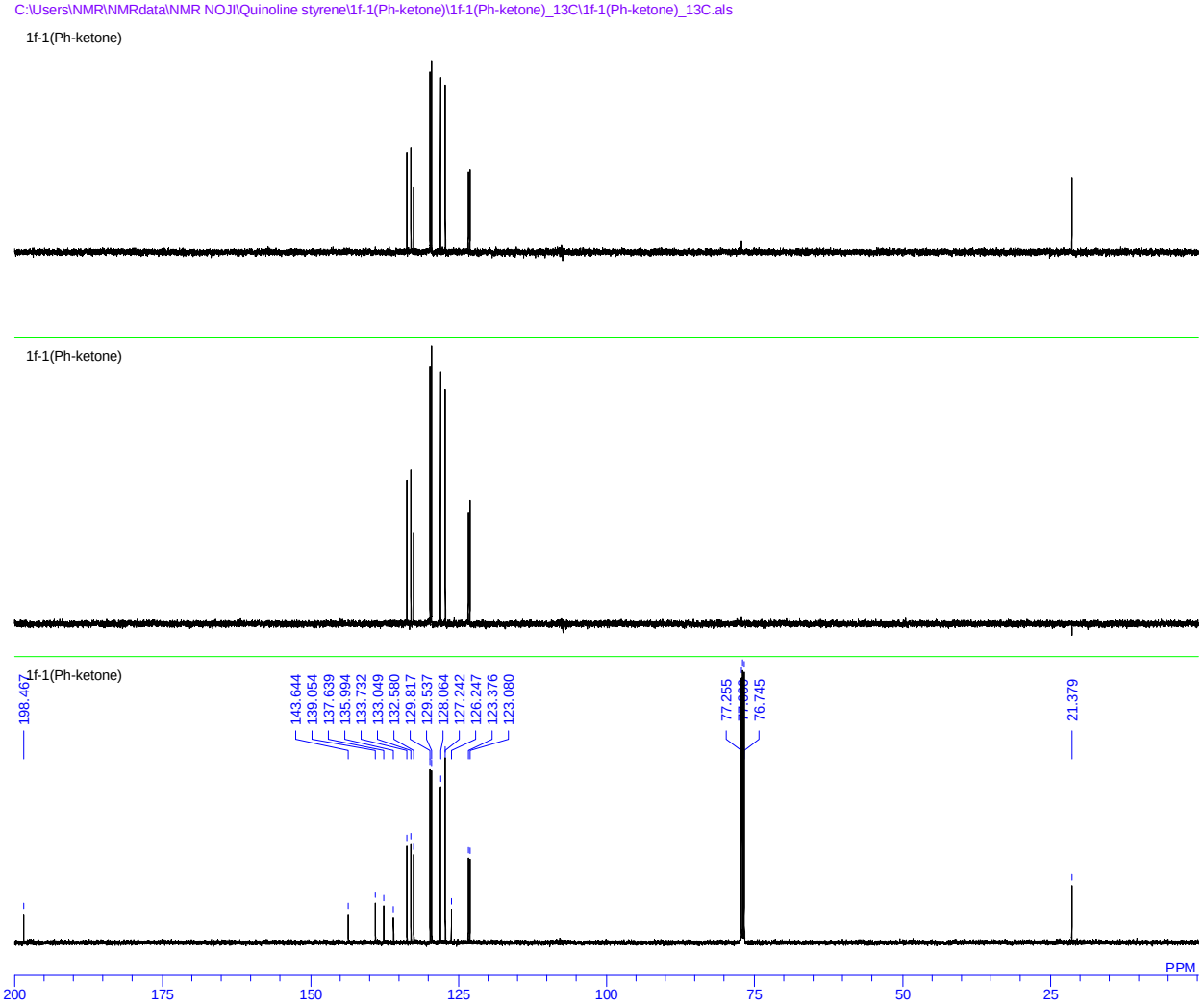


1e

^{1}H NMR spectrum of 1f-1



^{13}C NMR spectrum of 1f-1



DATIM	Mon Nov 23 19:12:05 2015
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OBNUC	13C
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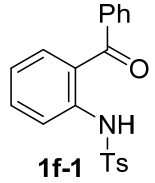
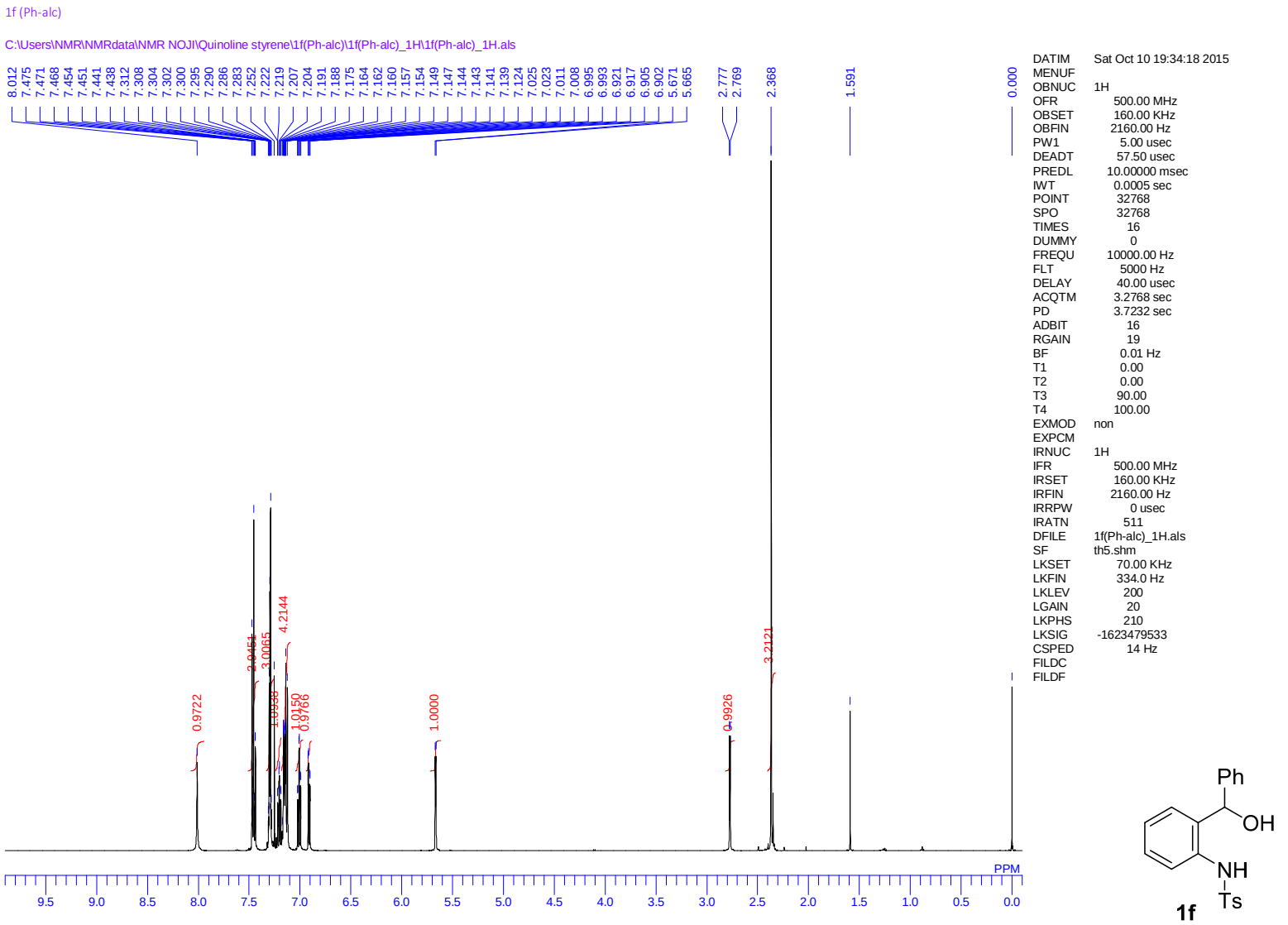
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.00 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	1f-1(Ph-ketone)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	1211945838
CSPED	12 Hz
FILDC	
FILDF	

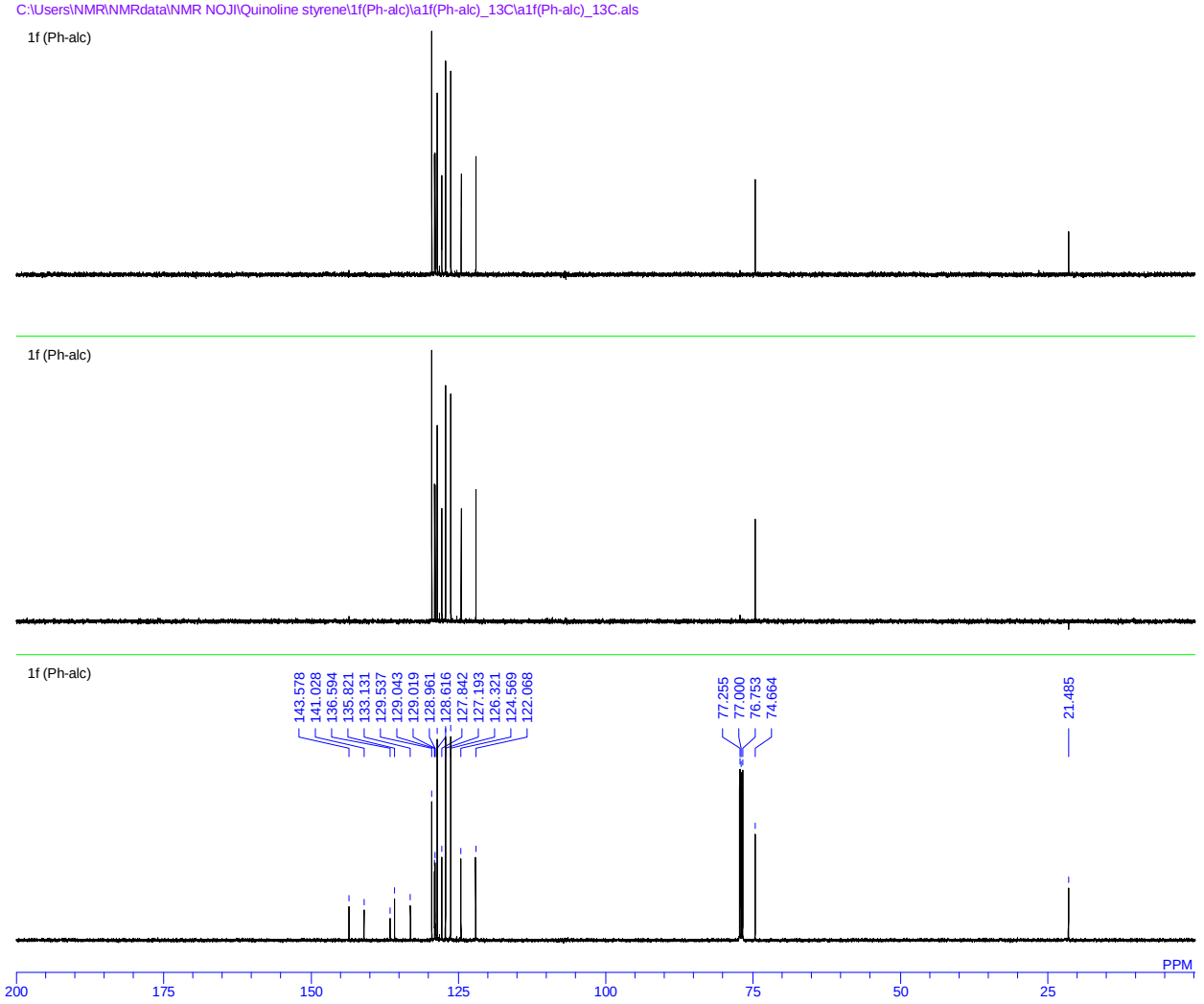


1f-1

^{1}H NMR spectrum of 1f



^{13}C NMR spectrum of 1f



DATIM	Sat Oct 10 20:15:38 2015
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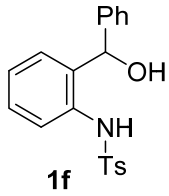
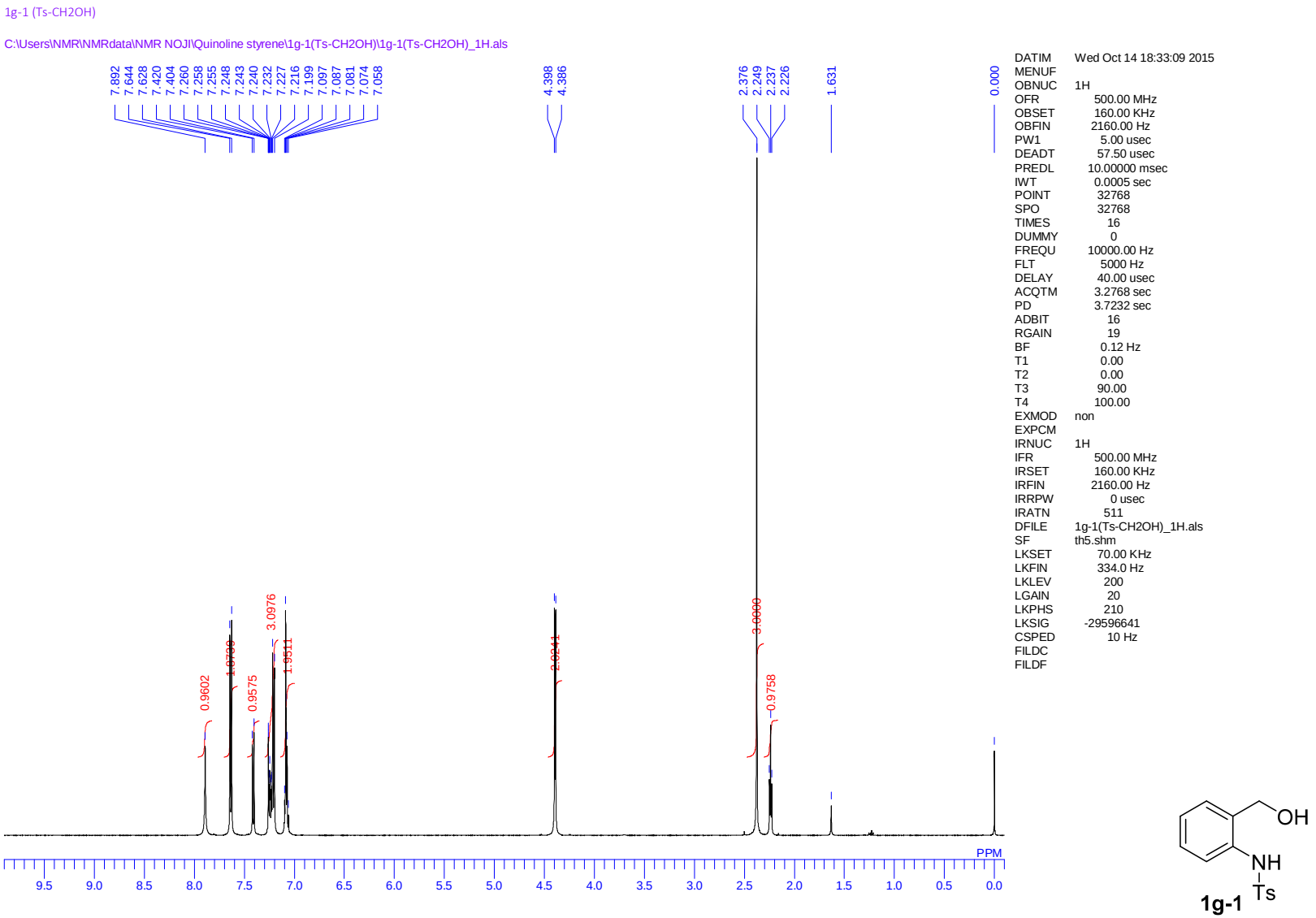
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.01 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	a1f(Ph-alc)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-776128229
CSPED	12 Hz
FILDC	
FILDF	

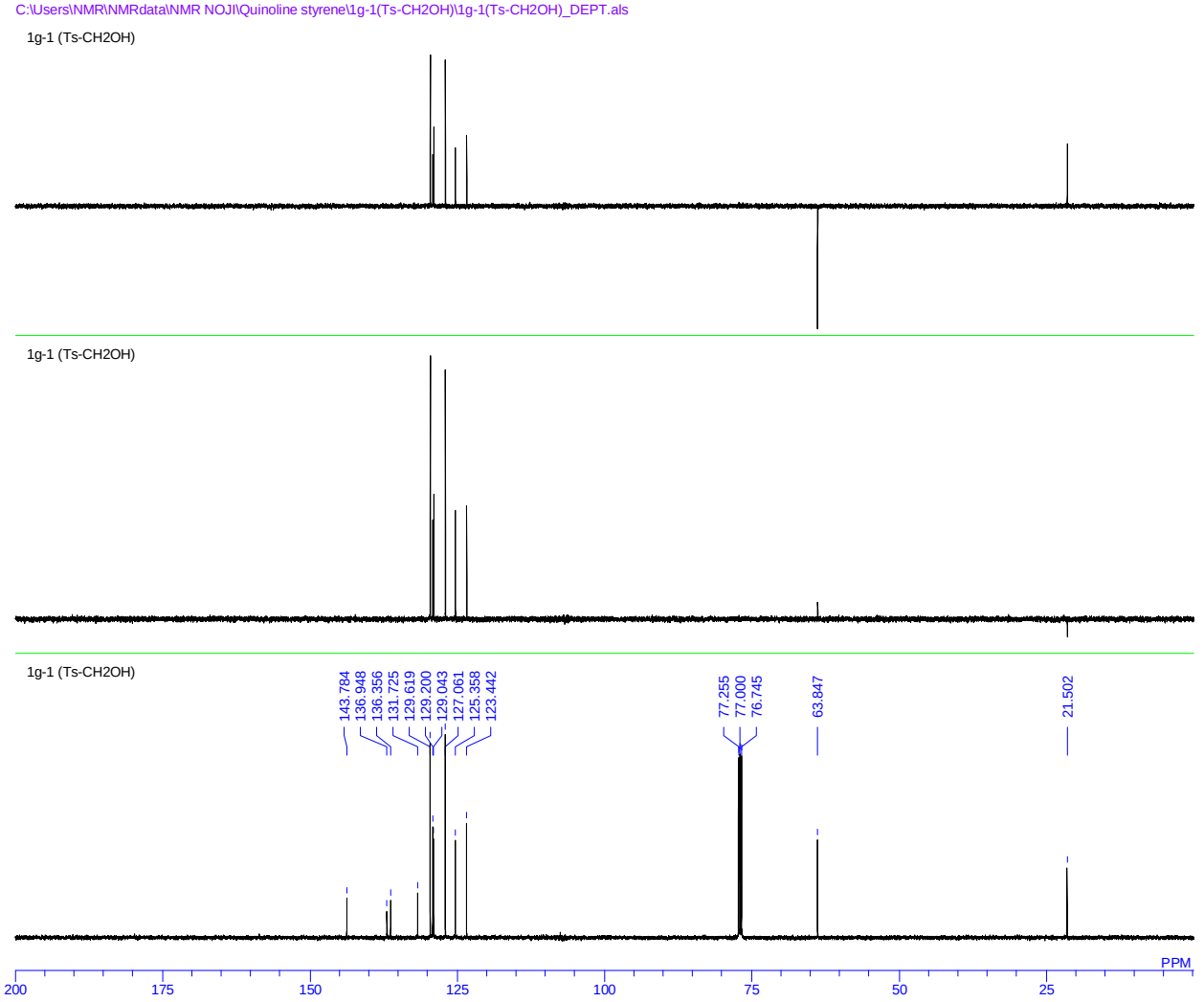


1f

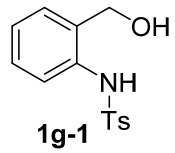
^{1}H NMR spectrum of 1g-1



^{13}C NMR spectrum of 1g-1

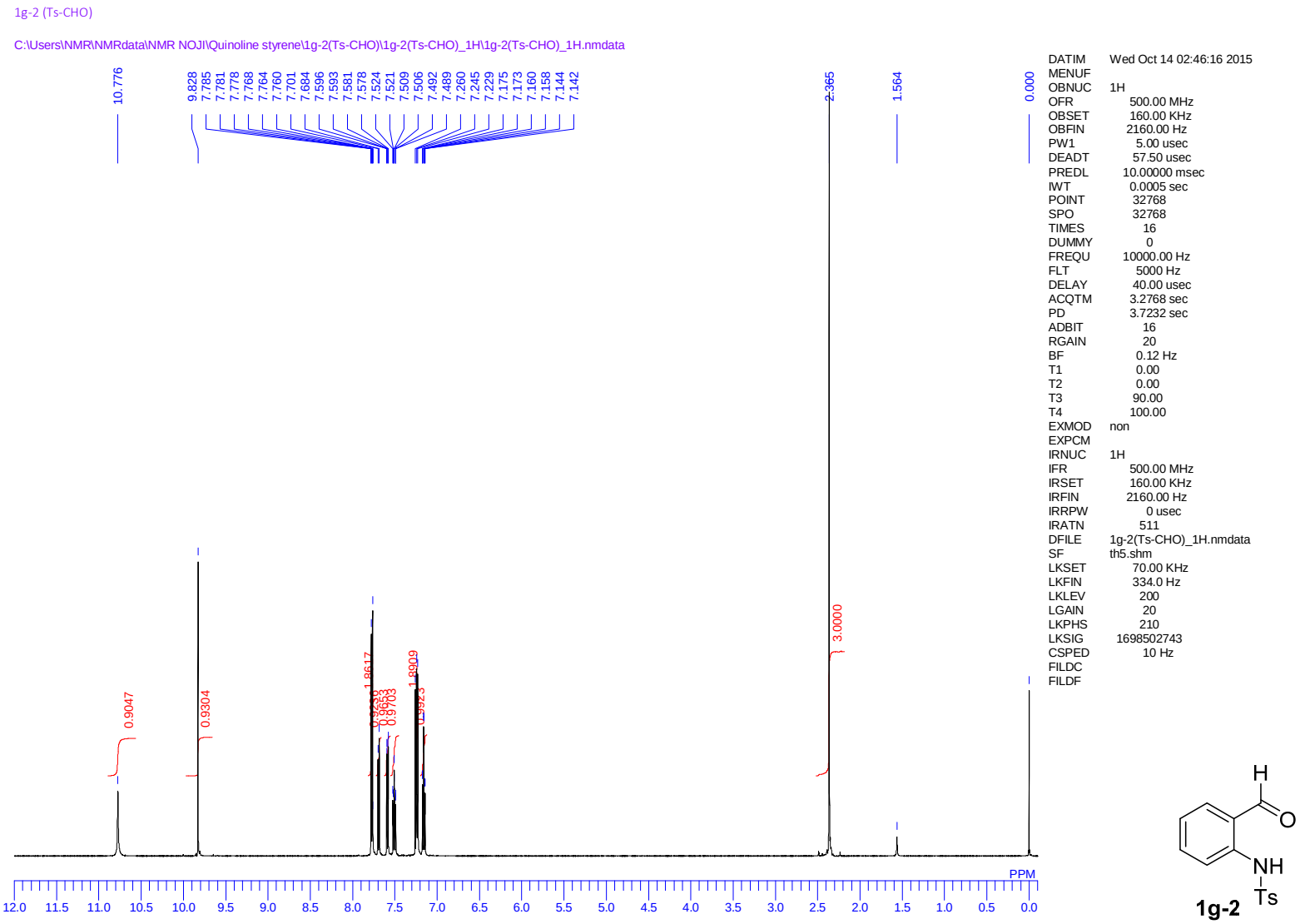


DATIM	Wed Oct 14 19:14:28 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	1g-1(Ts-CH2OH)_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-1287805795
CSPED	12 Hz
FILDC	
FILDF	

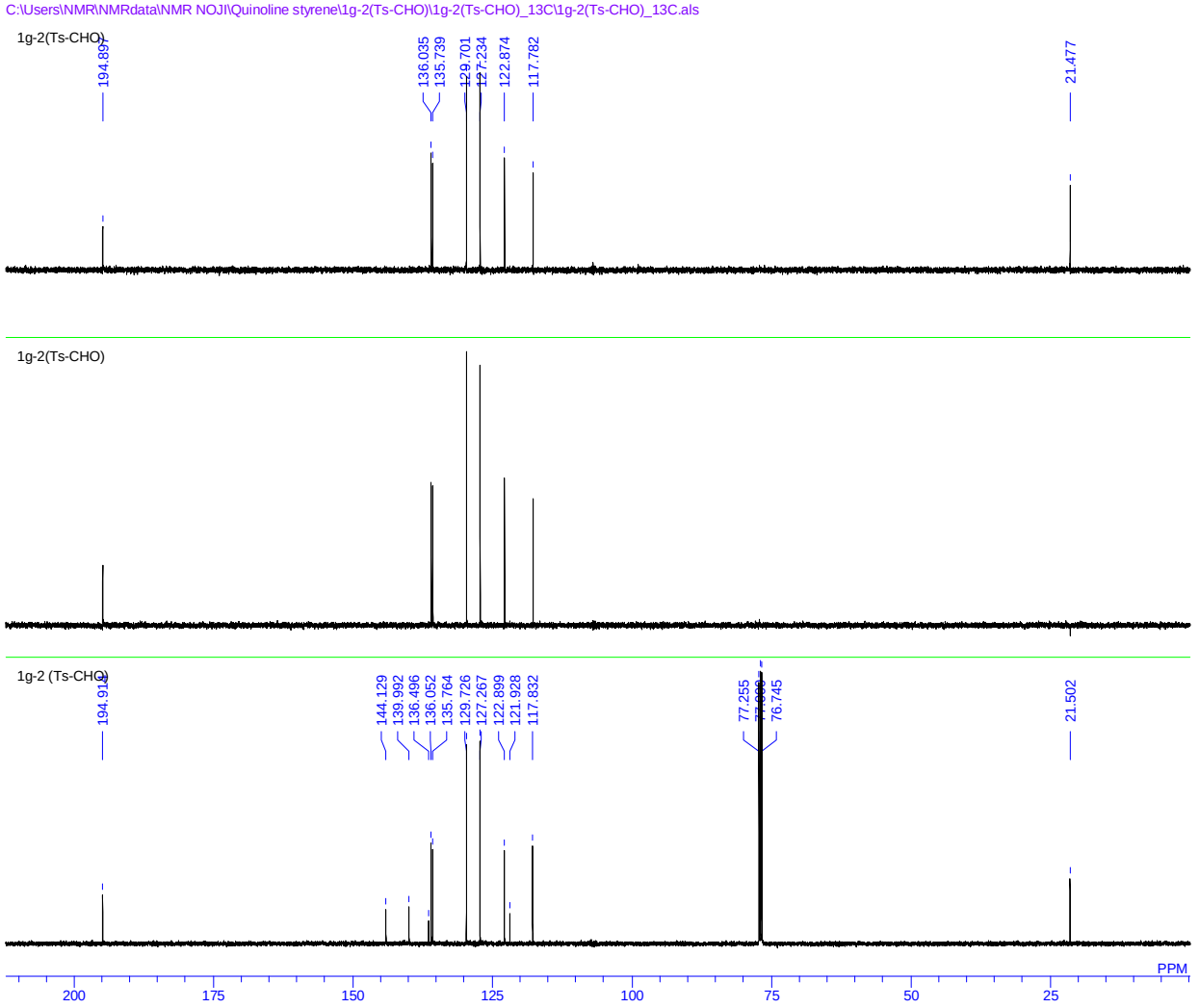


1g-1

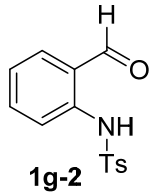
^{1}H NMR spectrum of 1g-2



^{13}C NMR spectrum of 1g-2

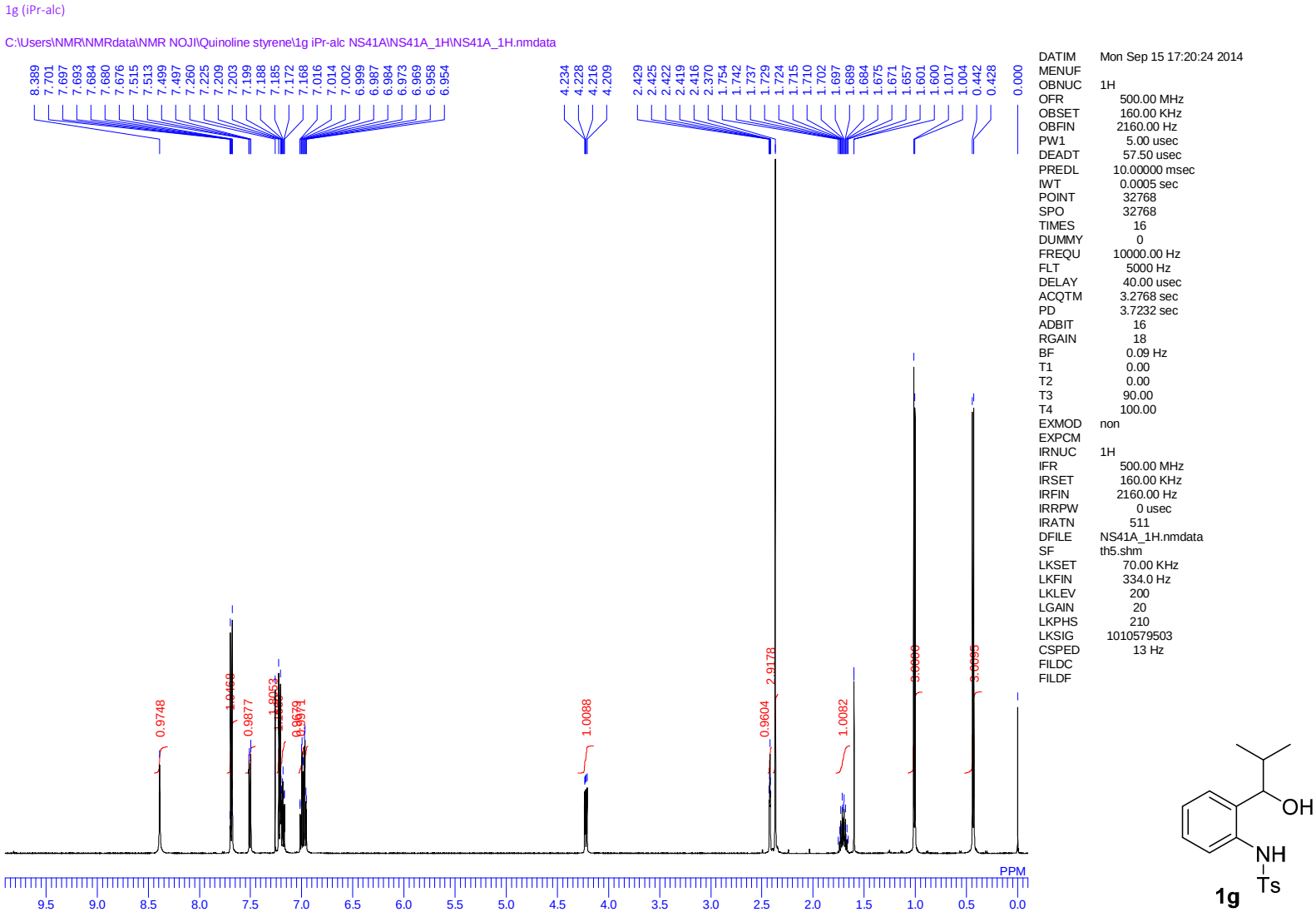


DATIM	Wed Oct 14 03:27:35 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	1g-2(Ts-CHO)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-2000761397
CSPED	10 Hz
FILDC	
FILDF	

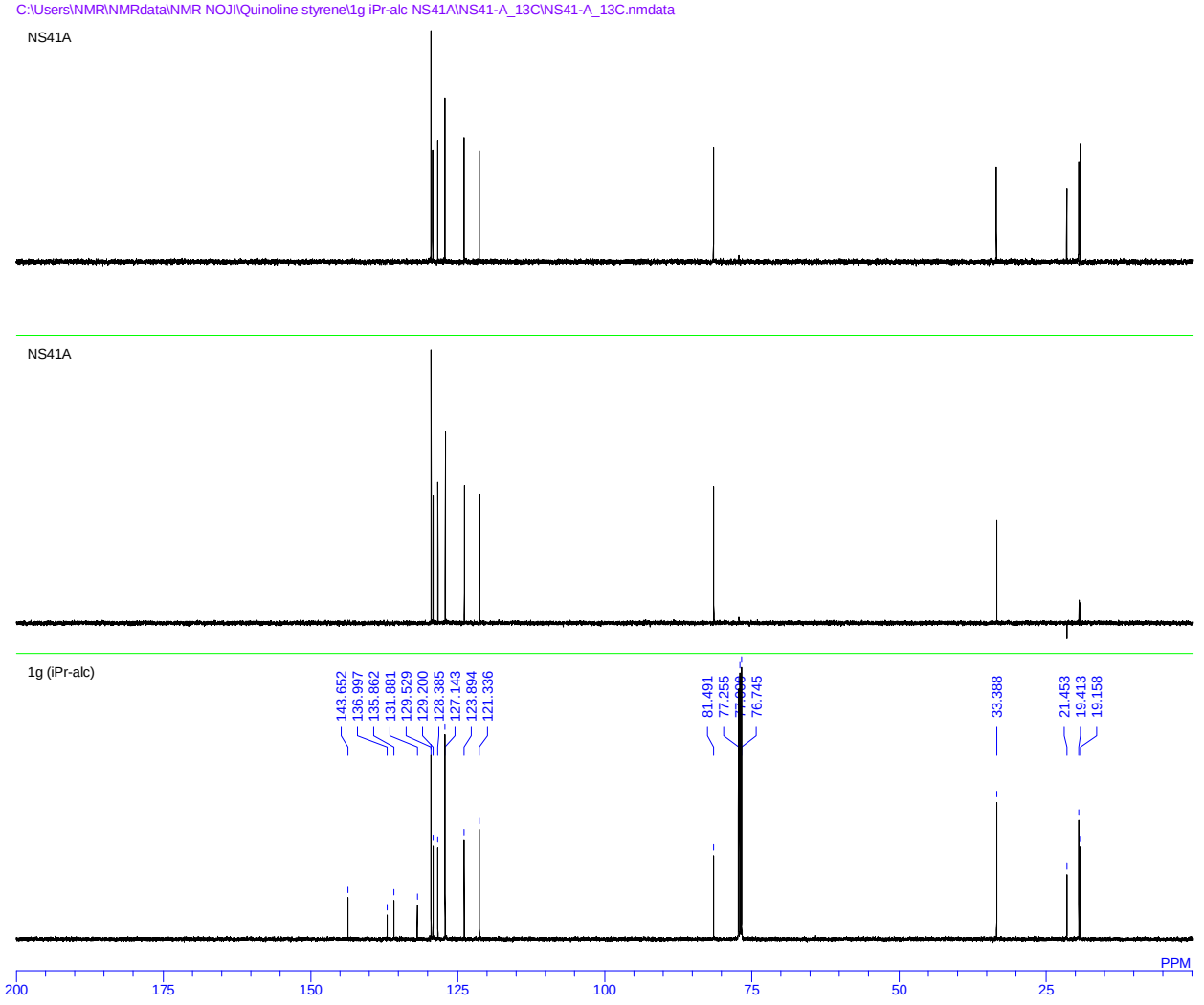


1g-2

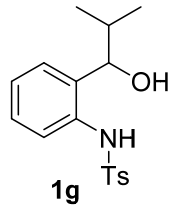
^{1}H NMR spectrum of 1g



^{13}C NMR spectrum of 1g

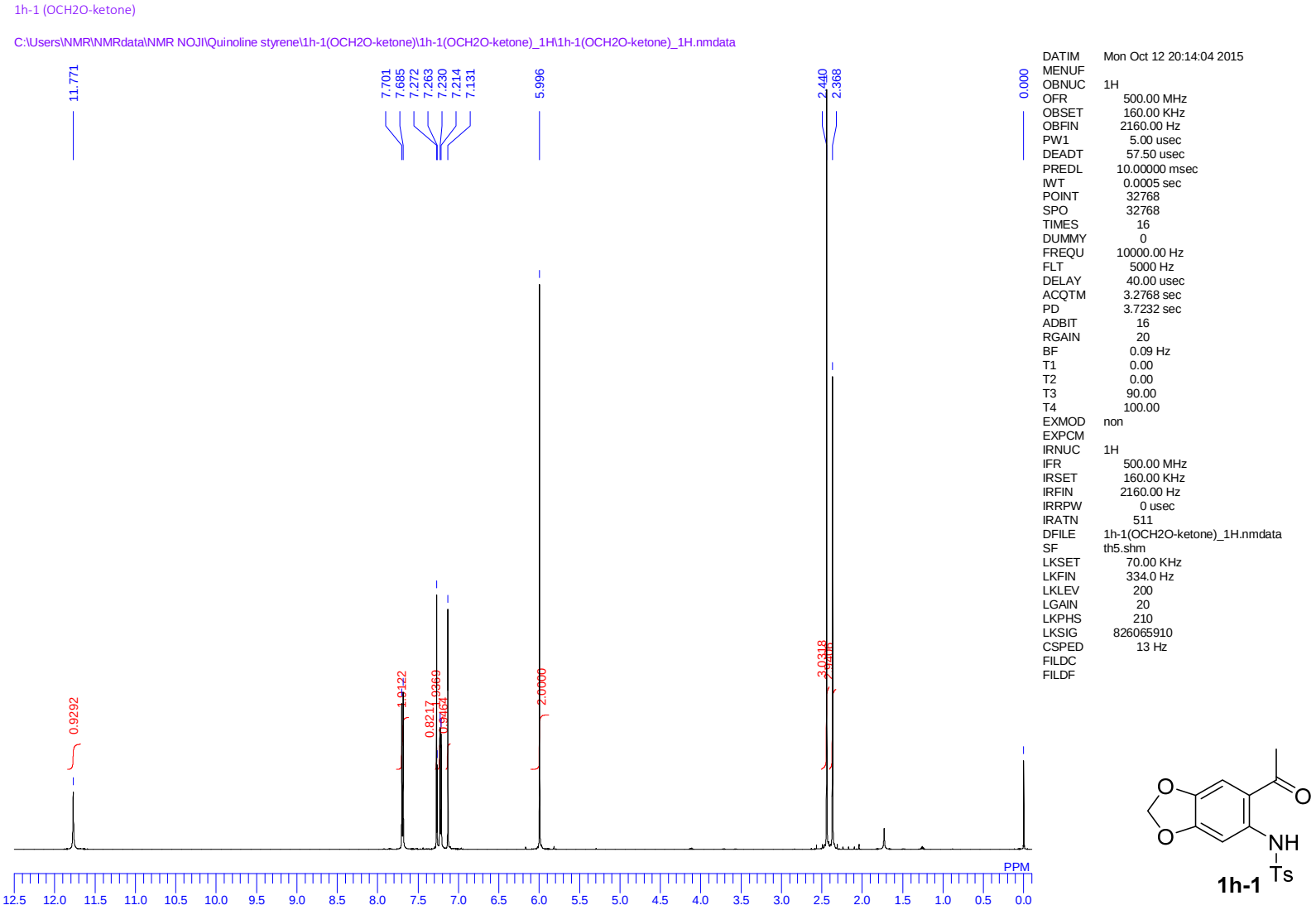


DATIM	Mon Sep 15 18:13:01 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	NS41-A_13C.nmdata
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	1019089845
CSPED	14 Hz
FILDC	
FILDF	

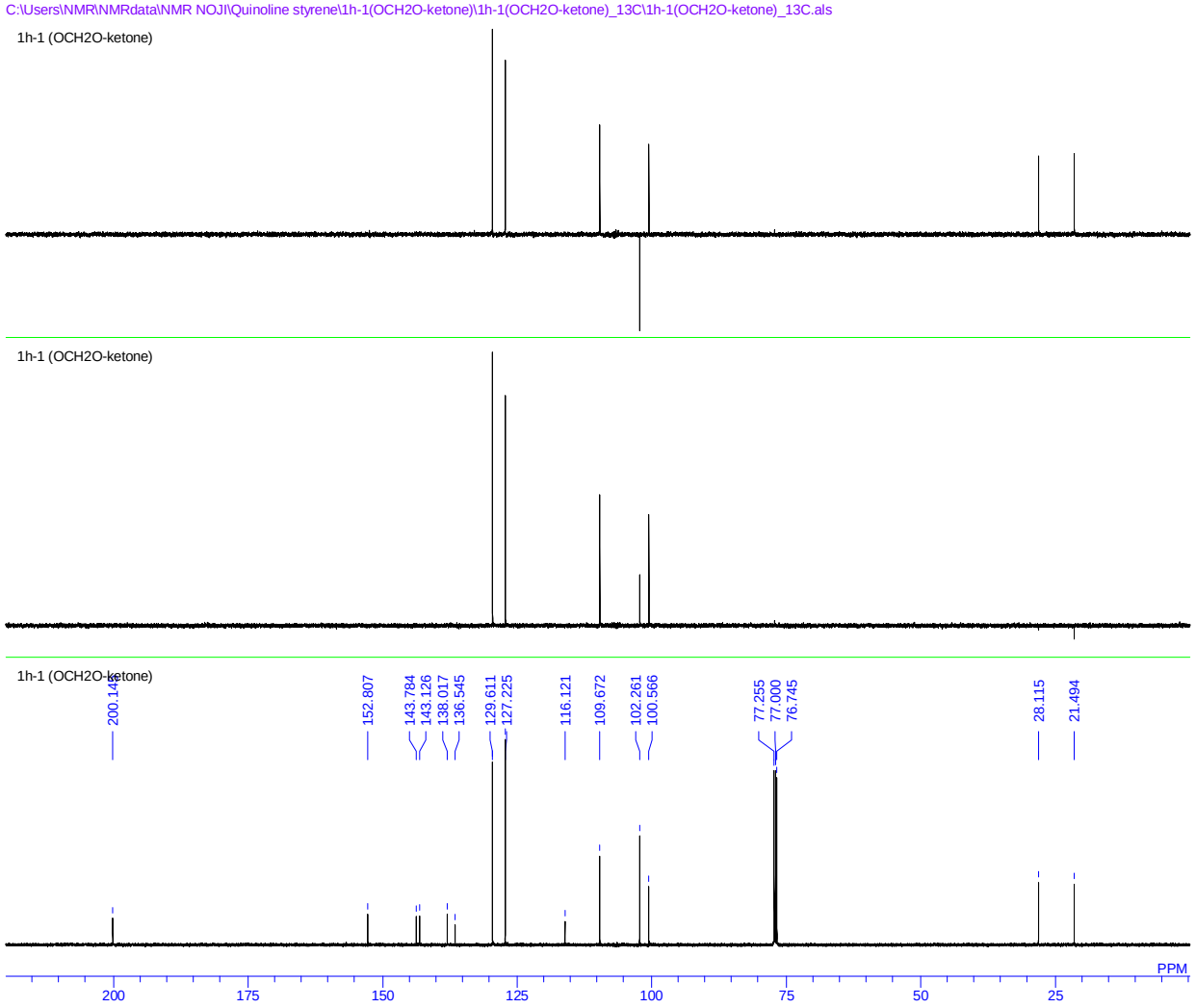


1g

^{1}H NMR spectrum of 1h-1



^{13}C NMR spectrum of 1h-1



DATIM	Mon Oct 12 21:06:34 2015
MENUF	
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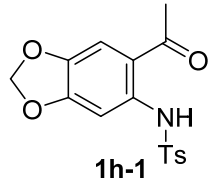
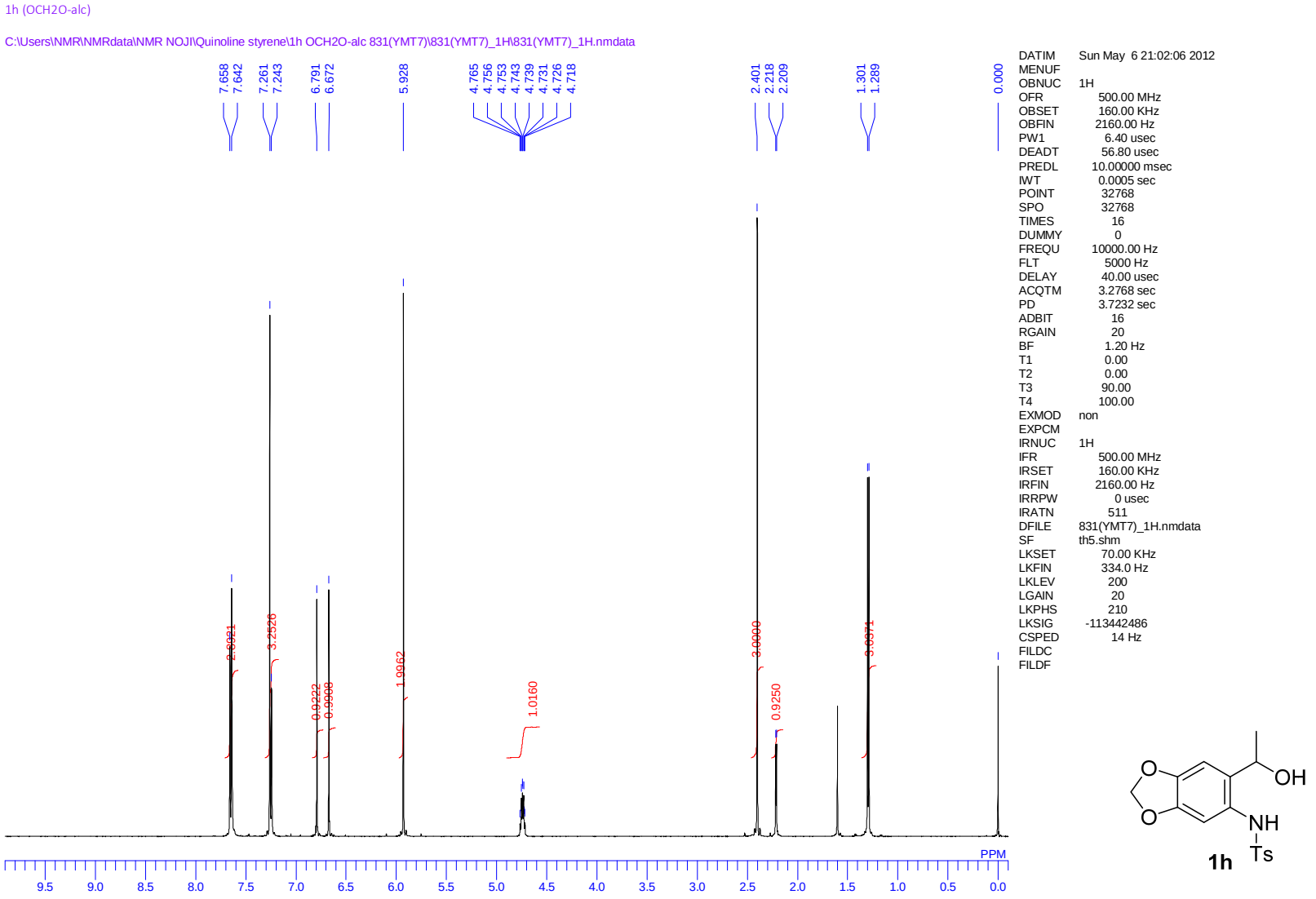
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	1h-1(OCH2O-ketone)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-557921211
CSPED	13 Hz
FILDC	
FILDF	

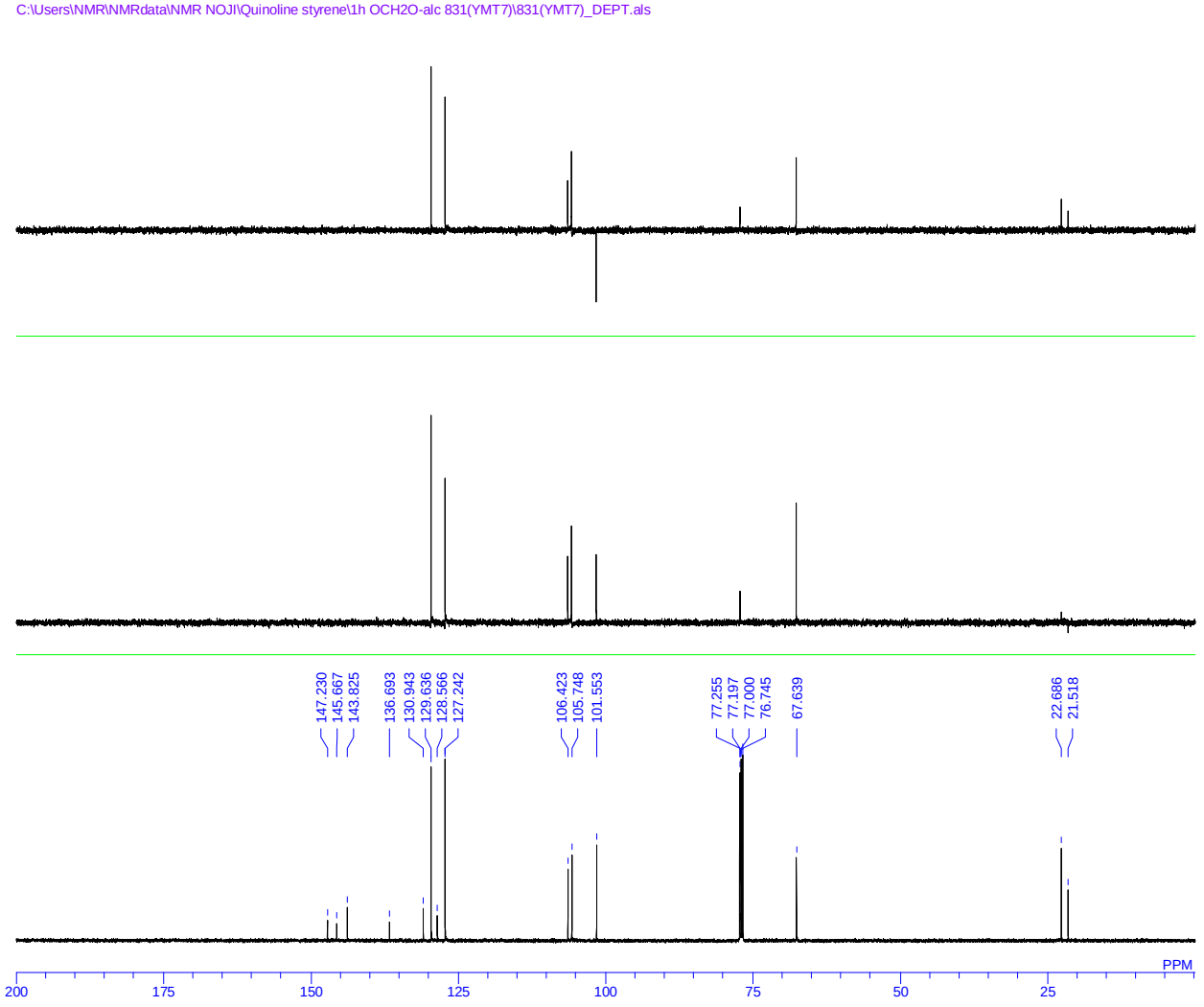


1h-1

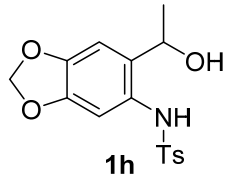
^{1}H NMR spectrum of 1h



^{13}C NMR spectrum of 1h

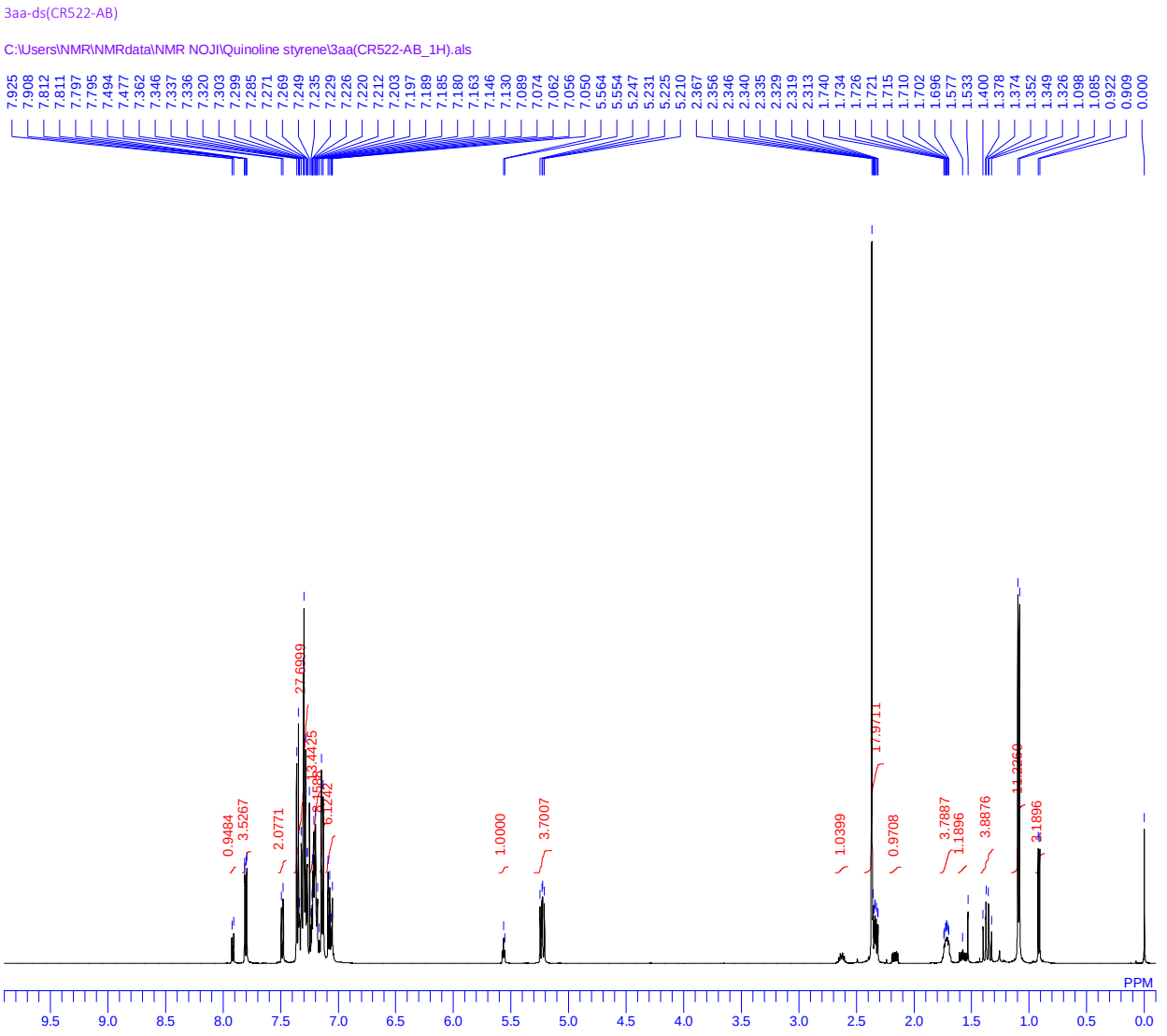


DATIM	Sun May 6 21:54:41 2012
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	5.40 usec
DEADT	10.00 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	831(YMT7)_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	10489
CSPED	13 Hz
FILDC	
FILDF	

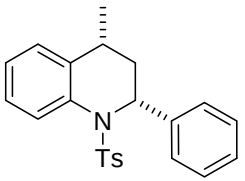


1h

^{1}H NMR spectrum of diastereomixture-3aa (*cis*-major)

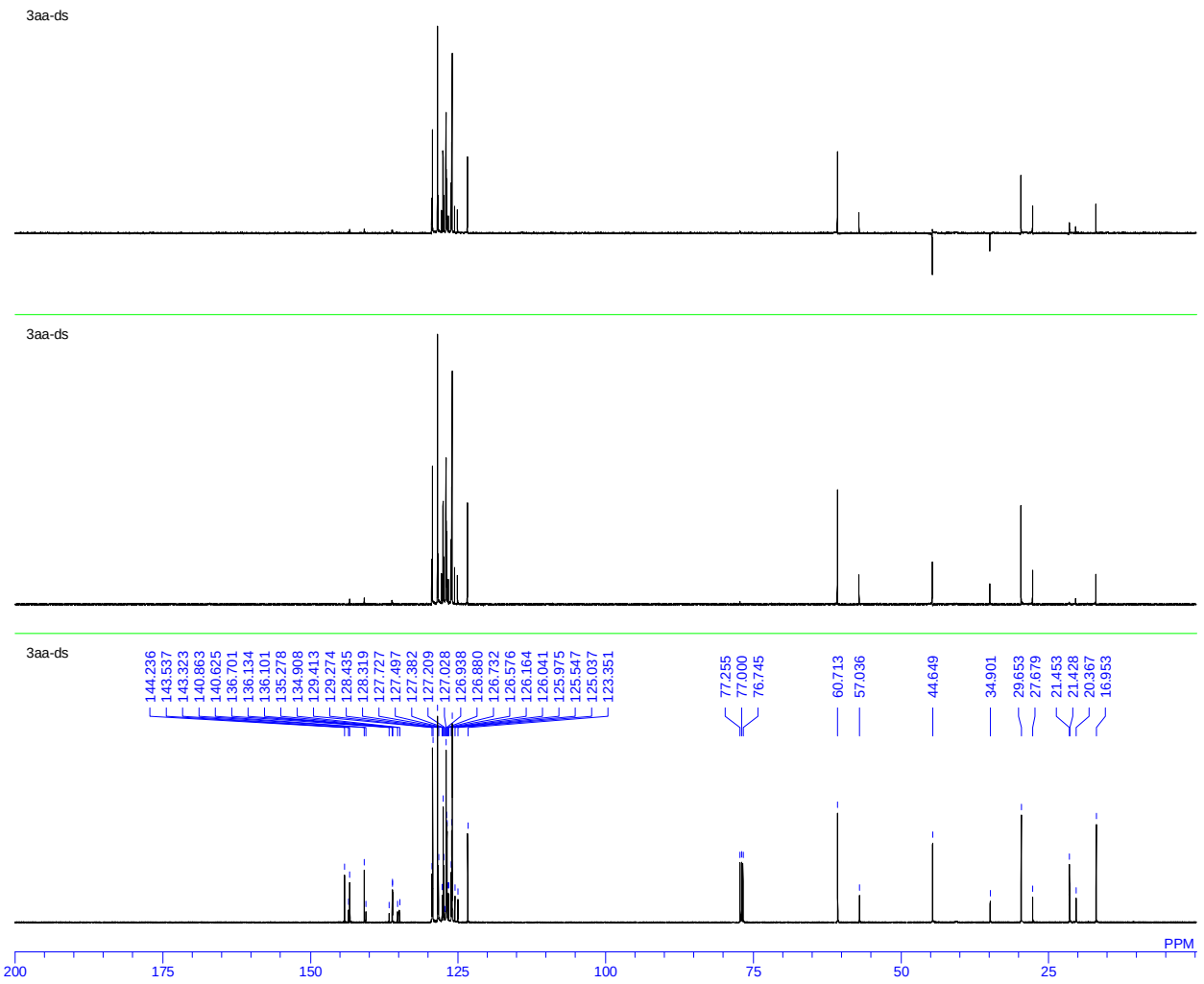


DATIM	Fri Nov 20 23:32:23 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.00 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3aa(CR522-AB_1H).als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	1664871078
CSPED	13 Hz
FILDC	
FILDF	

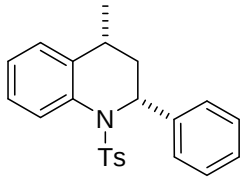


cis-**3aa** (major)

^{1}H NMR spectrum of diastereomixture-3aa (*cis*-major)

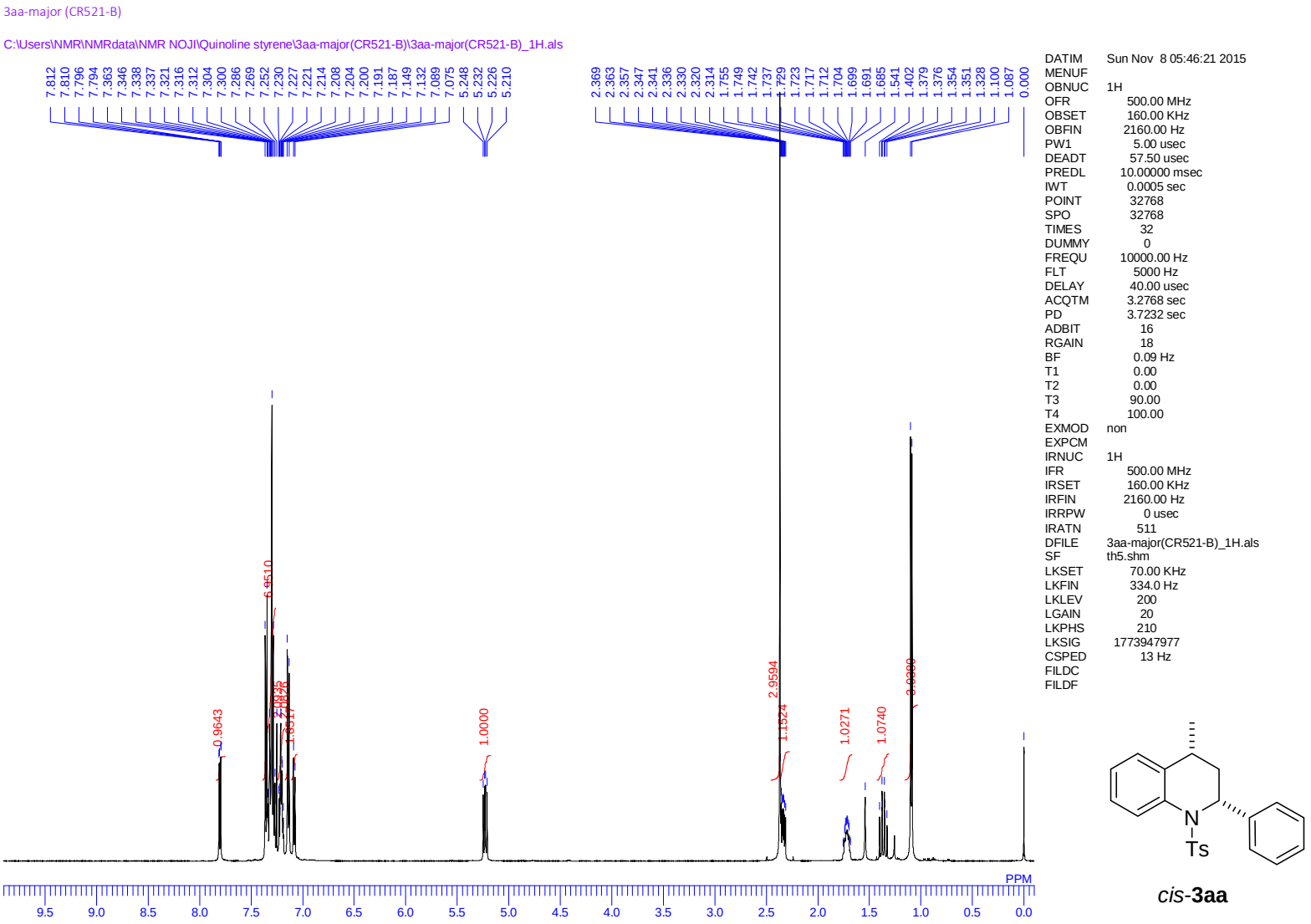


DATIM	Sat Nov 12 16:11:39 2011
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	5.40 usec
DEADT	10.00 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	784(MY2B)_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	9906
CSPED	12 Hz
FILDC	
FILDF	



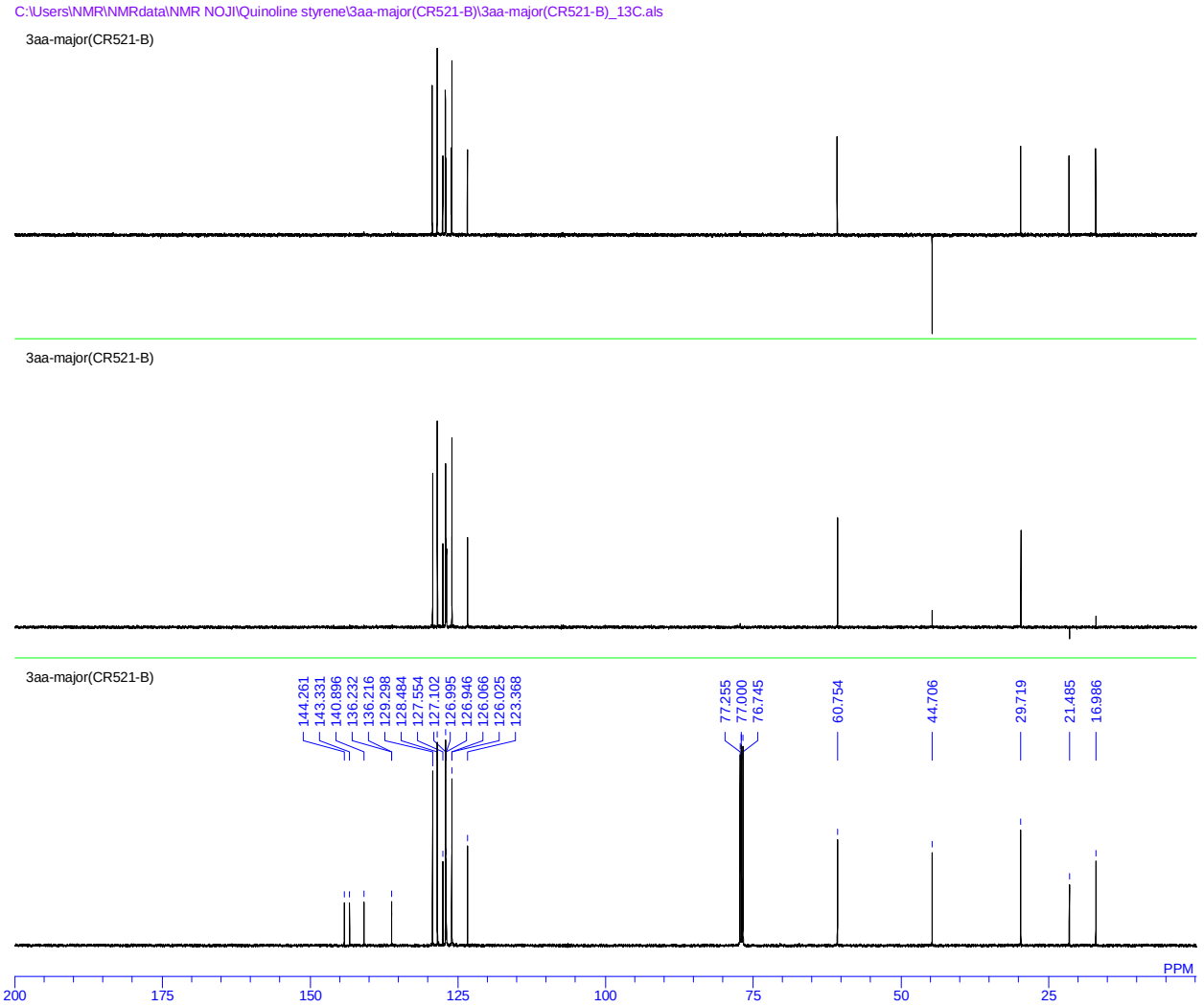
cis-**3aa** (major)

^{1}H NMR spectrum of *cis*-3aa (major)



cis-**3aa**

^{13}C NMR spectrum of *cis*-3aa (major)



DATIM	Sun Nov 8 07:30:05 2015
MENUF	
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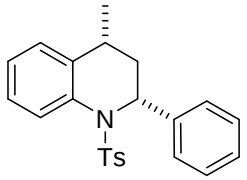
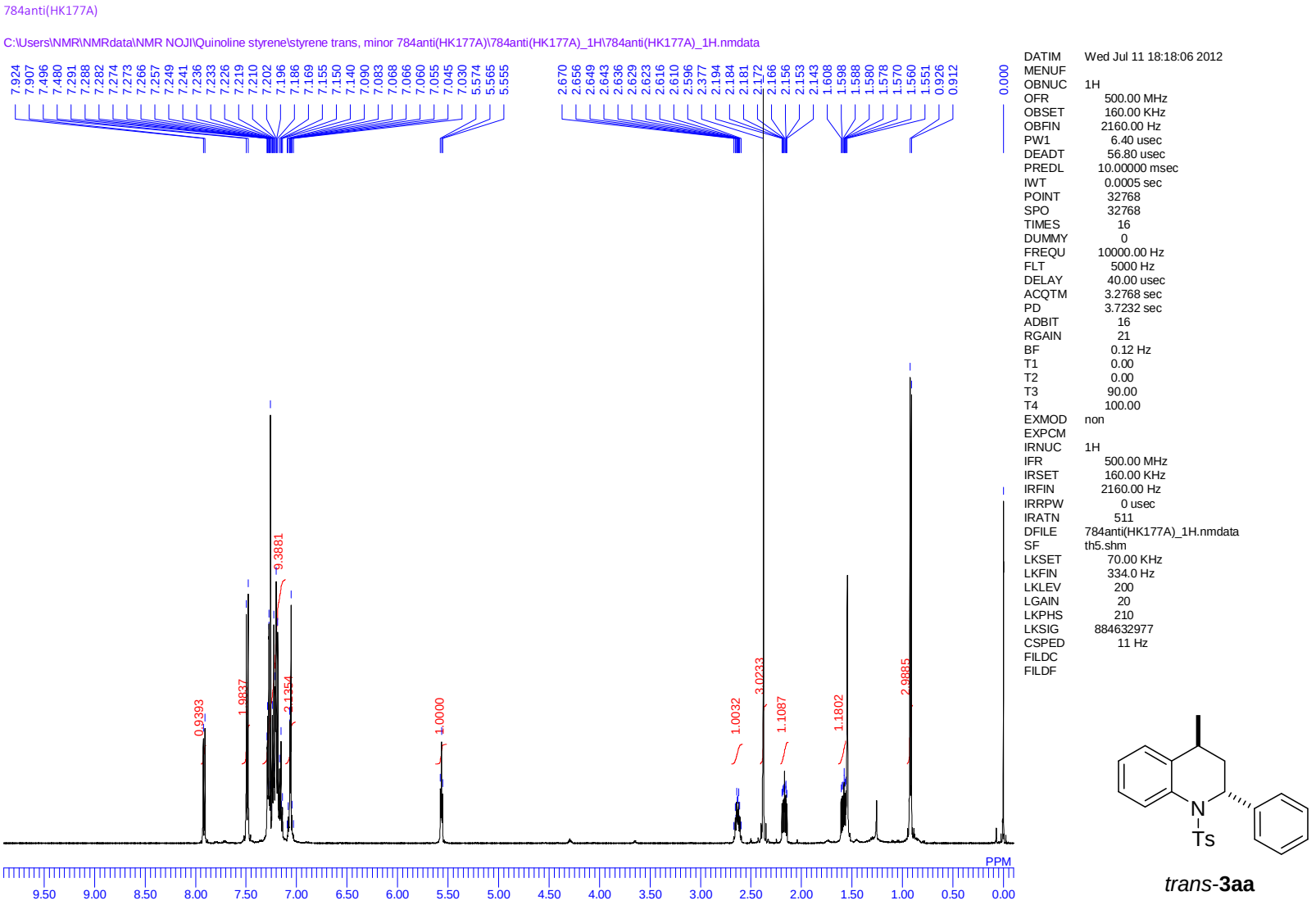
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3aa-major(CR521-B)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	30138
CSPED	12 Hz
FILDC	
FILDF	



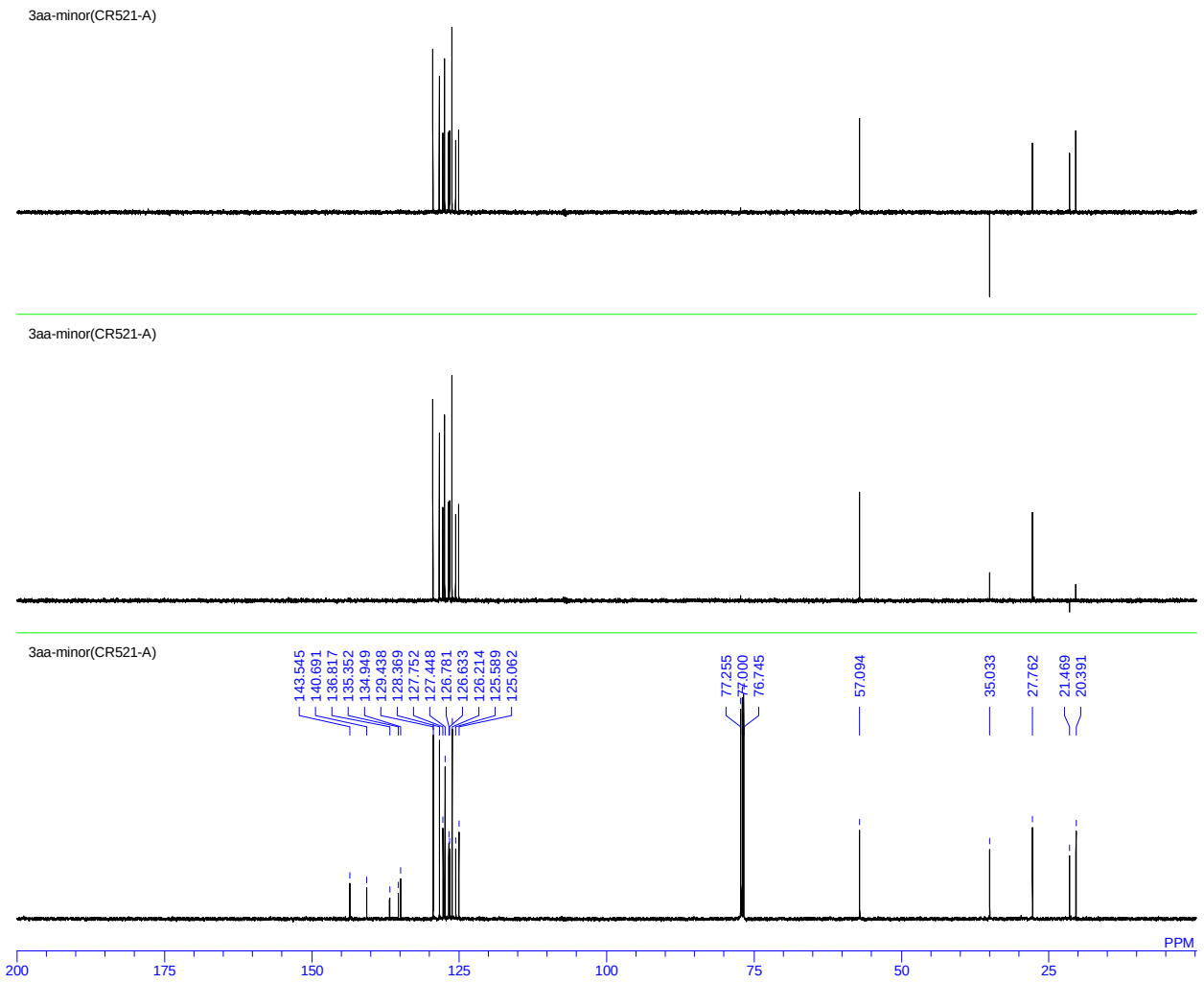
cis-**3aa**

^{1}H NMR spectrum of *trans*-3aa (minor)

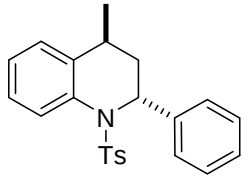


trans-**3aa**

^{13}C NMR spectrum of *trans*-3aa (minor)

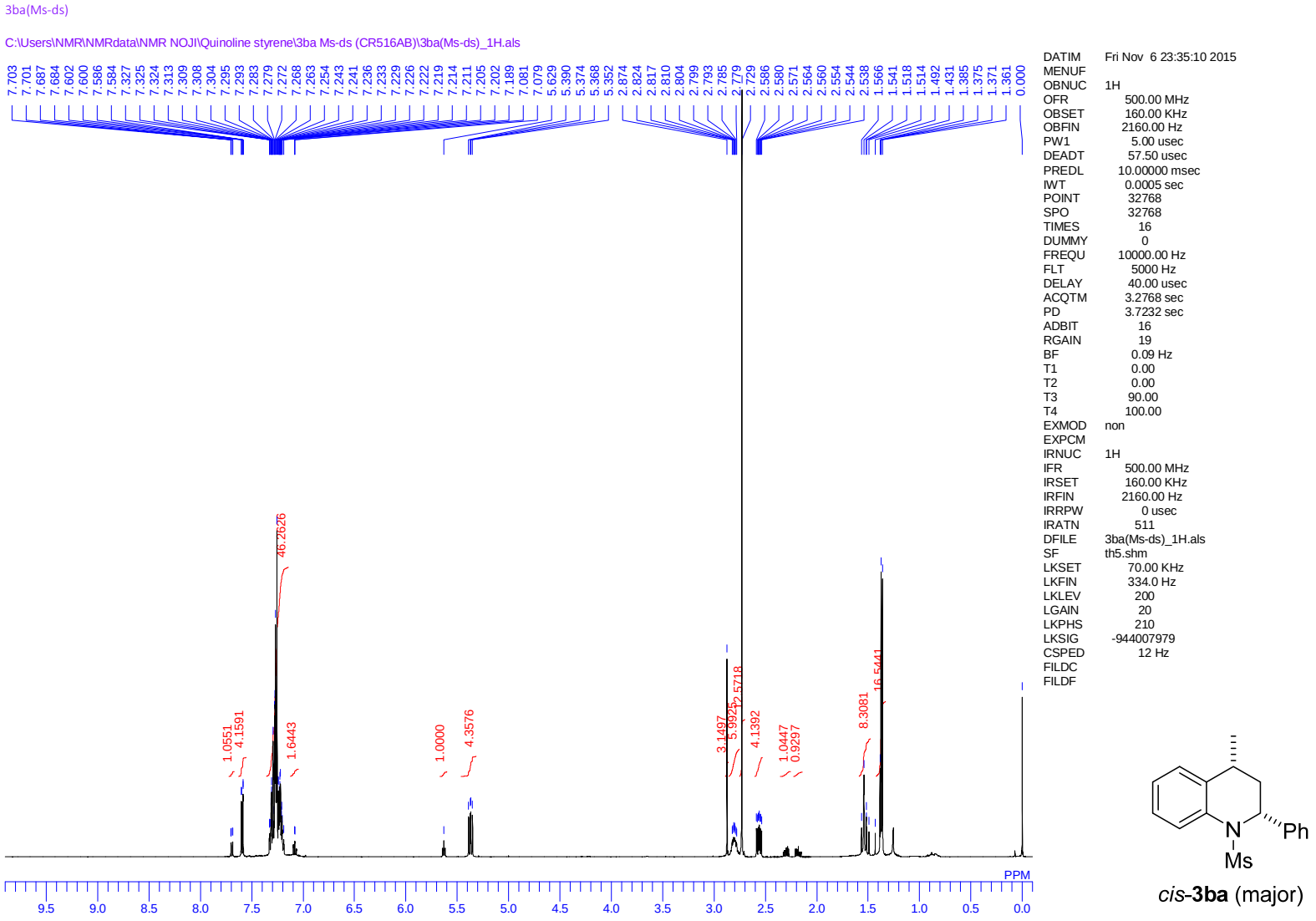


DATIM	Sun Nov 8 18:03:18 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3aa-minor(CR521-A)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	63099
CSPED	12 Hz
FILDC	
FILDF	



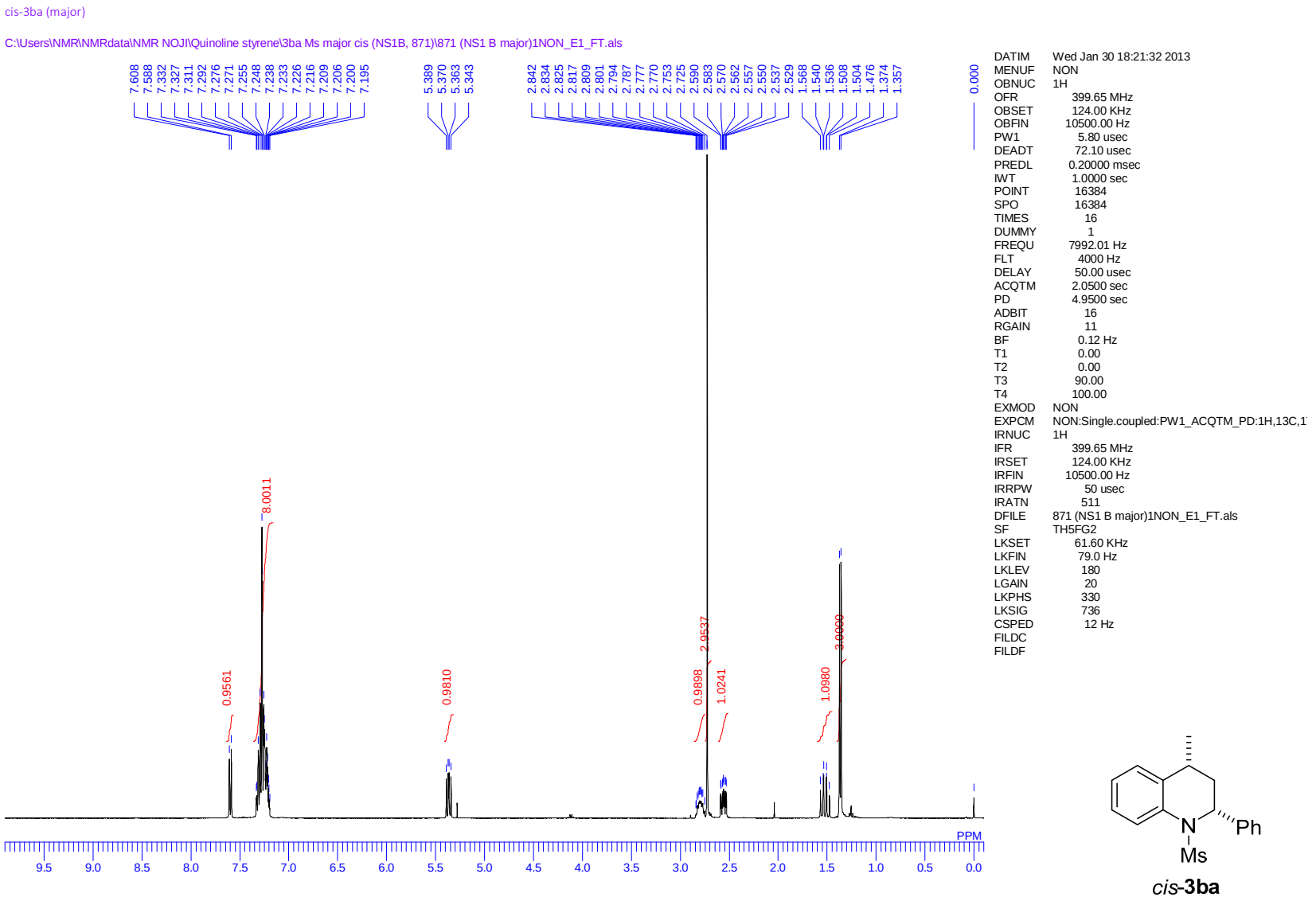
trans-**3aa**

^{1}H NMR spectrum of diastereomixture-3ba (*cis*-major)



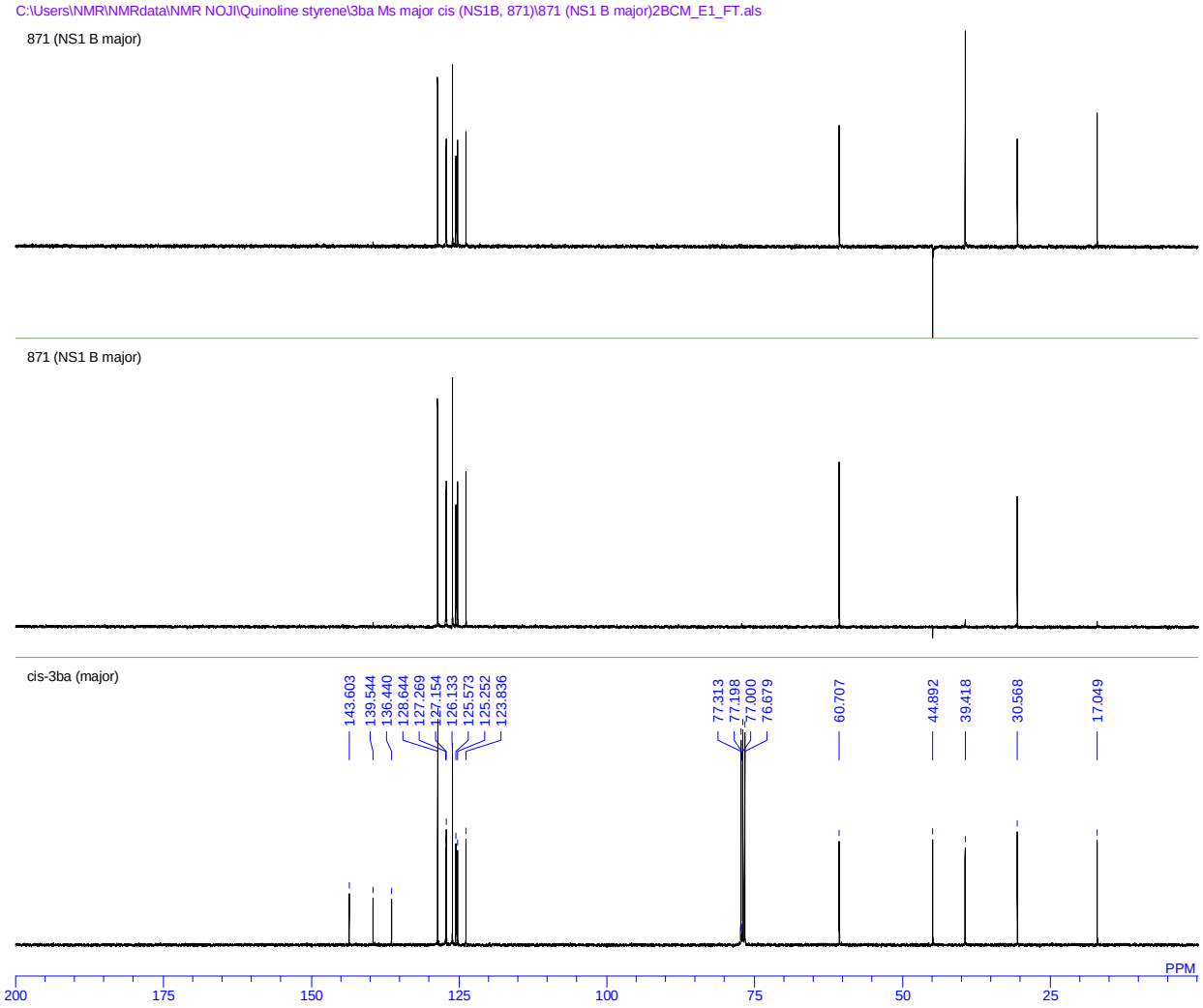
cis-**3ba** (major)

^{1}H NMR spectrum of *cis*-3ba (major)



cis-**3ba**

^{13}C NMR spectrum of *cis*-3ba (major)



DATIM	Wed Jan 30 19:02:00 2013
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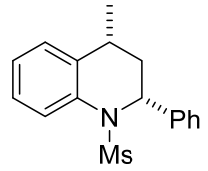
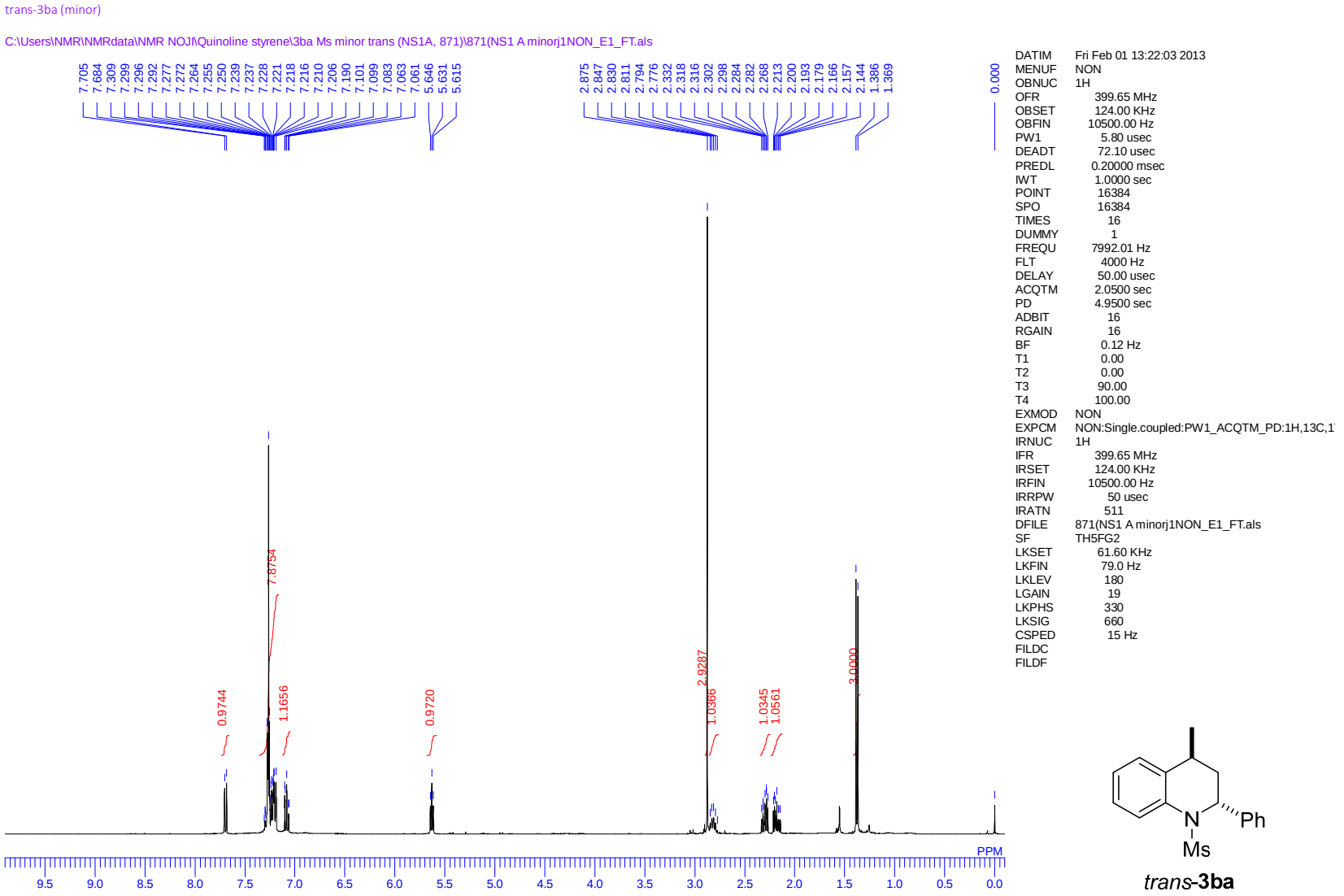
OBSET	125.00 KHz
OBFIN	10500.00 Hz
PW1	6.00 usec
DEADT	19.14 usec
PREDL	0.20000 msec
IWT	1.0000 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	27118.64 Hz
FLT	13550 Hz
DELAY	14.76 usec
ACQTM	1.2083 sec
PD	1.7920 sec
ADBIT	16
RGAIN	24
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	BCM
EXPCM	Bilevel.complete.decoupling:Set_IRRPW
IRNUC	1H
IFR	399.65 MHz
IRSET	124.00 KHz
IRFIN	10500.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	871 (NS1 B major)2BCM_E1_FT.als
SF	TH5FG2
LKSET	61.60 KHz
LKFIN	79.0 Hz
LKLEV	180
LGAIN	20
LKPHS	330
LKSIG	739
CSPED	16 Hz
FILDC	
FILDF	



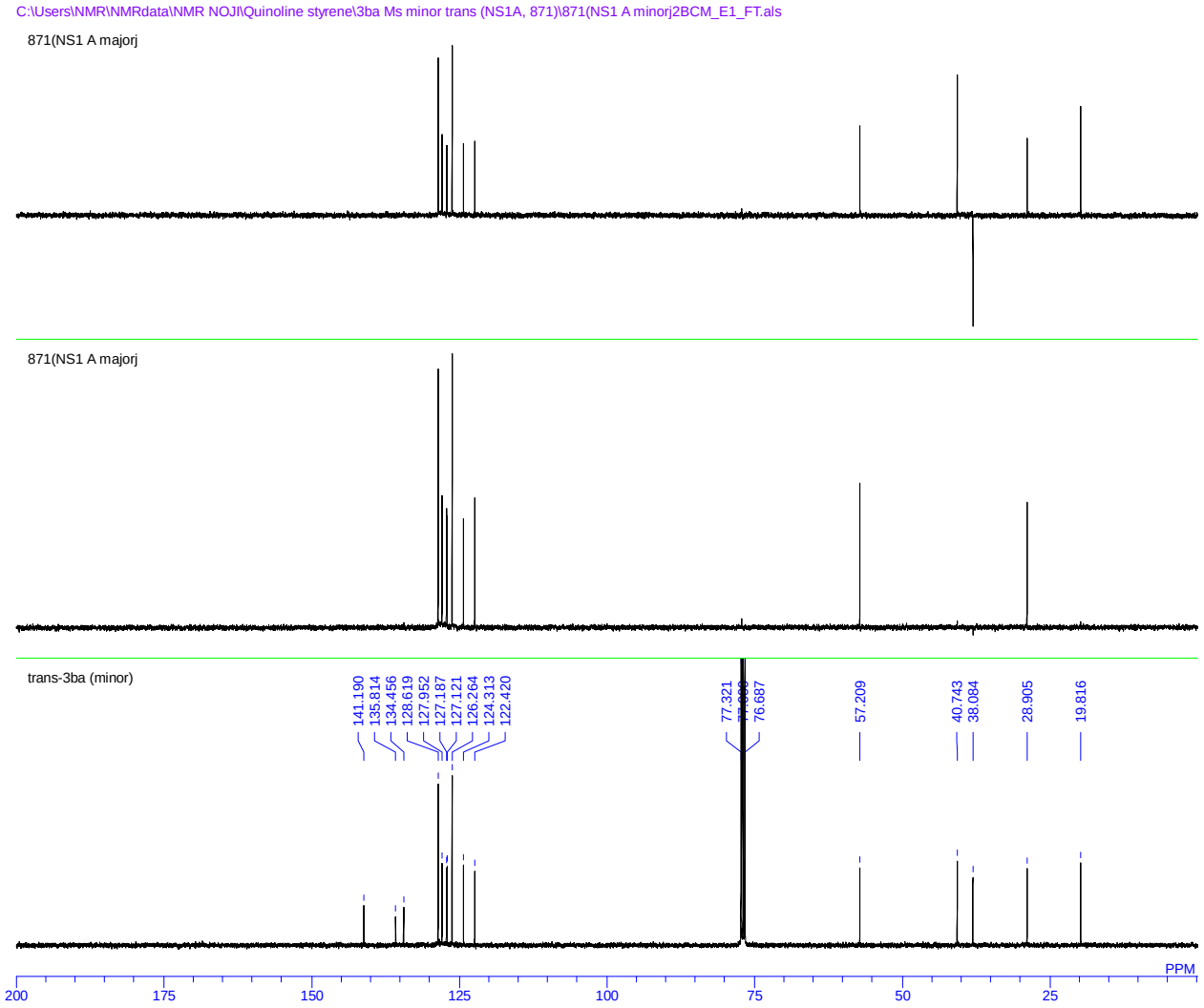
cis-**3ba**

^{1}H NMR spectrum of *trans*-3ba (minor)

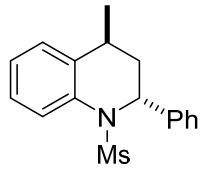


trans-**3ba**

^{13}C NMR spectrum of *trans*-3ba (minor)

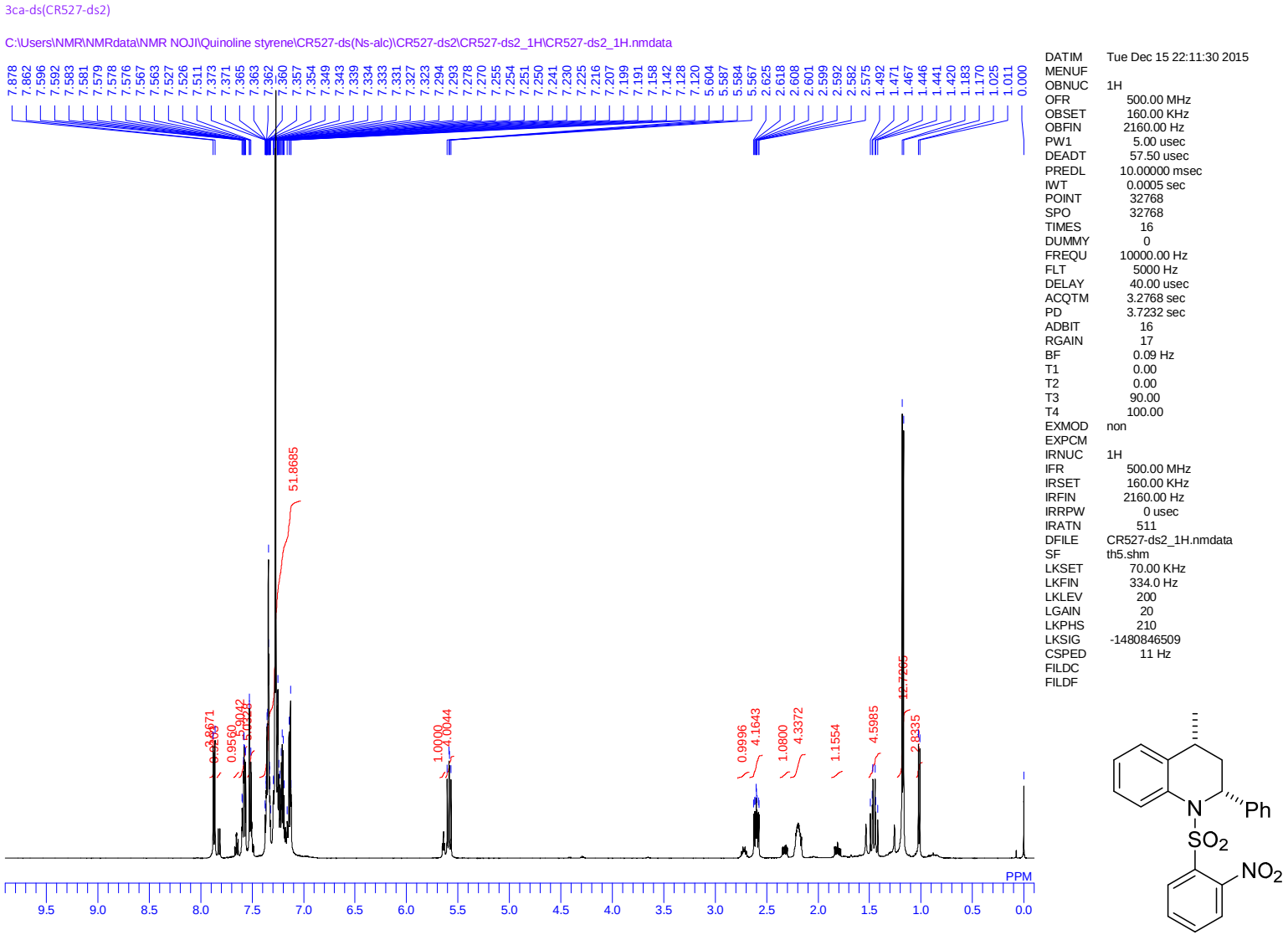


DATIM	Fri Feb 01 14:13:44 2013
MENUF	BCM
OBNUC	13C
OFR	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
PW1	6.00 usec
DEADT	19.14 usec
PREDL	0.20000 msec
IWT	1.0000 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	27118.64 Hz
FLT	13550 Hz
DELAY	14.76 usec
ACQTM	1.2083 sec
PD	1.7920 sec
ADBIT	16
RGAIN	25
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	BCM
EXPCM	Bilevel.complete.decoupling:Set_IRRPW
IRNUC	1H
IFR	399.65 MHz
IRSET	124.00 KHz
IRFIN	10500.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	871(NS1 A minorj2BCM_E1_FT.als
SF	TH5FG2
LKSET	61.60 KHz
LKFIN	79.0 Hz
LKLEV	180
LGAIN	19
LKPHS	330
LKSIG	634
CSPED	15 Hz
FILDC	
FILDF	



trans-**3ba**

^{1}H NMR spectrum of diastereomixture-3ca (*cis*-major)



DATIM	Tue Dec 15 22:11:30 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
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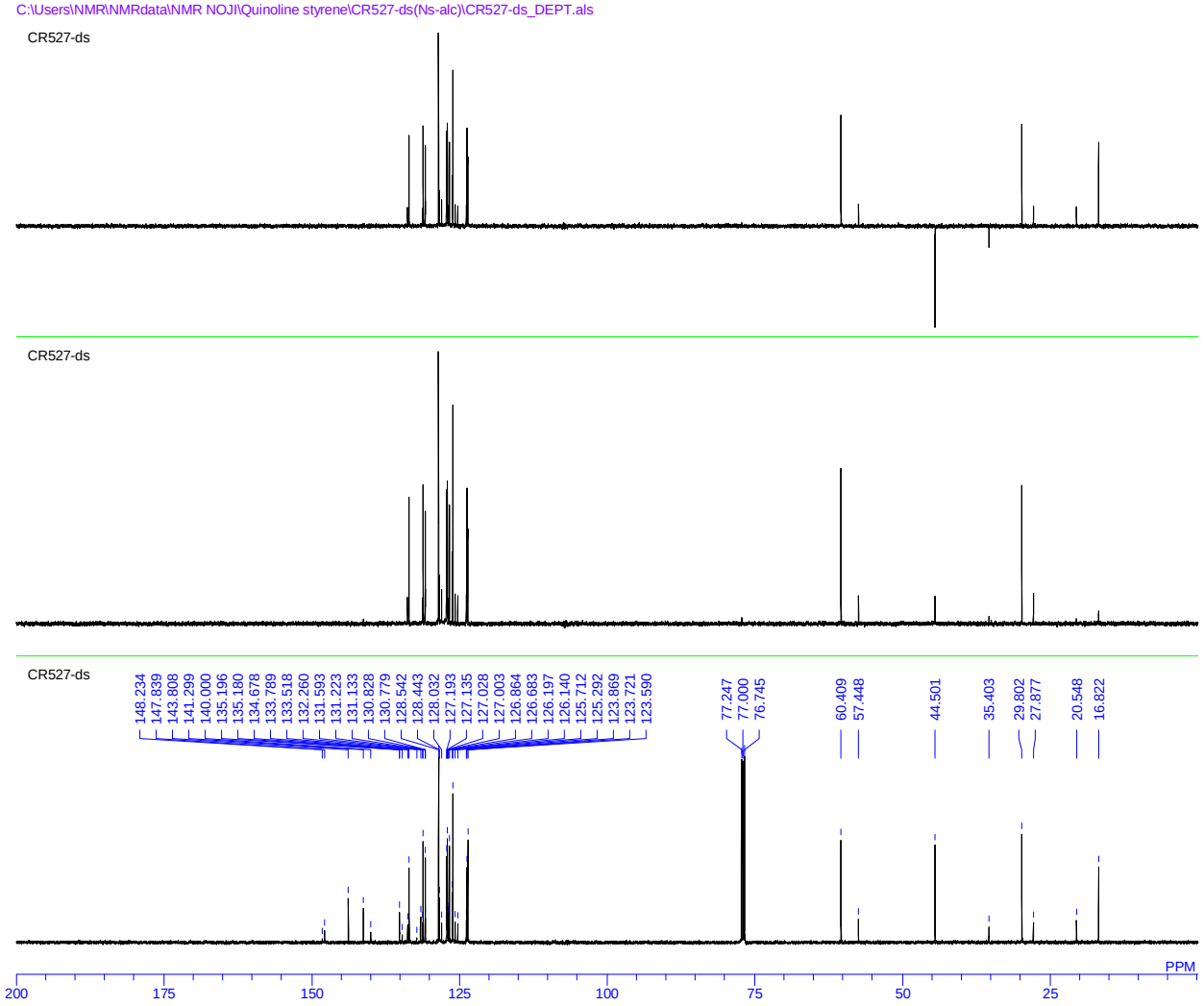
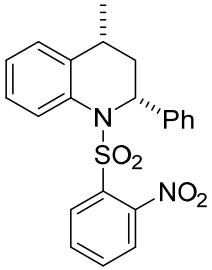
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-1480846509
CSPED	11 Hz
FILDC	
FILDF	

cis-**3ca** (major)

^{13}C NMR spectrum of diastereomixture-3ca (*cis*-major)

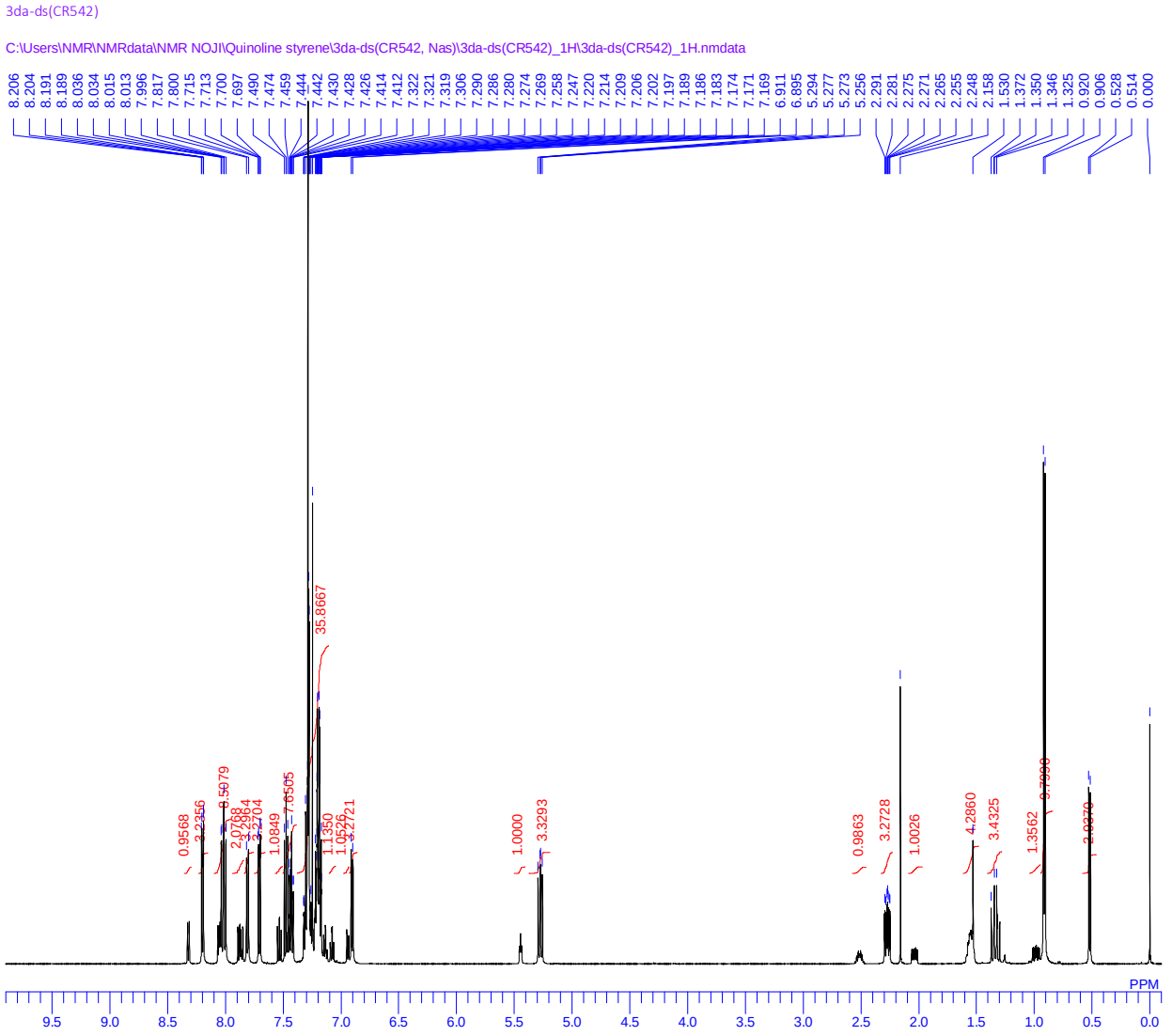


DATIM	Tue Dec 15 20:25:52 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR527-ds_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	4166
CSPED	13 Hz
FILDC	
FILDF	

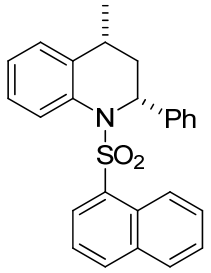


cis-**3ca** (major)

^{1}H NMR spectrum of diastereomixture-3da (*cis*-major)

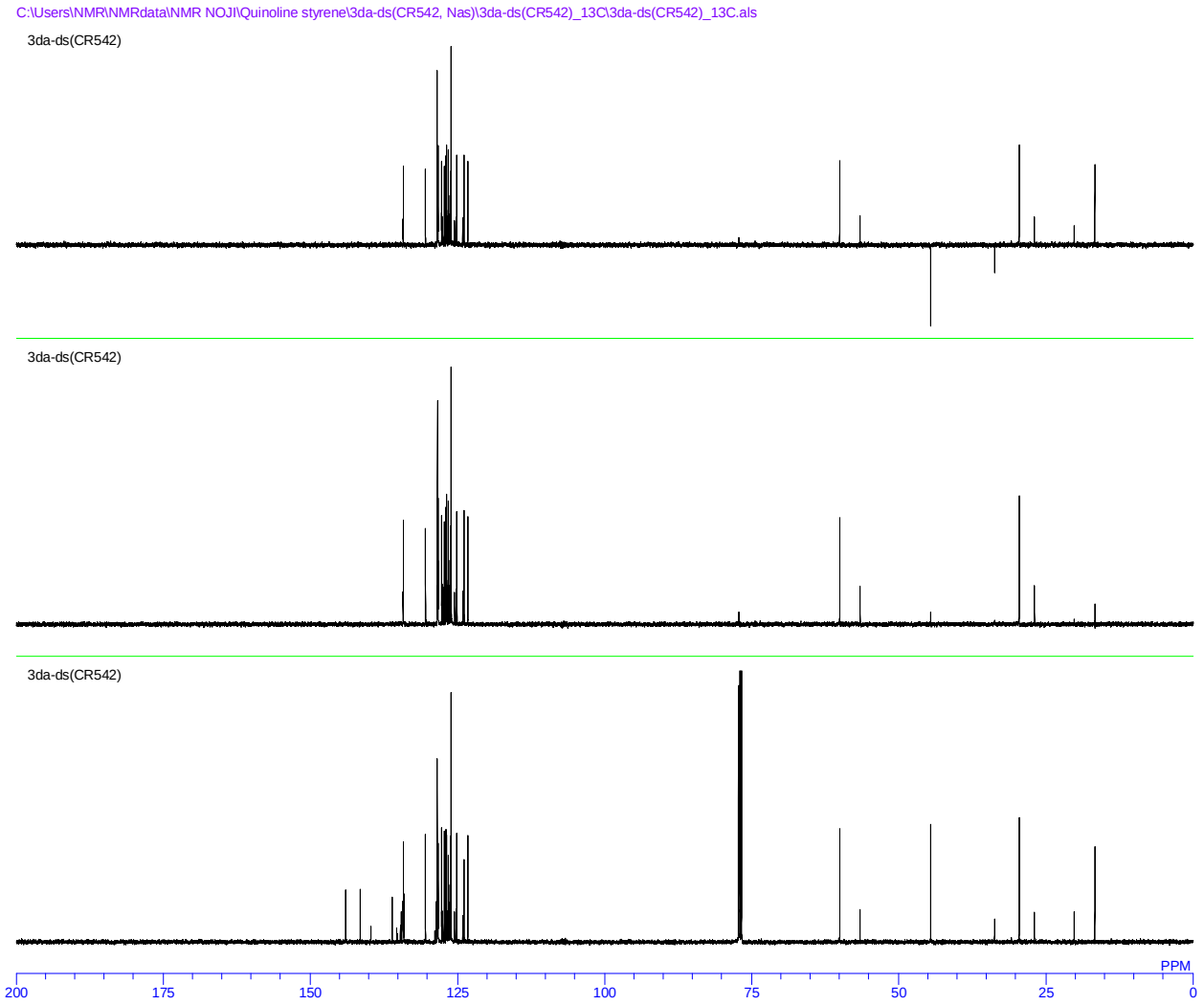


DATIM	Wed Jan 20 21:17:41 2016
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3da-ds(CR542)_1H.nmdata
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	1044070204
CSPED	12 Hz
FILDC	
FILDF	

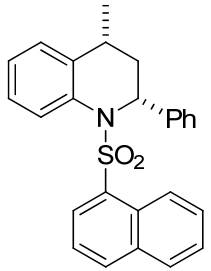


cis-**3da** (major)

^{13}C NMR spectrum of diastereomixture-3da (*cis*-major)

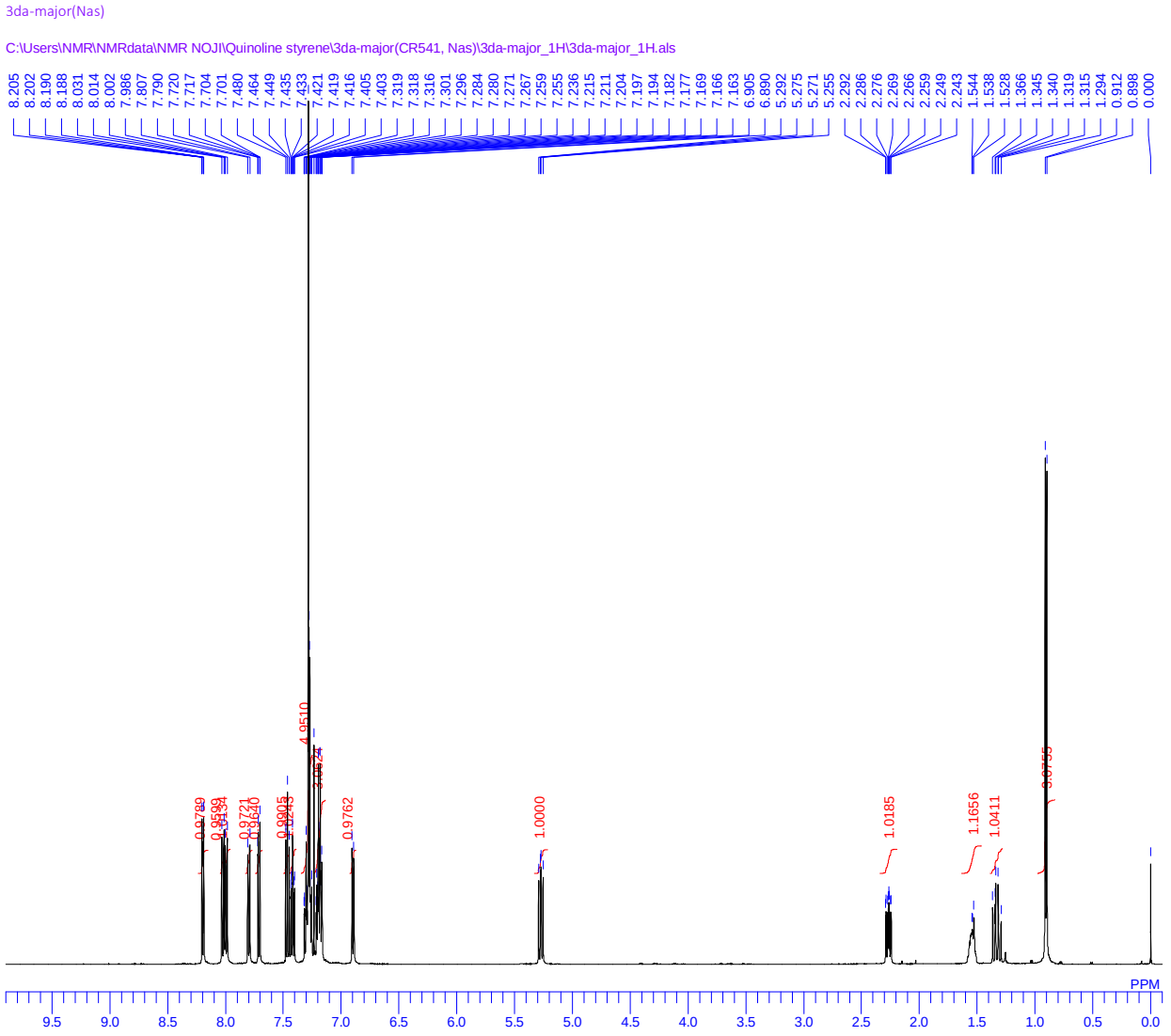


DATIM	Wed Jan 20 22:10:20 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3da-ds(CR542)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	792634726
CSPED	13 Hz
FILDC	
FILDF	



cis-**3da** (major)

^{1}H NMR spectrum of *cis*-3da (major)



DATIM	Wed Jan 20 18:59:27 2016
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	14
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
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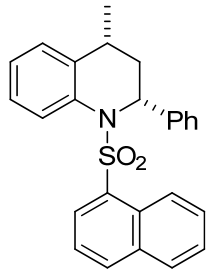
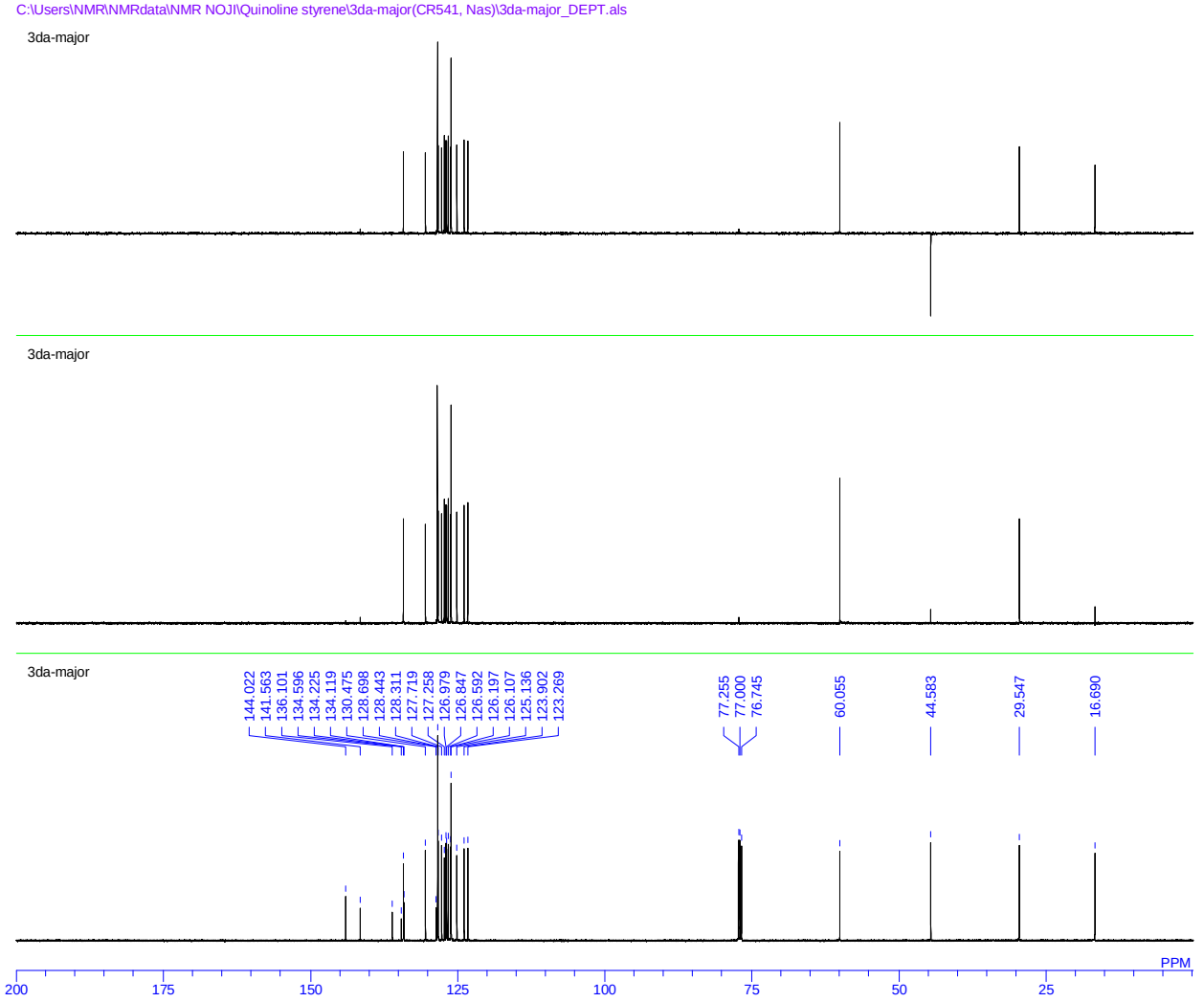
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	356258145
CSPED	13 Hz
FILDC	
FILDF	

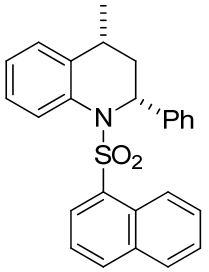


cis-**3da**

^{13}C NMR spectrum of *cis*-3da (major)

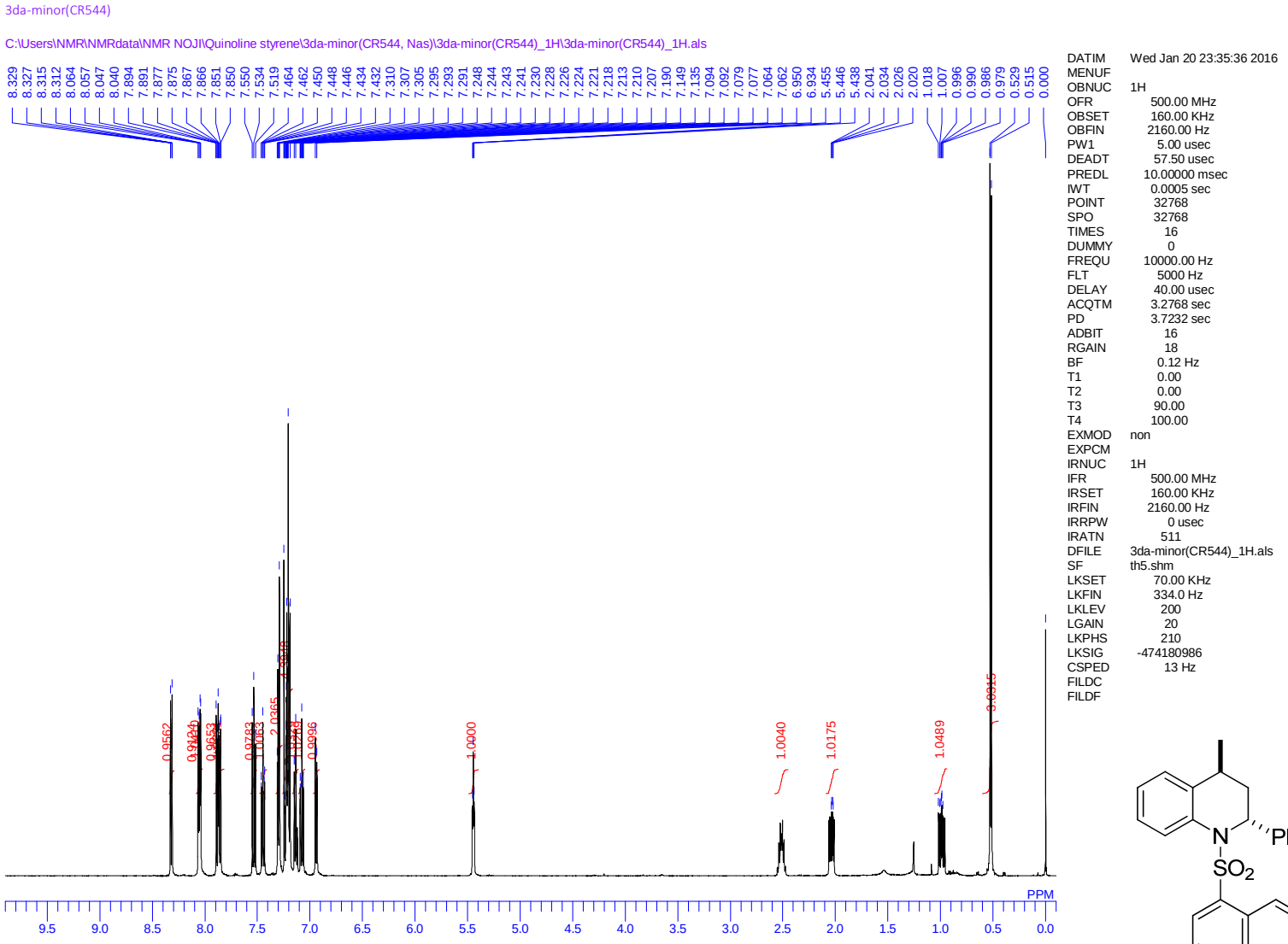


DATIM	Wed Jan 20 19:52:00 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3da-major_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	20490
CSPED	11 Hz
FILDC	
FILDF	



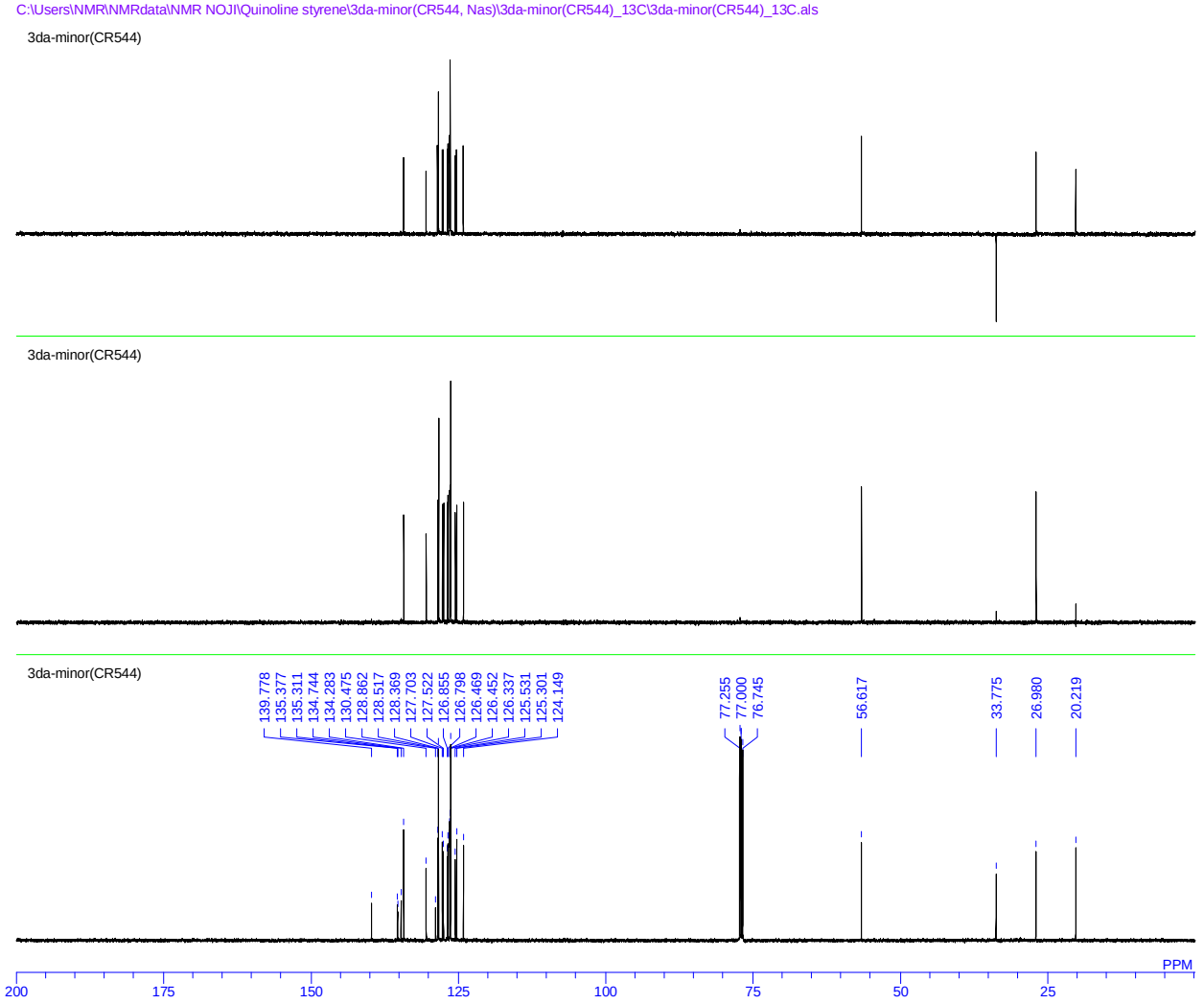
cis-**3da**

^{1}H NMR spectrum of *trans*-3da (minor)

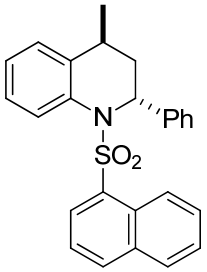


trans-**3da**

^{13}C NMR spectrum of *trans*-3da (minor)

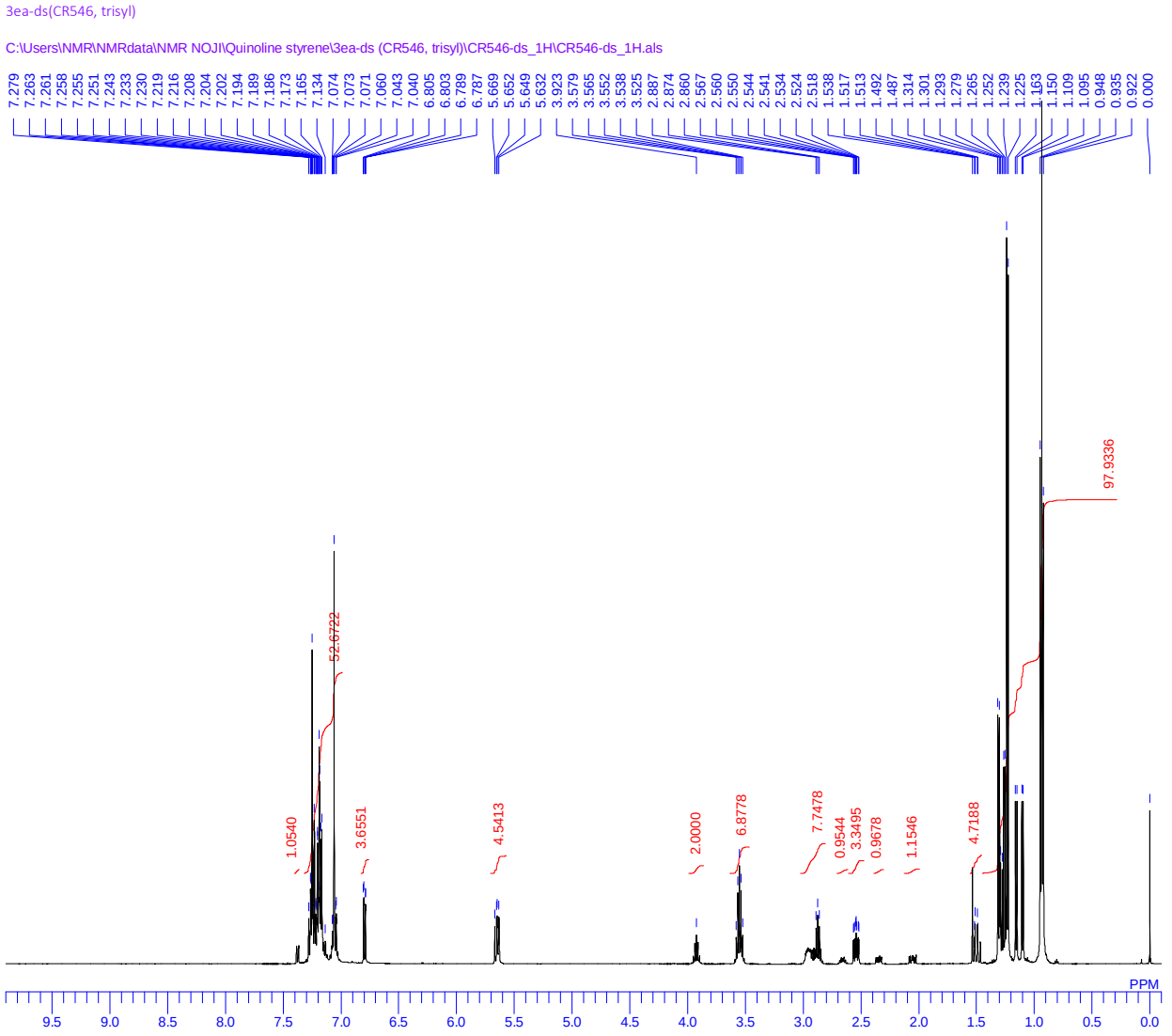


DATIM	Thu Jan 21 00:28:11 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3da-minor(CR544)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	700337804
CSPED	11 Hz
FILDC	
FILDF	



trans-**3da**

^{1}H NMR spectrum of diastereomixture-3ea (*cis*-major)



DATIM	Sat Jan 30 16:56:01 2016
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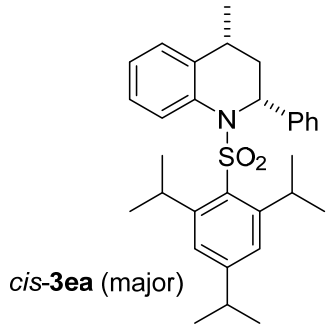
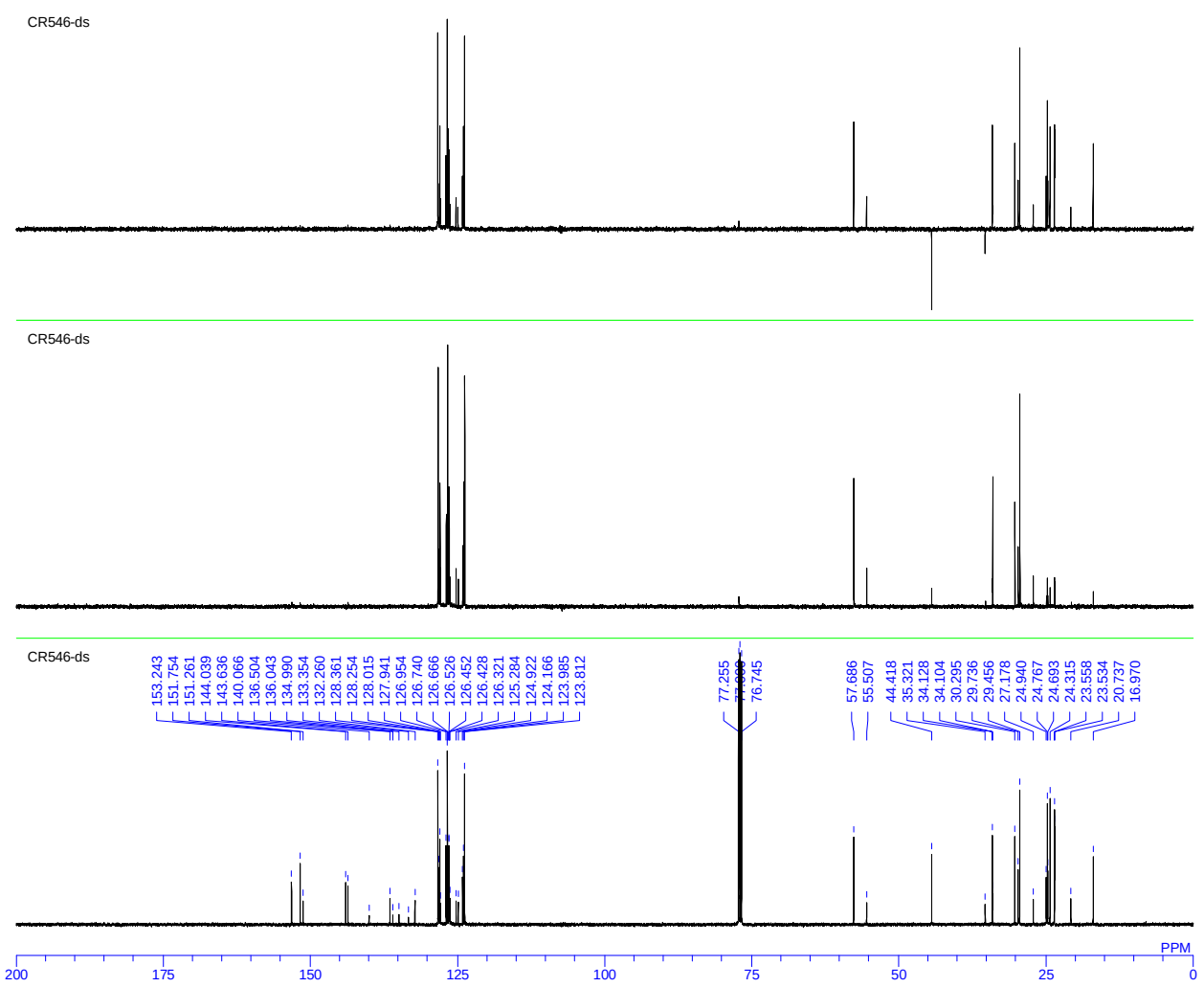
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	32
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR546-ds_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	64988
CSPED	11 Hz
FILDC	
FILDF	

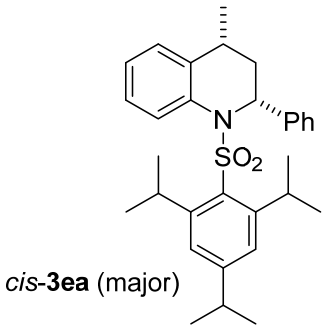


cis-**3ea** (major)

^{13}C NMR spectrum of diastereomixture-3ea (*cis*-major)

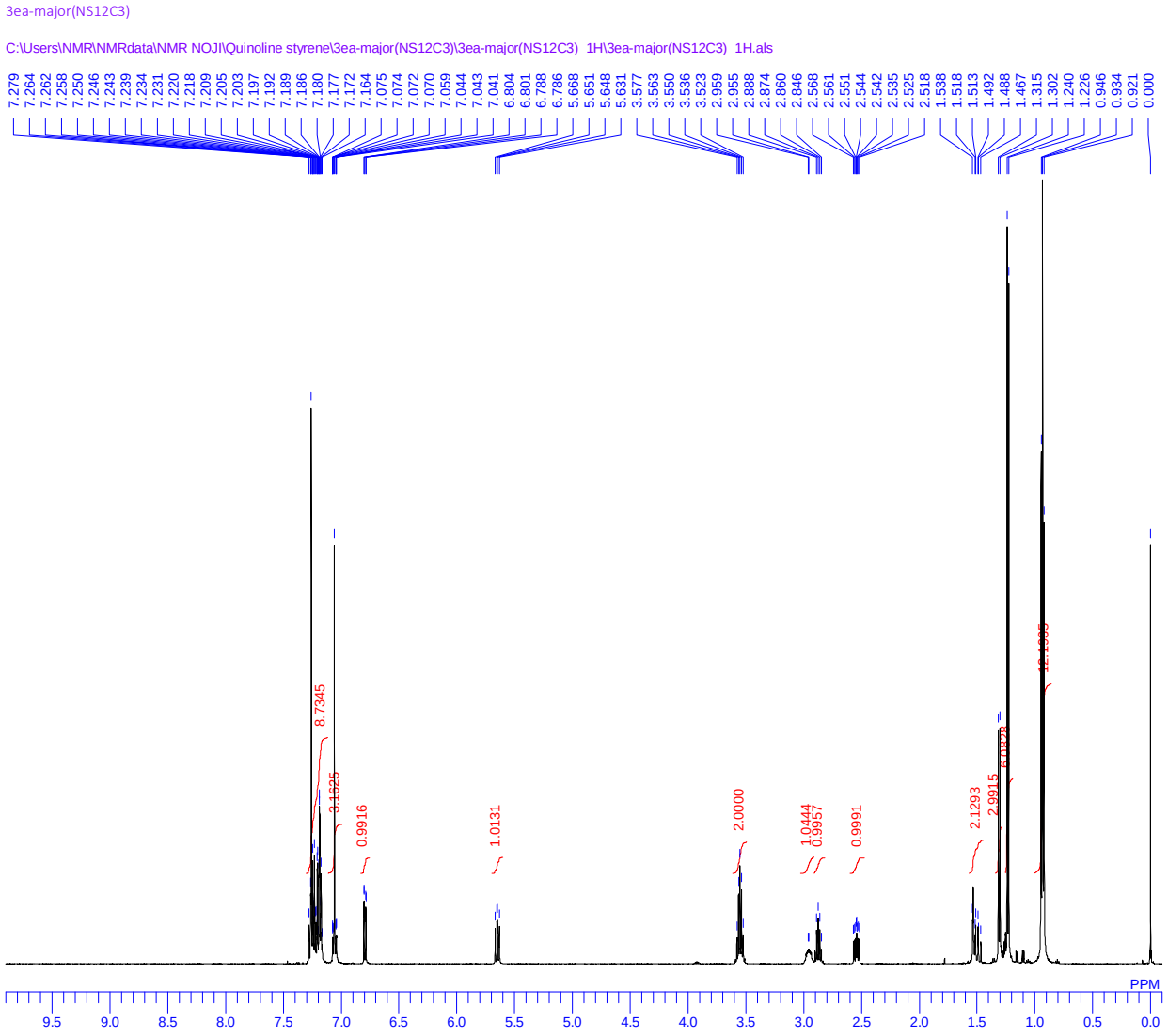


DATIM	Sat Jan 30 18:39:41 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR546-ds_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	8892
CSPED	12 Hz
FILDC	
FILDF	

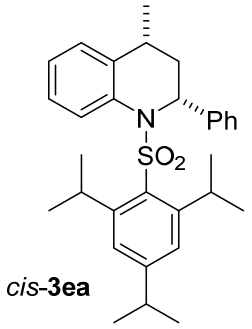


cis-**3ea** (major)

^{1}H NMR spectrum of *cis*-3ea (major)

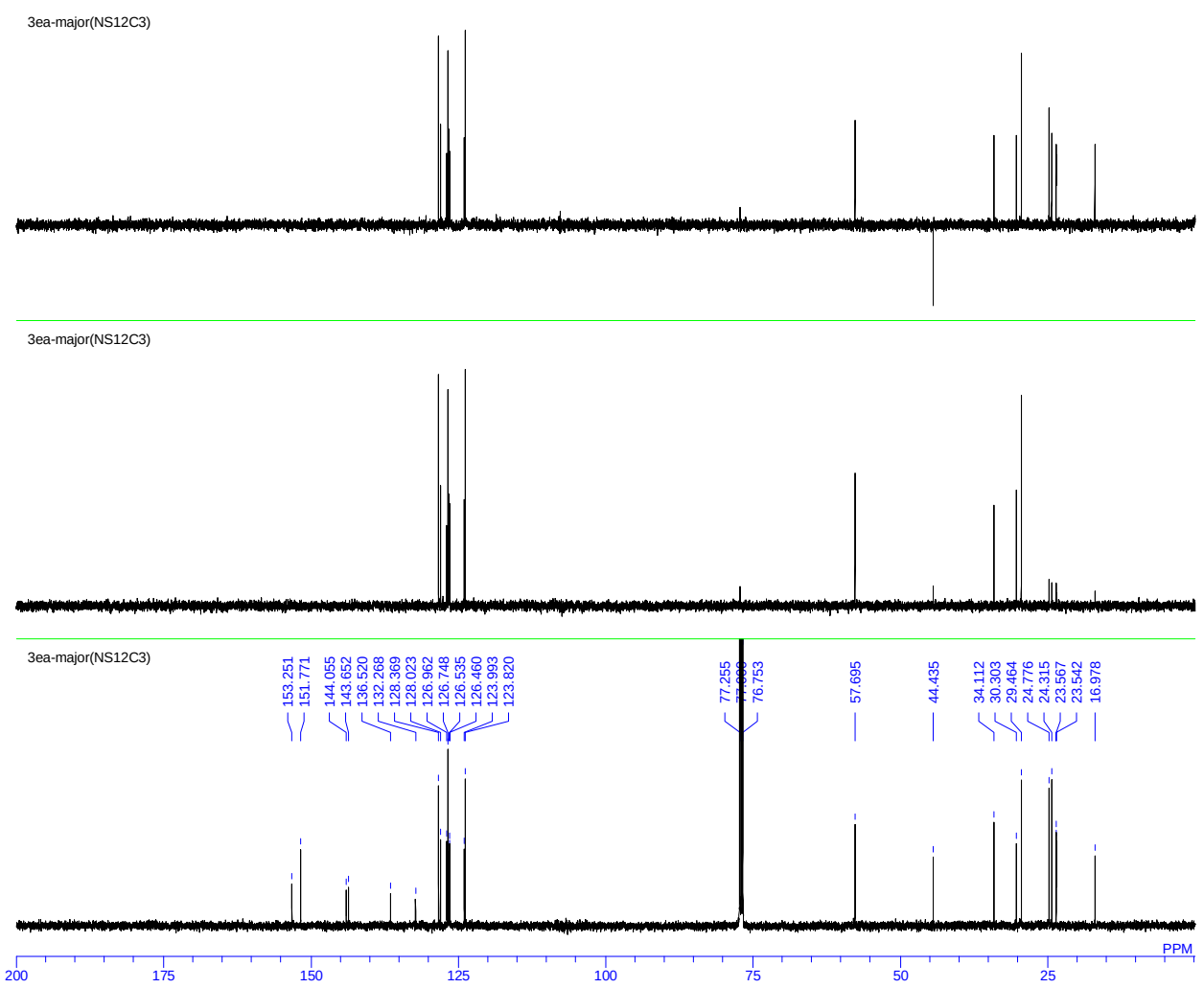


DATIM Tue Feb 2 20:58:22 2016
MENUF
OBNUC 1H
OFR 500.00 MHz
OBSET 160.00 KHz
OBFIN 2160.00 Hz
PW1 5.00 usec
DEADT 57.50 usec
PREDL 10.00000 msec
IWT 0.0005 sec
POINT 32768
SPO 32768
TIMES 32
DUMMY 0
FREQU 10000.00 Hz
FLT 5000 Hz
DELAY 40.00 usec
ACQTM 3.2768 sec
PD 3.7232 sec
ADBIT 16
RGAIN 22
BF 0.09 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD non
EXPCM
IRNUC 1H
IFR 500.00 MHz
IRSET 160.00 KHz
IRFIN 2160.00 Hz
IRRPW 0 usec
IRATN 511
DFILE 3ea-major(NS12C3)_1H.als
SF th5.shm
LKSET 70.00 KHz
LKFIN 334.0 Hz
LKLEV 200
LGAIN 20
LKPHS 210
LKSIG 448389616
CSPED 19 Hz
FILDC
FILDF

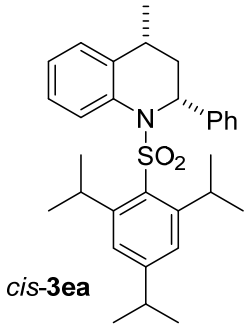


cis-**3ea**

^{13}C NMR spectrum of *cis*-3ea (major)

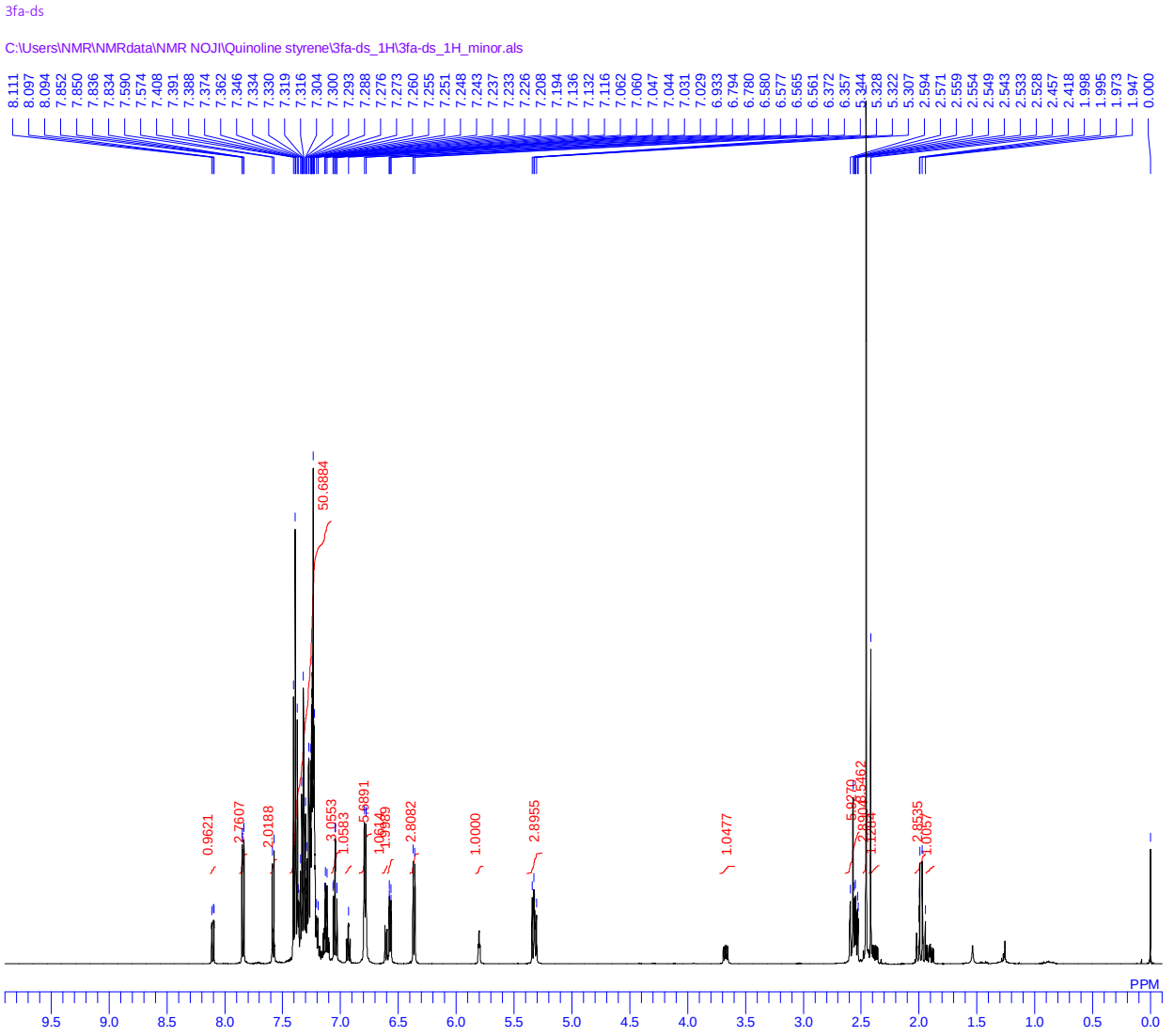


DATIM	Tue Feb 2 22:42:06 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3ea-major(NS12C3)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-583127561
CSPED	11 Hz
FILDC	
FILDF	

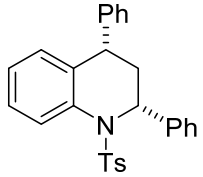


cis-**3ea**

^{1}H NMR spectrum of diastereomixture-3fa (*cis*-major)

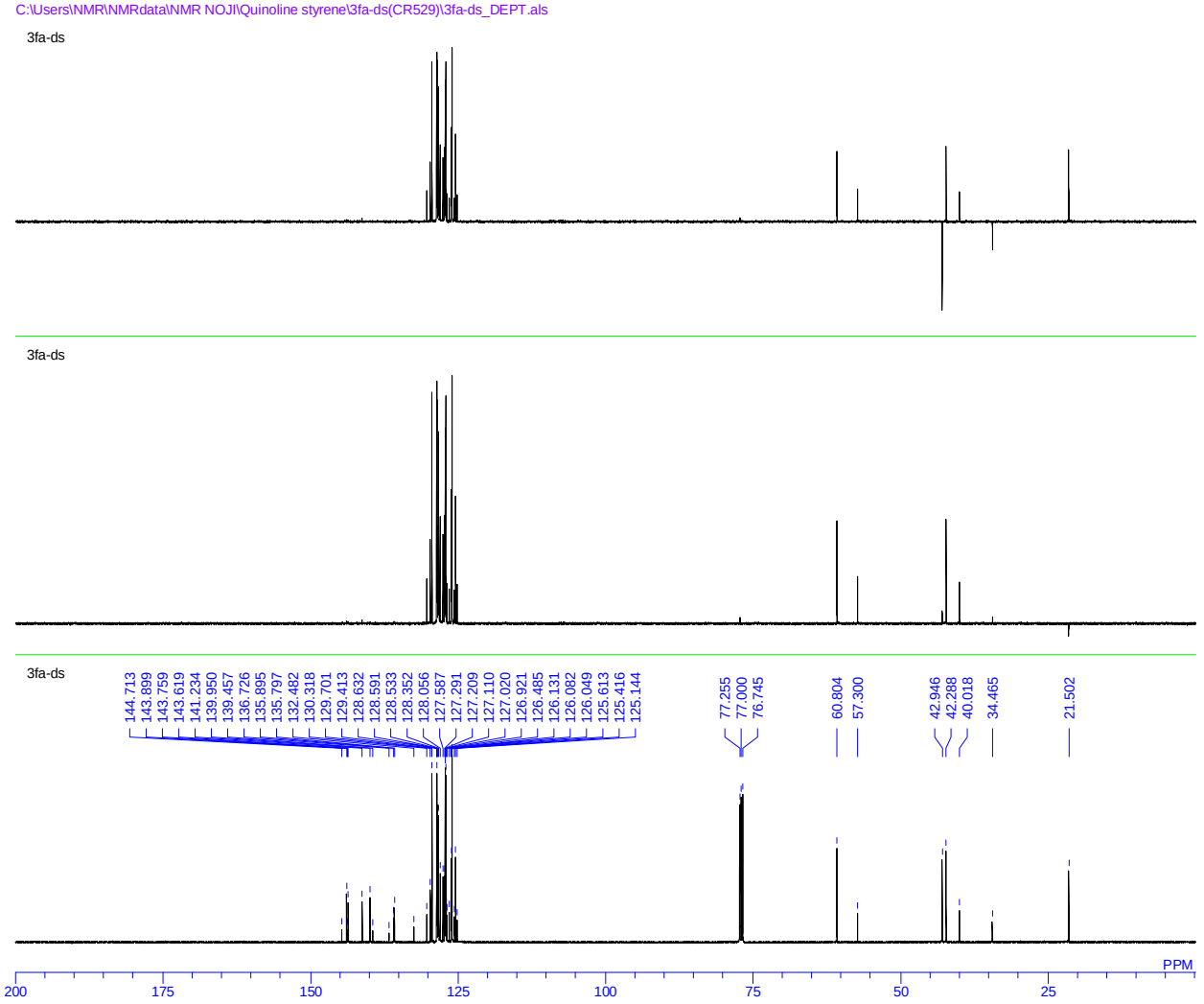


DATIM	Mon Dec 28 21:01:59 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	32
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	15
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3fa-ds_1H_minor.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	29293
CSPED	11 Hz
FILDC	
FILDF	

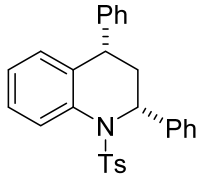


cis-**3fa** (major)

^{13}C NMR spectrum of diastereomixture-3fa (*cis*-major)

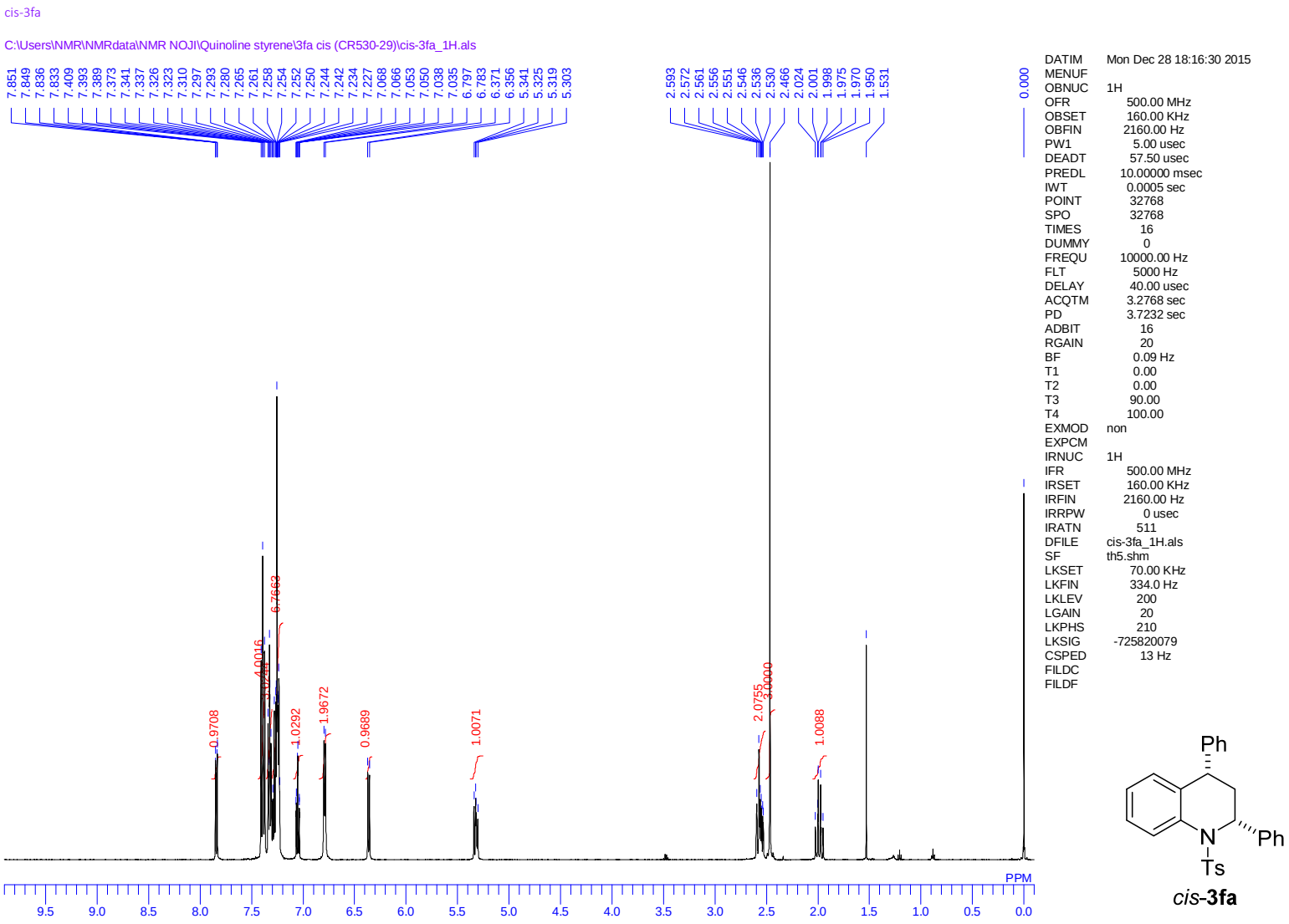


DATIM	Mon Dec 28 22:45:42 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3fa-ds_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	41124
CSPED	11 Hz
FILDC	
FILDF	

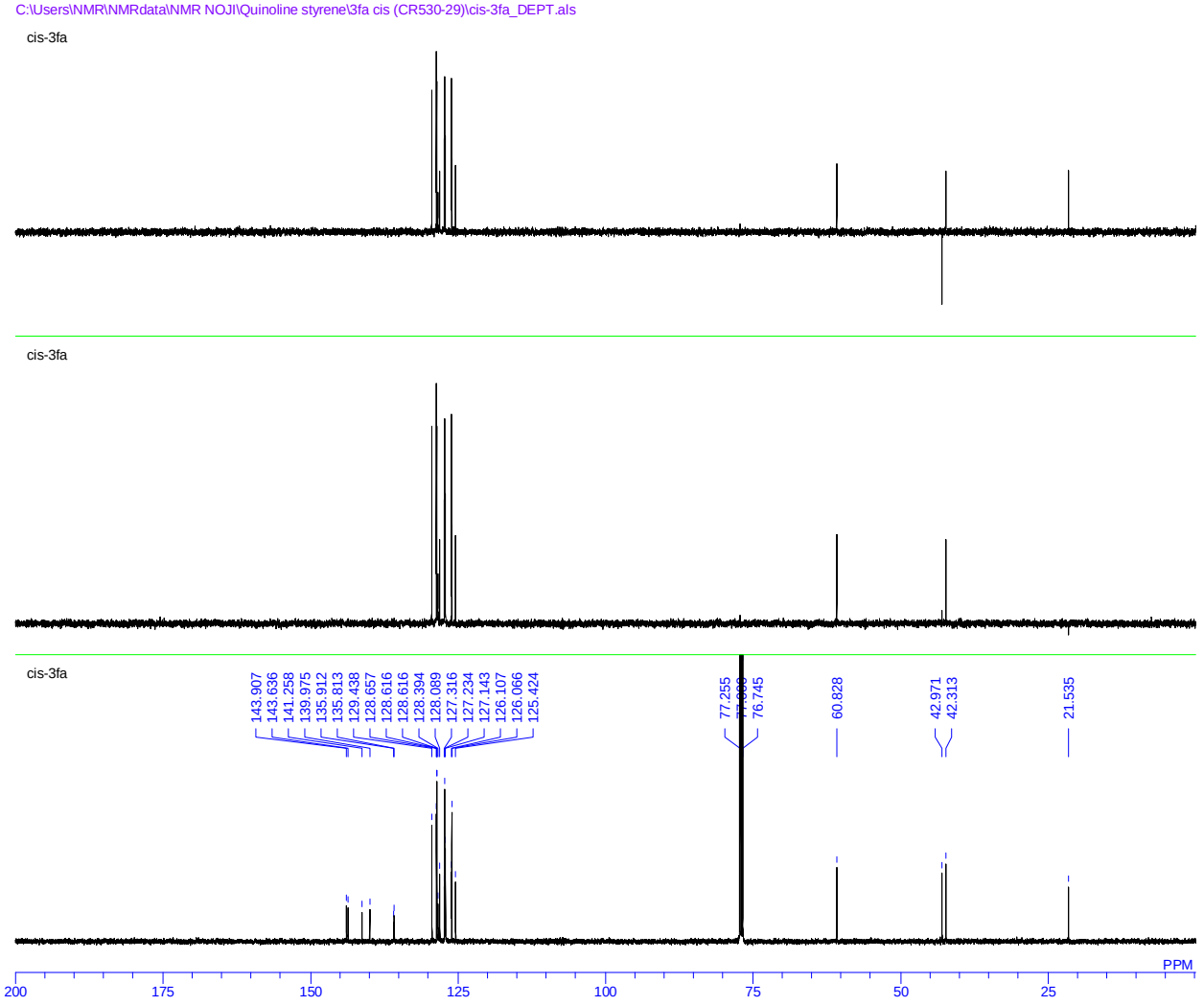


cis-**3fa** (major)

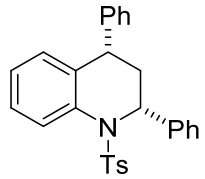
^{1}H NMR spectrum of *cis*-3fa (major)



^{13}C NMR spectrum of *cis*-3fa (major)

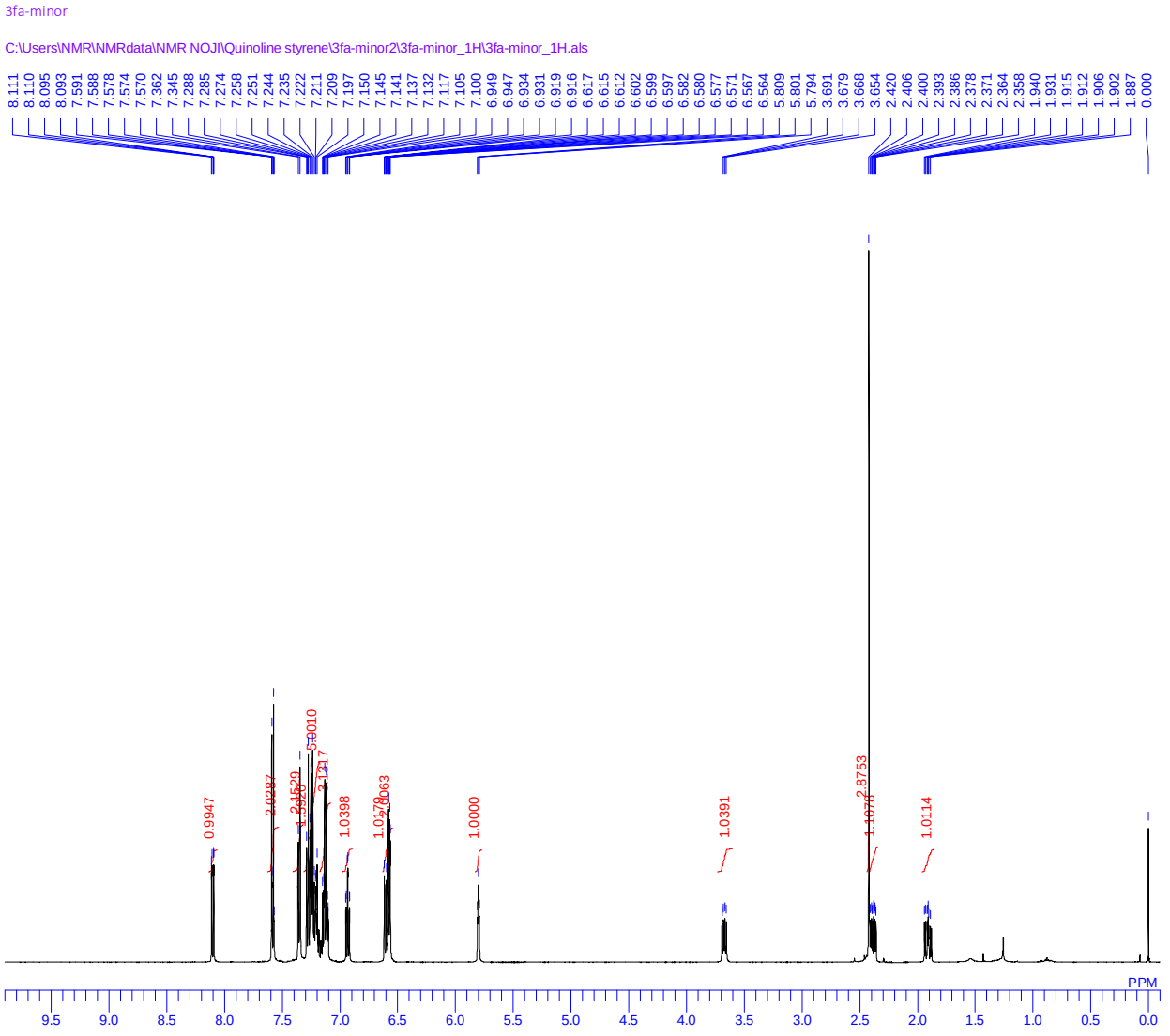


DATIM Mon Dec 28 19:09:01 2015
MENUF
OBNUC 13C
OFR 125.65 MHz
OBSET 120.00 KHz
OBFIN 7958.00 Hz
PW1 4.40 usec
DEADT 15.50 usec
PREDL 10.00000 msec
IWT 0.0100 sec
POINT 32768
SPO 32768
TIMES 1024
DUMMY 1
FREQU 33898.30 Hz
FLT 16950 Hz
DELAY 11.80 usec
ACQTM 0.9667 sec
PD 2.0333 sec
ADBIT 16
RGAIN 28
BF 0.09 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD bcm
EXPCM error_expcm
IRNUC 1H
IFR 500.00 MHz
IRSET 160.00 KHz
IRFIN 2160.00 Hz
IRRPW 0 usec
IRATN 511
DFILE cis-3fa_DEPT.als
SF th5.shm
LKSET 70.00 KHz
LKFIN 334.0 Hz
LKLEV 200
LGAIN 20
LKPHS 210
LKSIG 486
CSPED 10 Hz
FILDC
FILDF

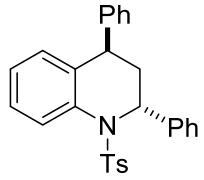


cis-**3fa**

^{1}H NMR spectrum of *trans*-3fa (minor)

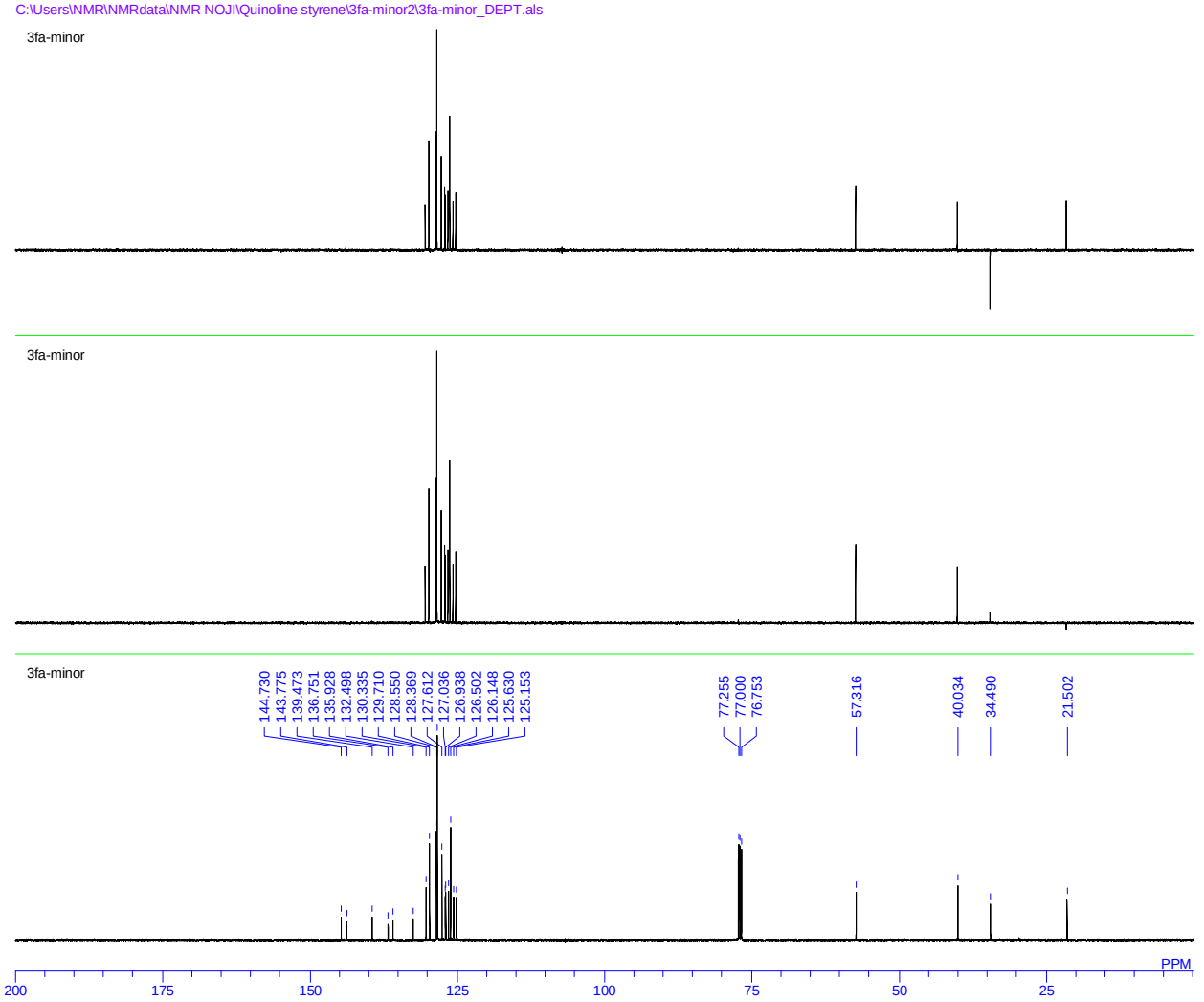


DATIM	Wed Dec 30 18:50:07 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3fa-minor_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-4488546
CSPED	10 Hz
FILDC	
FILDF	

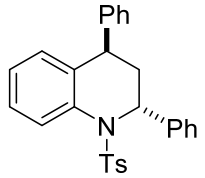


trans-**3fa**

^{13}C NMR spectrum of *trans*-3fa (minor)

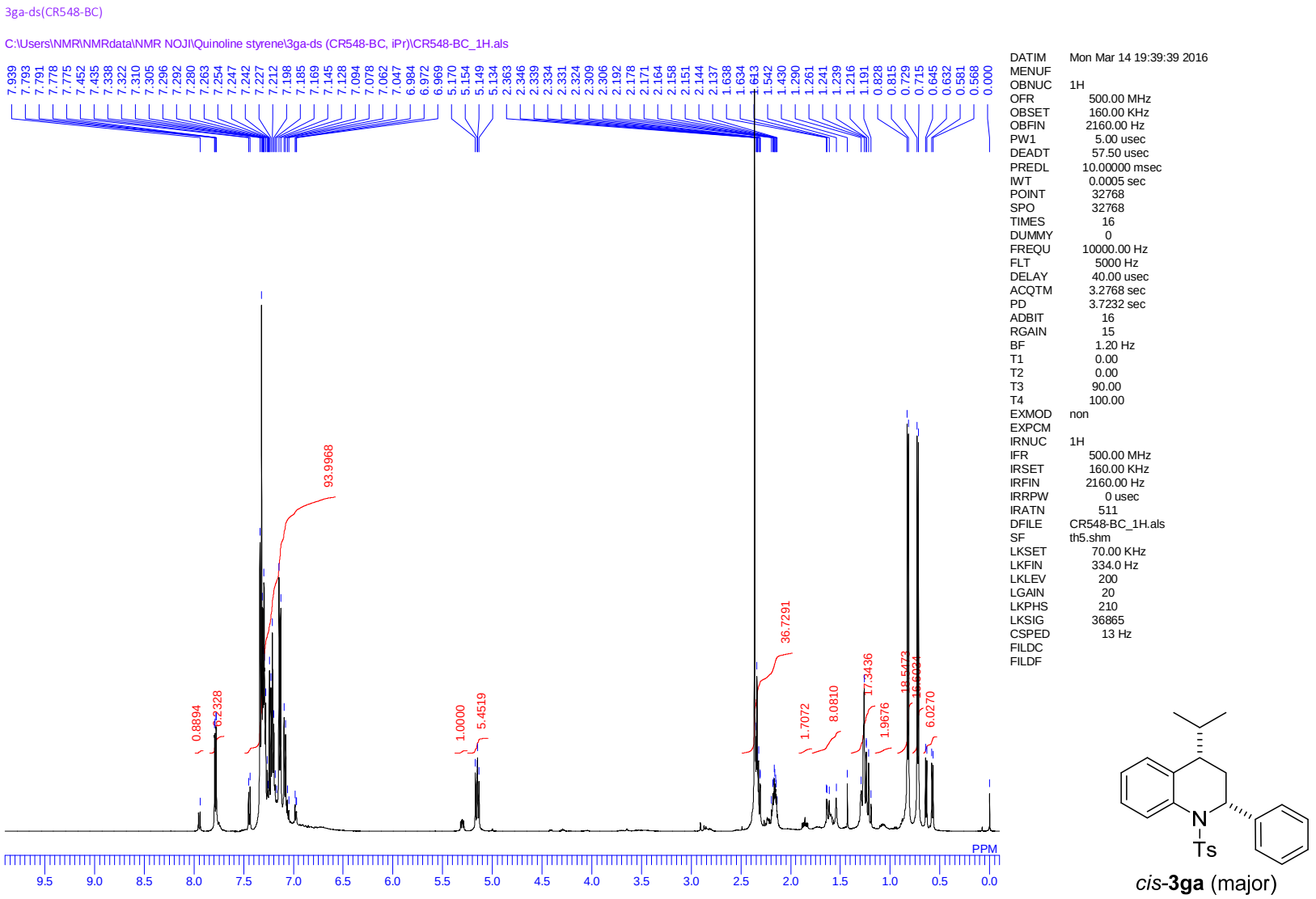


DATIM	Wed Dec 30 19:42:38 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3fa-minor_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	19564
CSPED	10 Hz
FILDC	
FILDF	

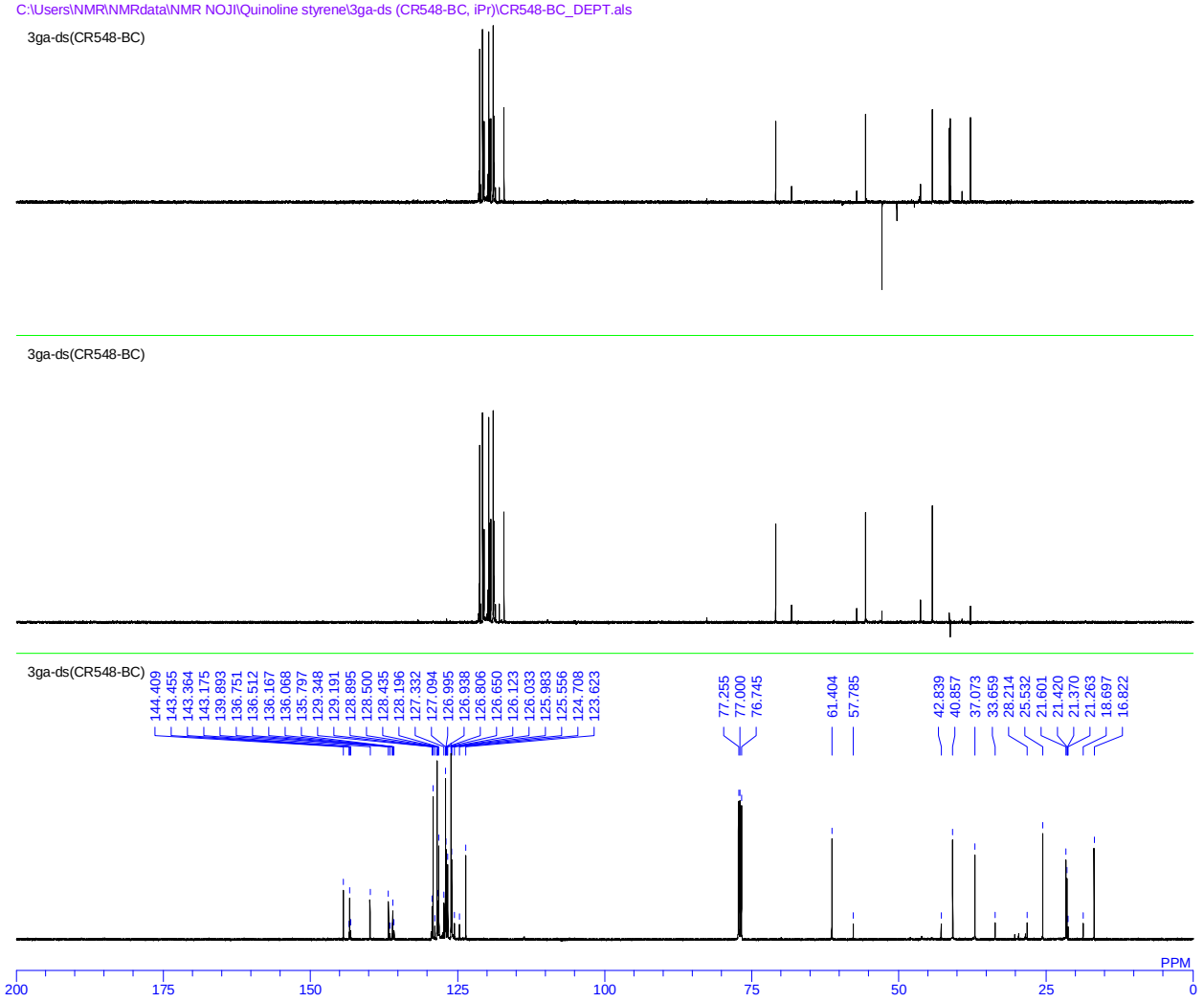


trans-**3fa**

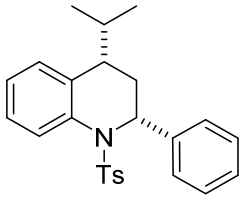
^{1}H NMR spectrum of diastereomixture-3ga (*cis*-major)



^{13}C NMR spectrum of diastereomixture-3ga (*cis*-major)

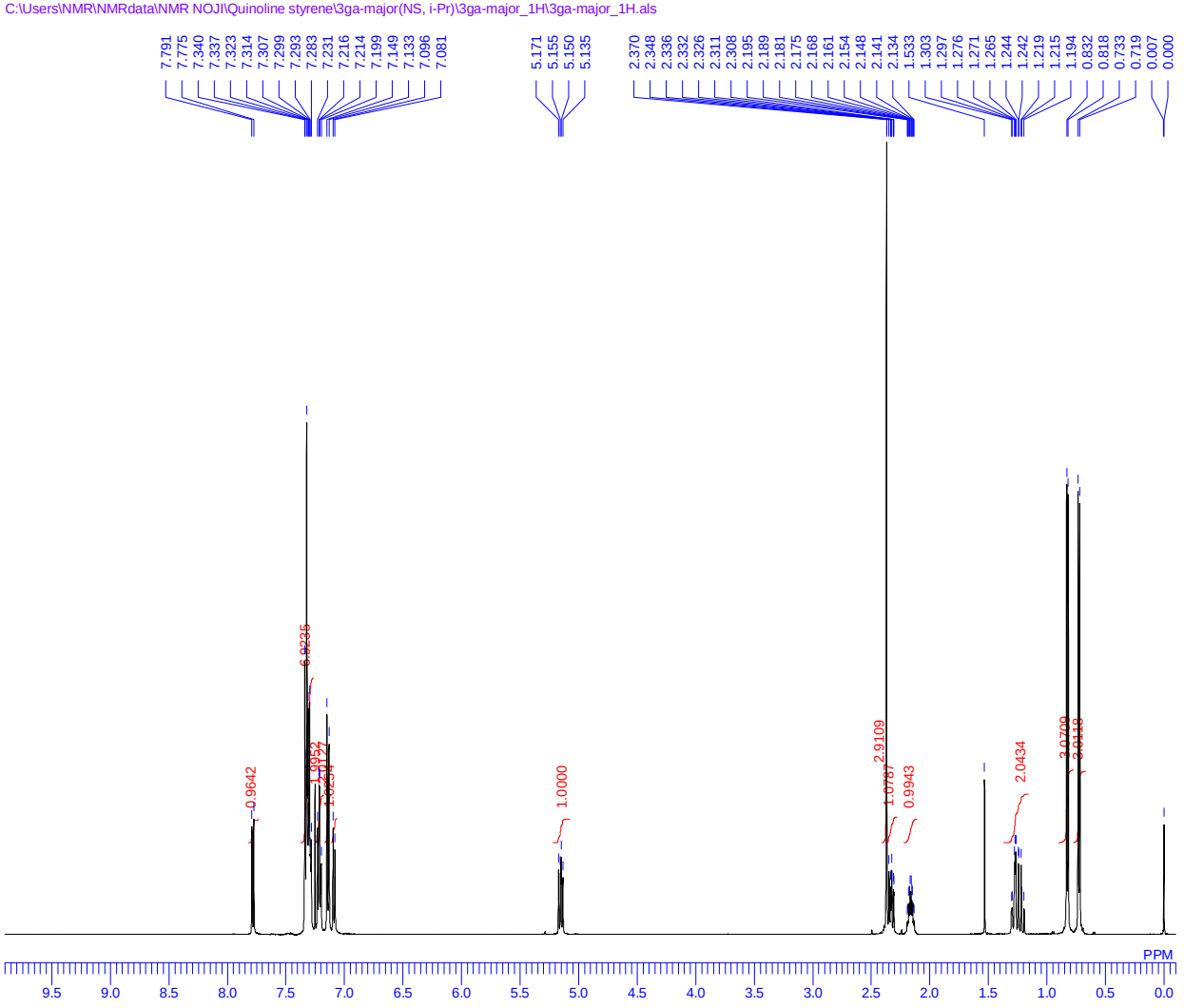


DATIM	Mon Mar 14 21:23:31 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR548-BC_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	8843
CSPED	11 Hz
FILDC	
FILDF	

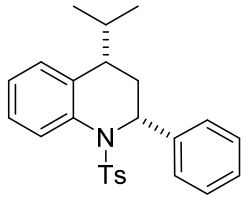


cis-**3ga** (major)

^{1}H NMR spectrum of *cis*-3ga (major)

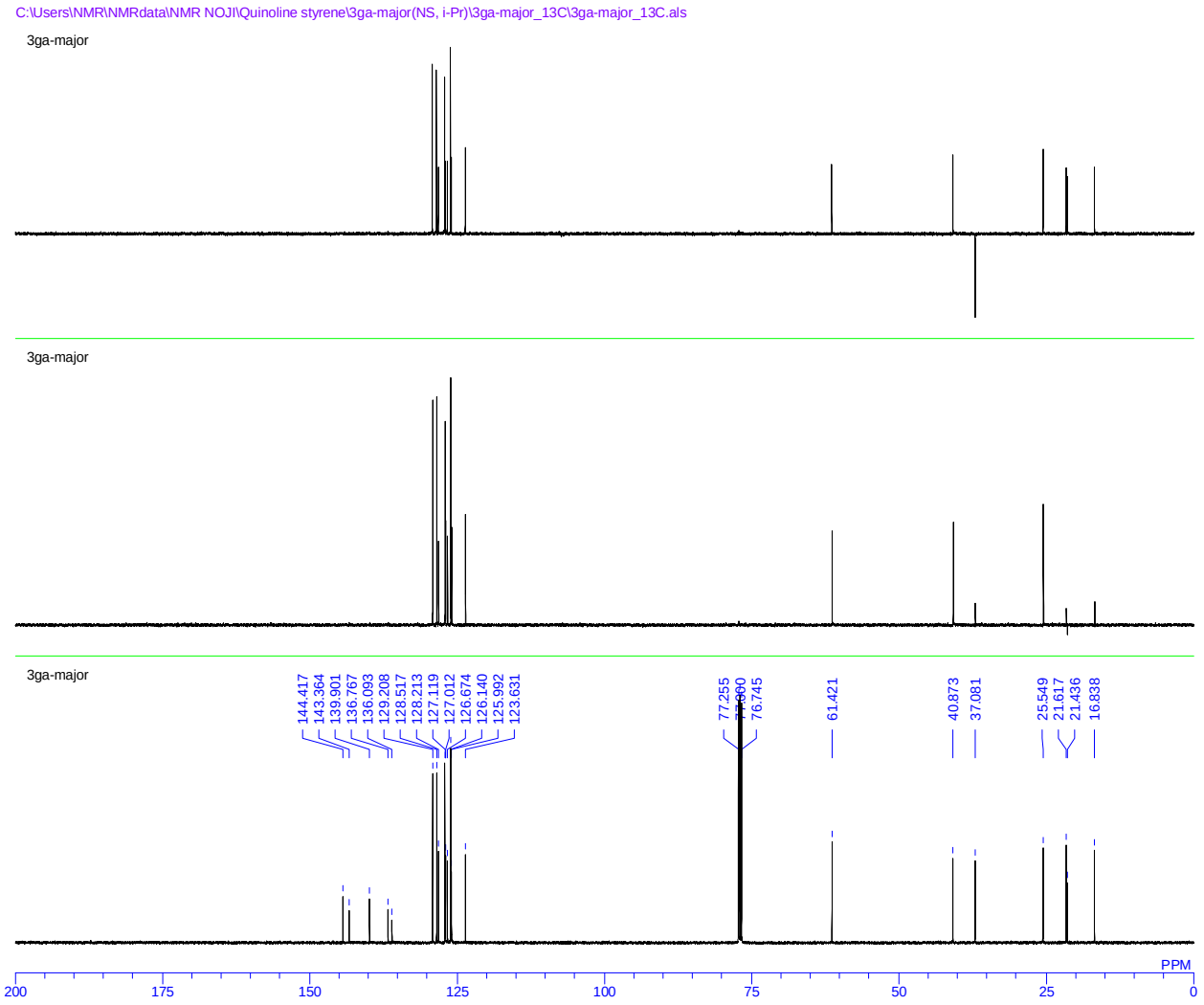


DATIM	Mon Feb 15 17:51:17 2016
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	19
BF	1.21 Hz
T1	0.00
T2	0.00
T3	70.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3ga-major_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	26881
CSPED	12 Hz
FILDC	
FILDF	

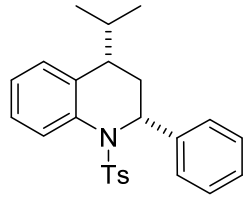


cis-**3ga**

^{13}C NMR spectrum of *cis*-3ga (major)

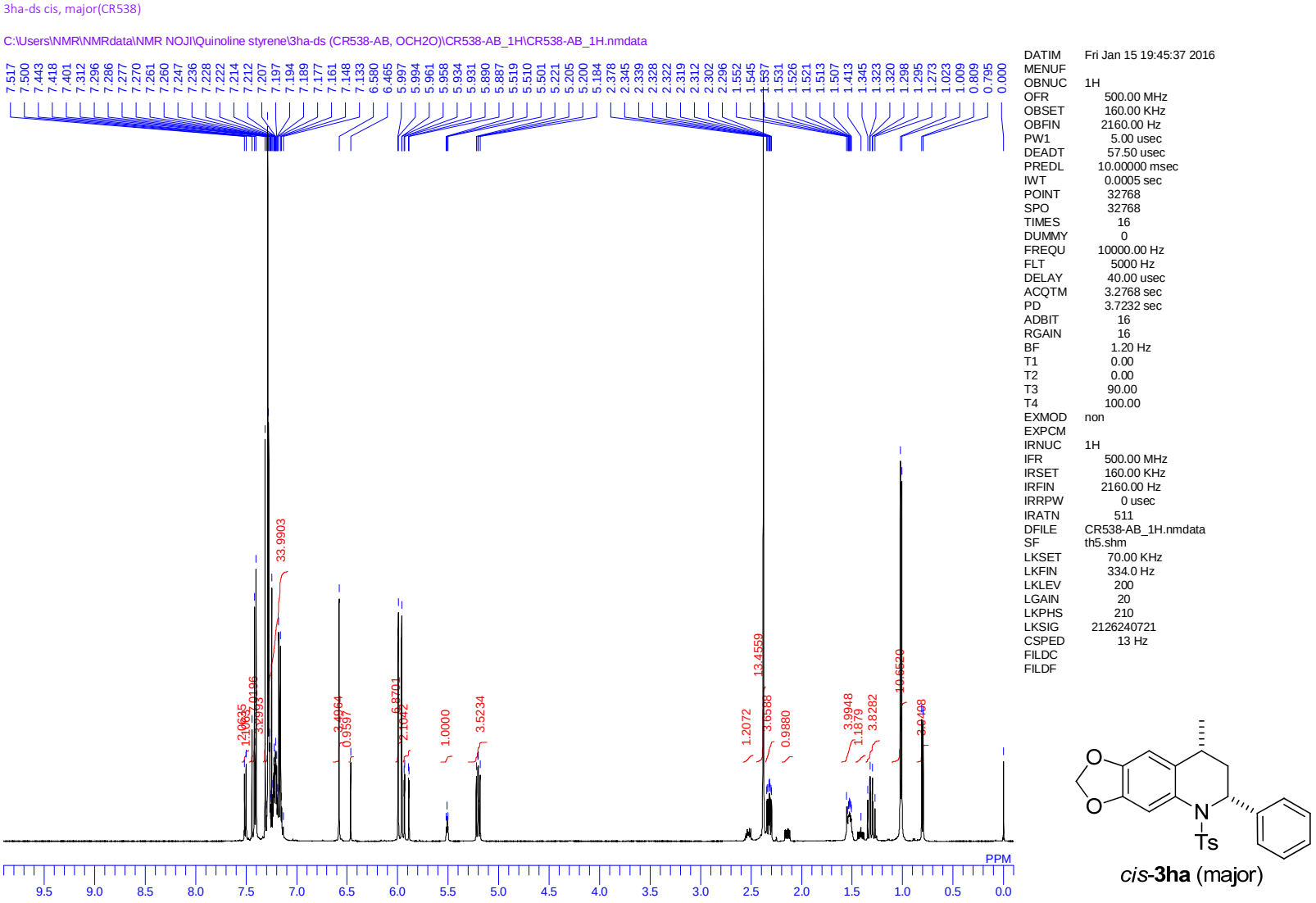


DATIM	Mon Feb 15 19:35:02 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.21 Hz
T1	0.00
T2	0.00
T3	70.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3ga-major_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	37396
CSPED	12 Hz
FILDC	
FILDF	

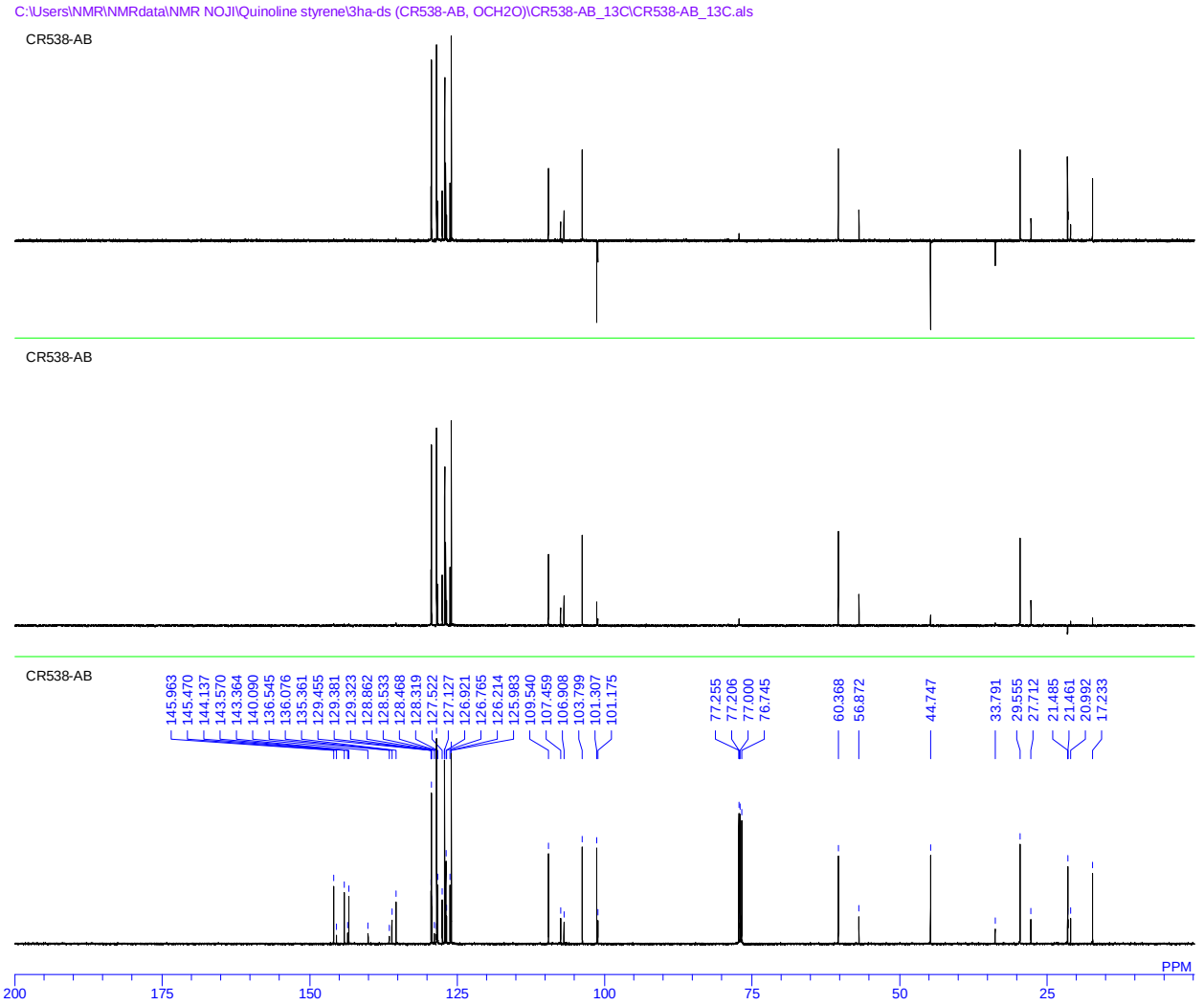


cis-**3ga**

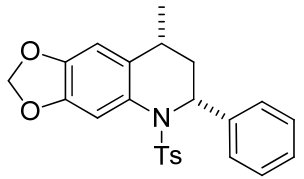
^{1}H NMR spectrum of diastereomixture-3ha (*cis*-major)



^{13}C NMR spectrum of diastereomixture-3ha (*cis*-major)

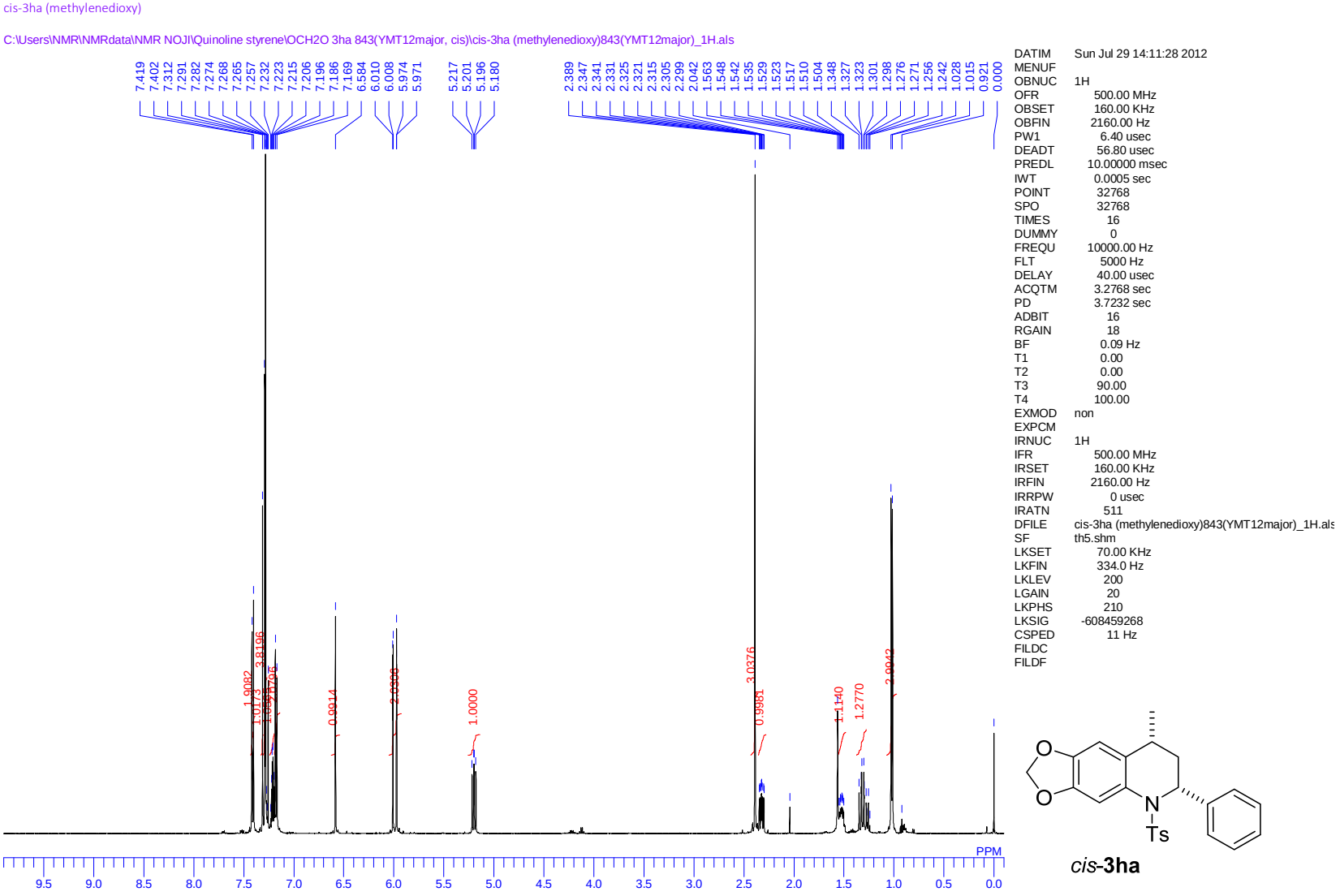


DATIM	Fri Jan 15 20:38:08 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR538-AB_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-599926122
CSPED	10 Hz
FILDC	
FILDF	

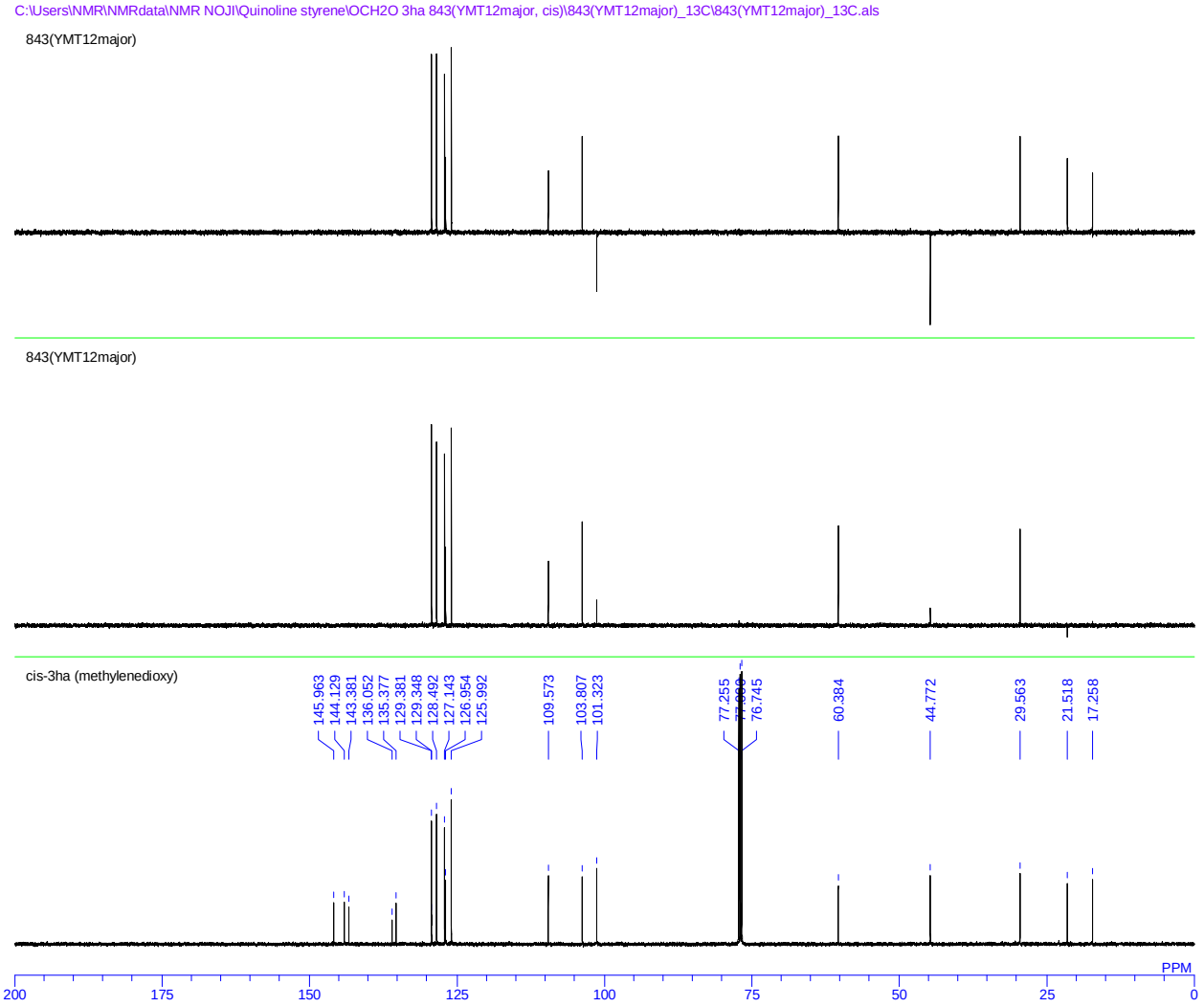


cis-**3ha** (major)

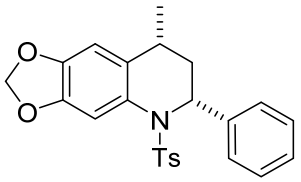
^{1}H NMR spectrum of *cis*-3ha (major)



^{13}C NMR spectrum of *cis*-3ha (major)

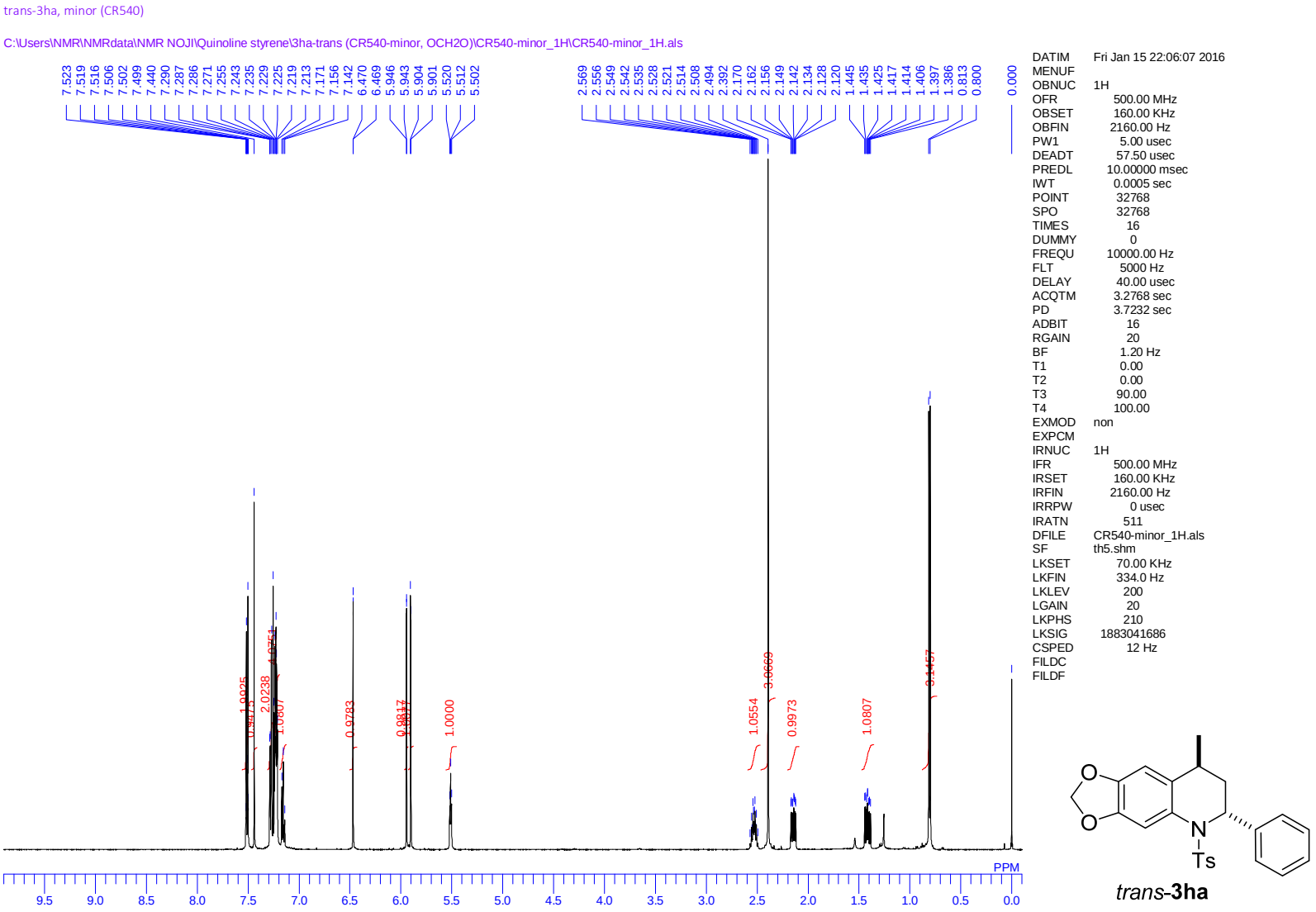


DATIM	Sun Jul 29 15:03:52 2012
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	5.40 usec
DEADT	10.00 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	843(YMT12major)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	129864346
CSPED	12 Hz
FILDC	
FILDF	

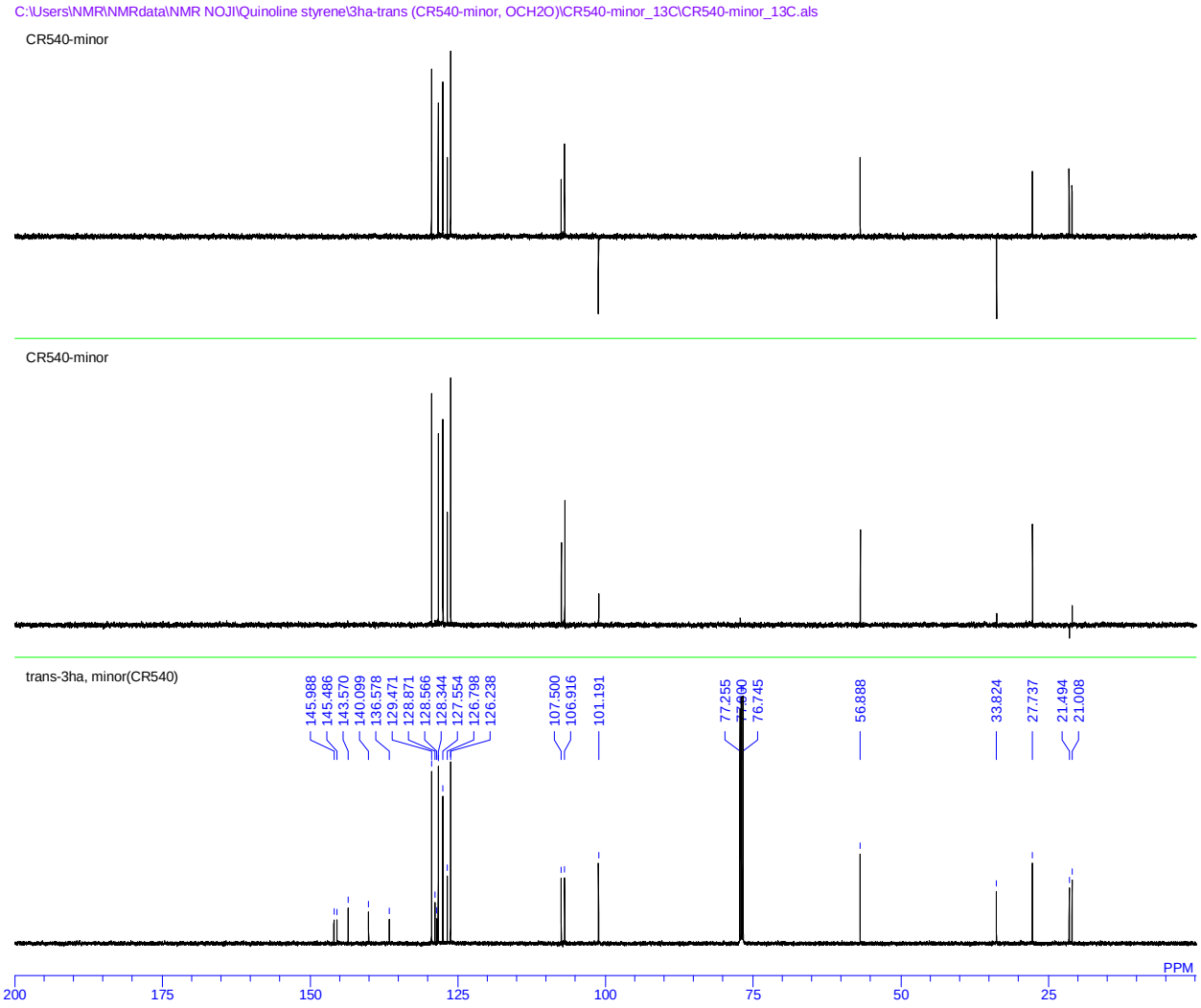


cis-**3ha**

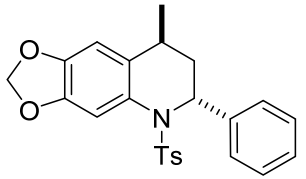
^{1}H NMR spectrum of *trans*-3ha (minor)



^{13}C NMR spectrum of *trans*-3ha (minor)

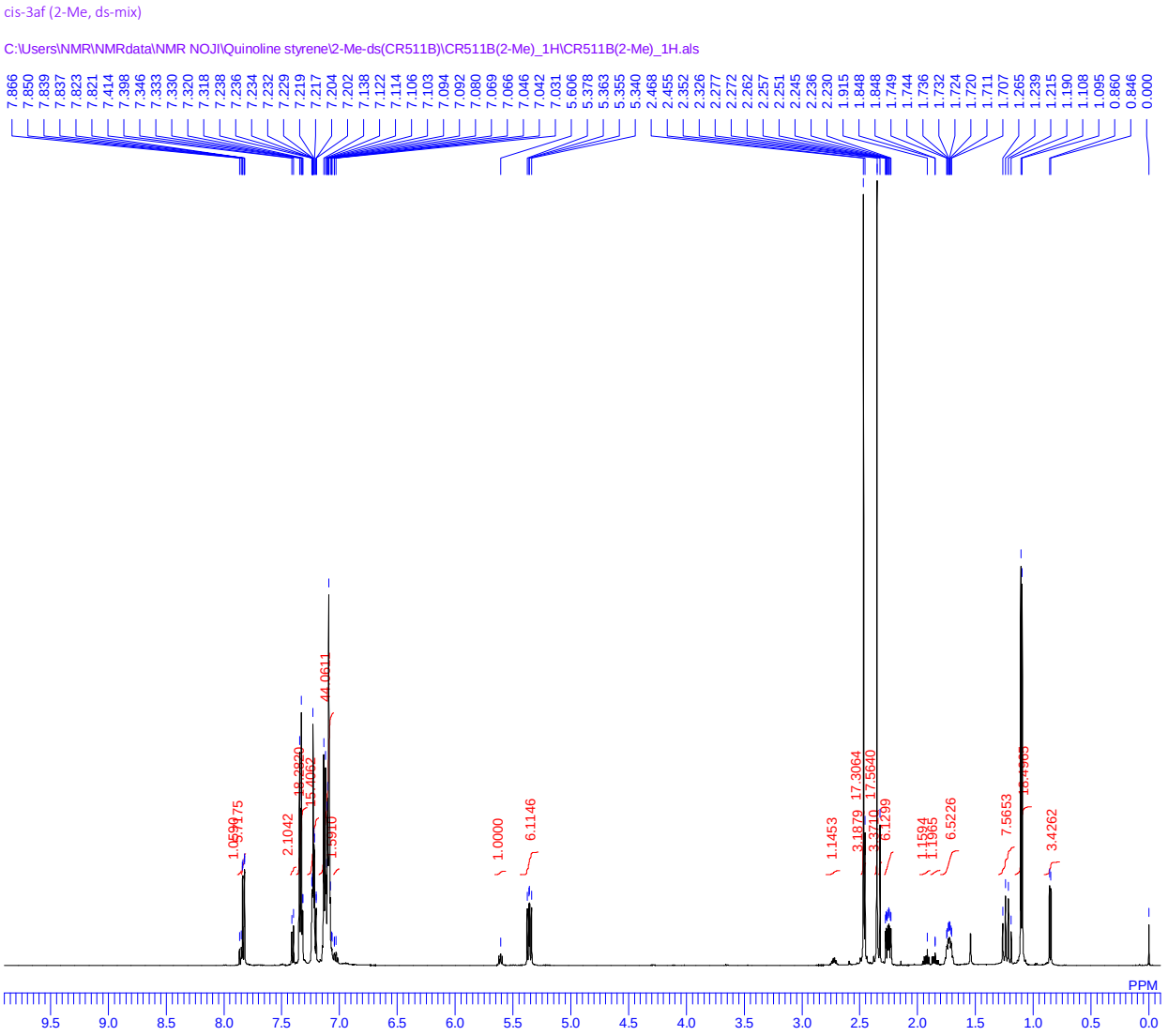


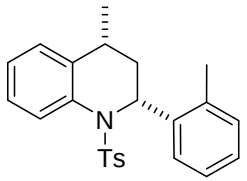
DATIM	Fri Jan 15 22:58:39 2016
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR540-minor_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	29274317
CSPED	13 Hz
FILDC	
FILDF	



trans-**3ha**

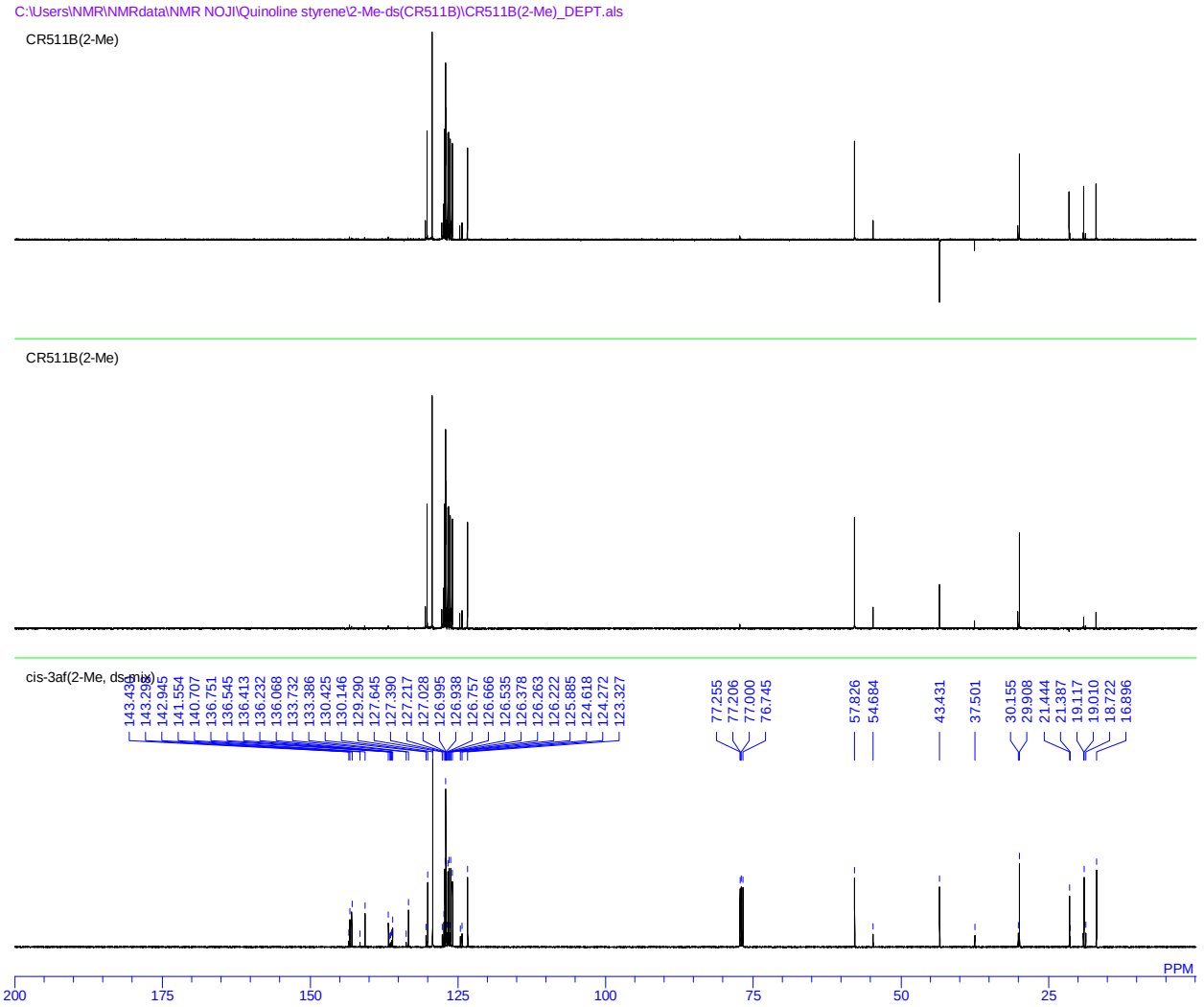
^{1}H NMR spectrum of diastereomixture-3ab (*cis*-major)



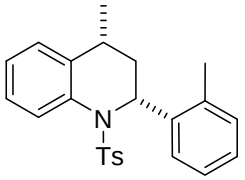


cis-**3ab** (major)

^{13}C NMR spectrum of diastereomixture-3ab (*cis*-major)

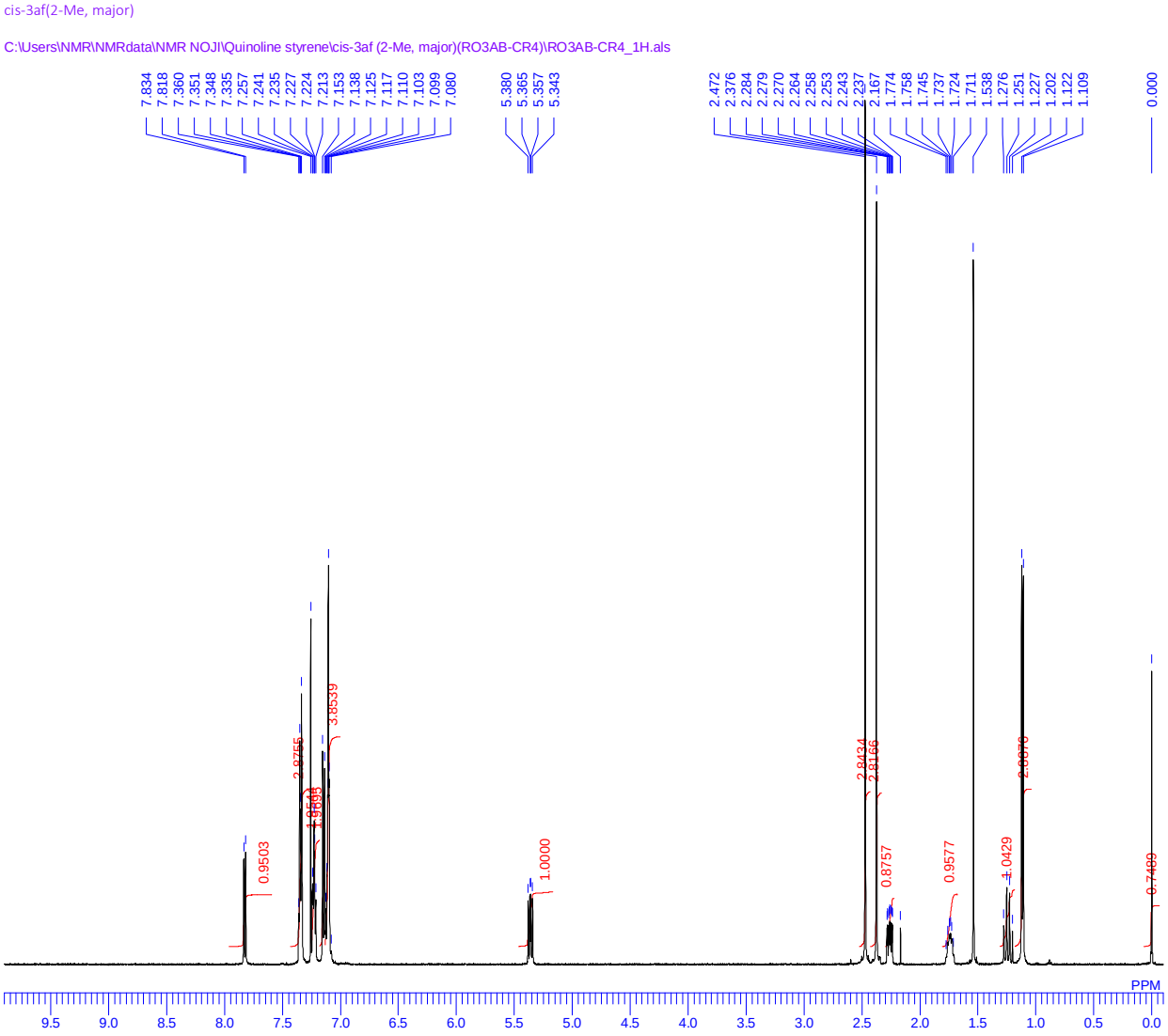


DATIM	Tue Jul 7 21:00:28 2015
DF	
COMNT	cis-3af(2-Me, ds-mix)
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
PW2	50.00 usec
PW3	12.00 usec
PI1	5660.0000 msec
PI2	0.2500 msec
PI3	1.0000 msec
LOOP1	1
POINT	32768
SPO	32768
SCANS	1024
DUMMY	1
FREQU	33898.30 Hz
ACQTM	0.9667 sec
PD	2.0333 sec
RGAIN	28
BF	0.12 Hz
EXMOD	bcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
CSPED	12 Hz
CTEMP	29.8 c
XE	25153.72 Hz
XS	62.07 Hz

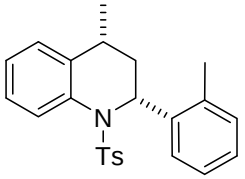


cis-**3ab** (major)

^{1}H NMR spectrum of *cis*-3ab (major)

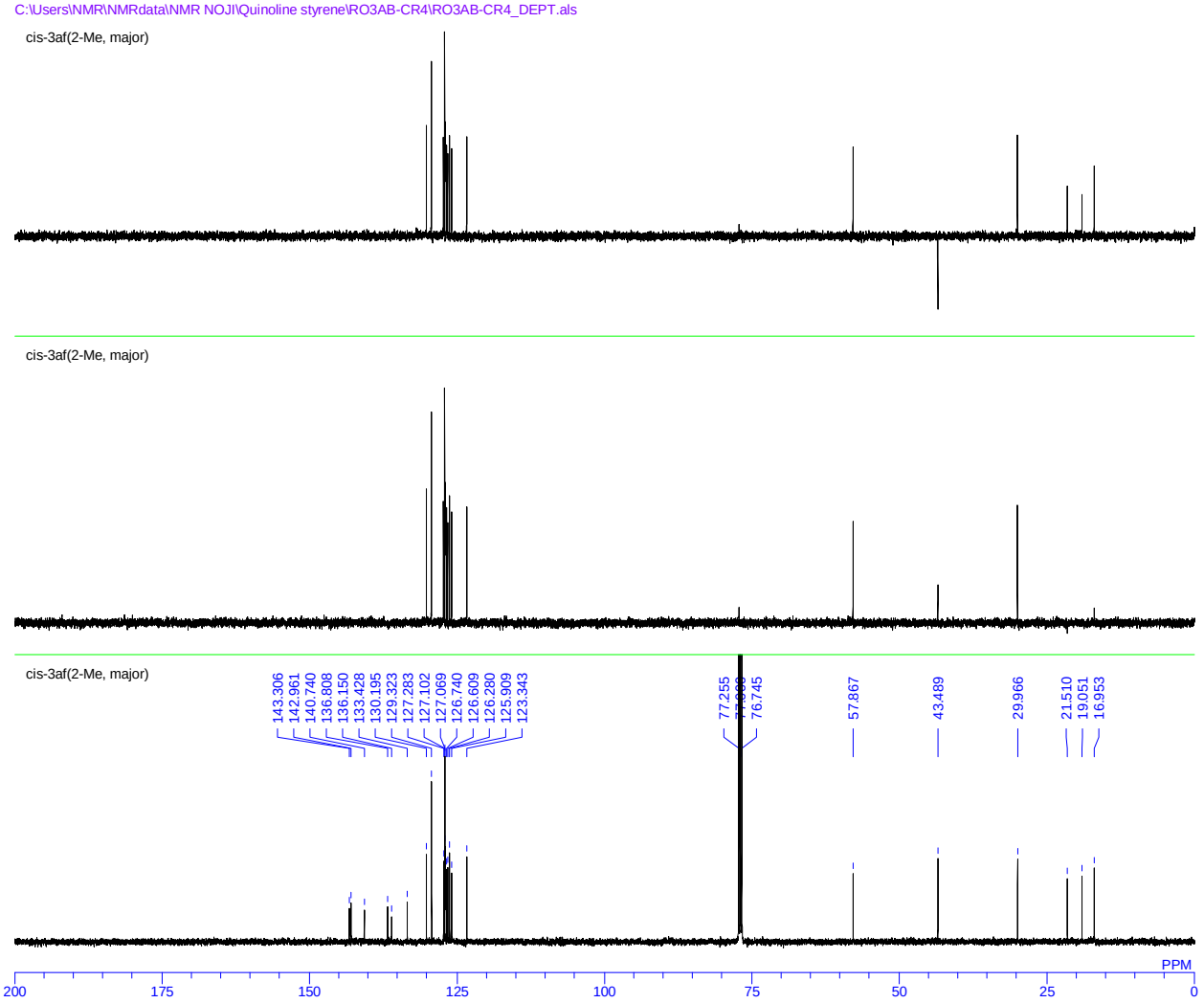


DATIM	Fri May 23 18:53:37 2014
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	23
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	RO3AB-CR4_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	37466
CSPED	13 Hz
FILDC	
FILDF	

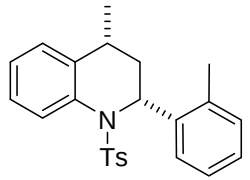


***cis*-3ab**

^{13}C NMR spectrum of *cis*-3ab (major)

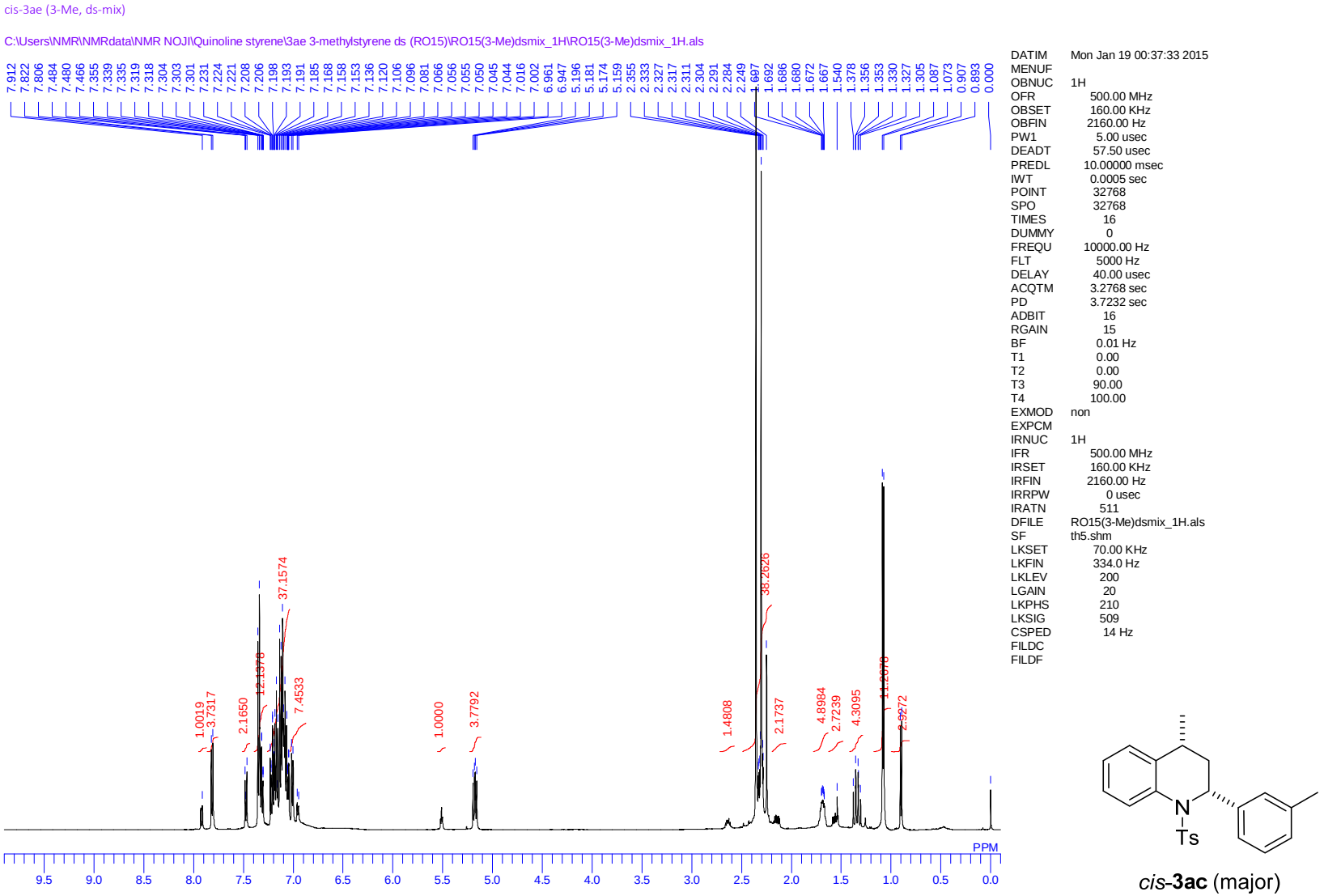


DATIM	Fri May 23 20:37:22 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	RO3AB-CR4_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	9283
CSPED	15 Hz
FILDC	
FILDF	

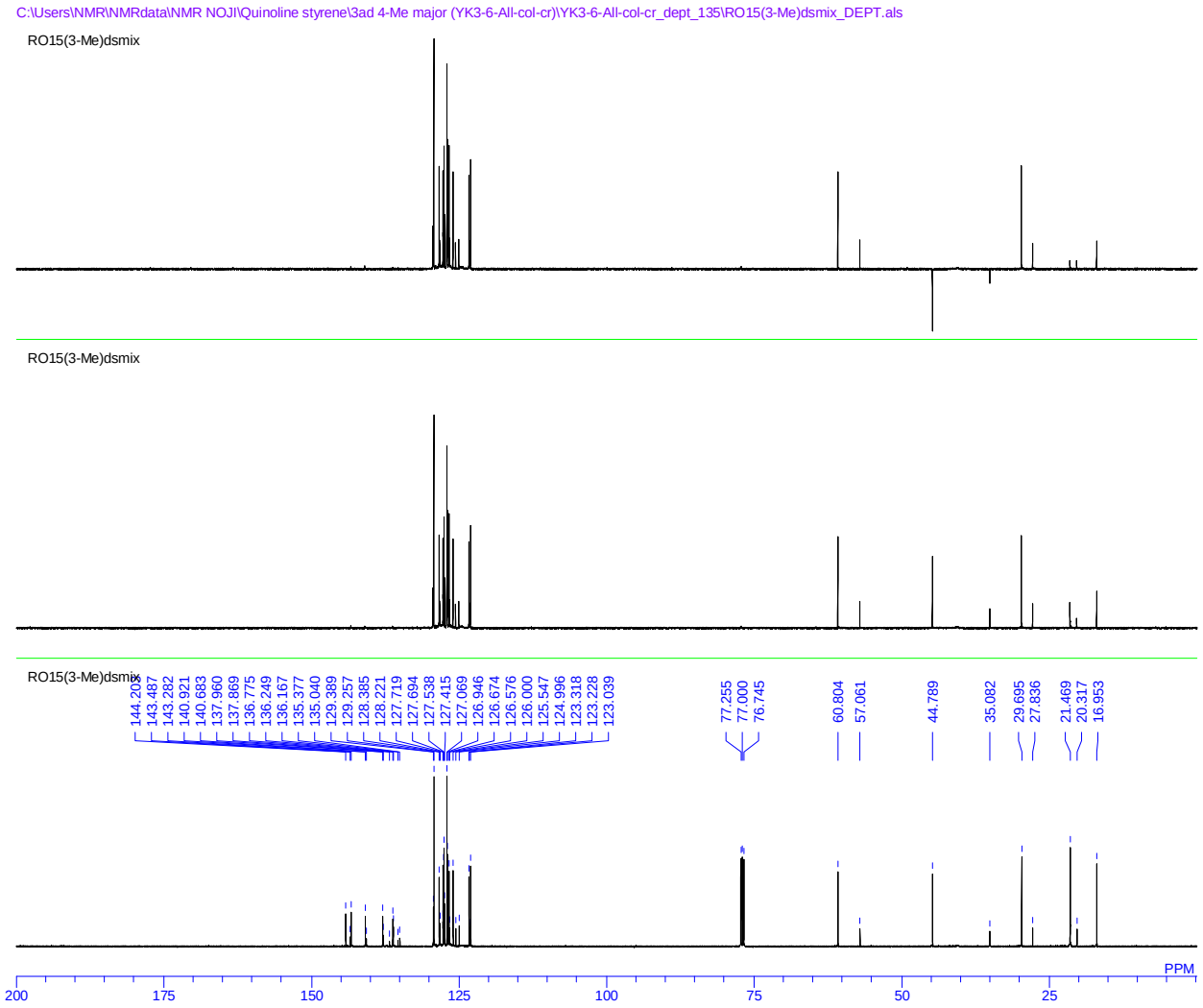


cis-**3ab**

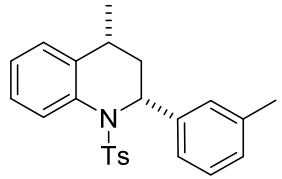
^{1}H NMR spectrum of diastereomixture-3ac (*cis*-major)



^{13}C NMR spectrum of diastereomixture-3ac (*cis*-major)

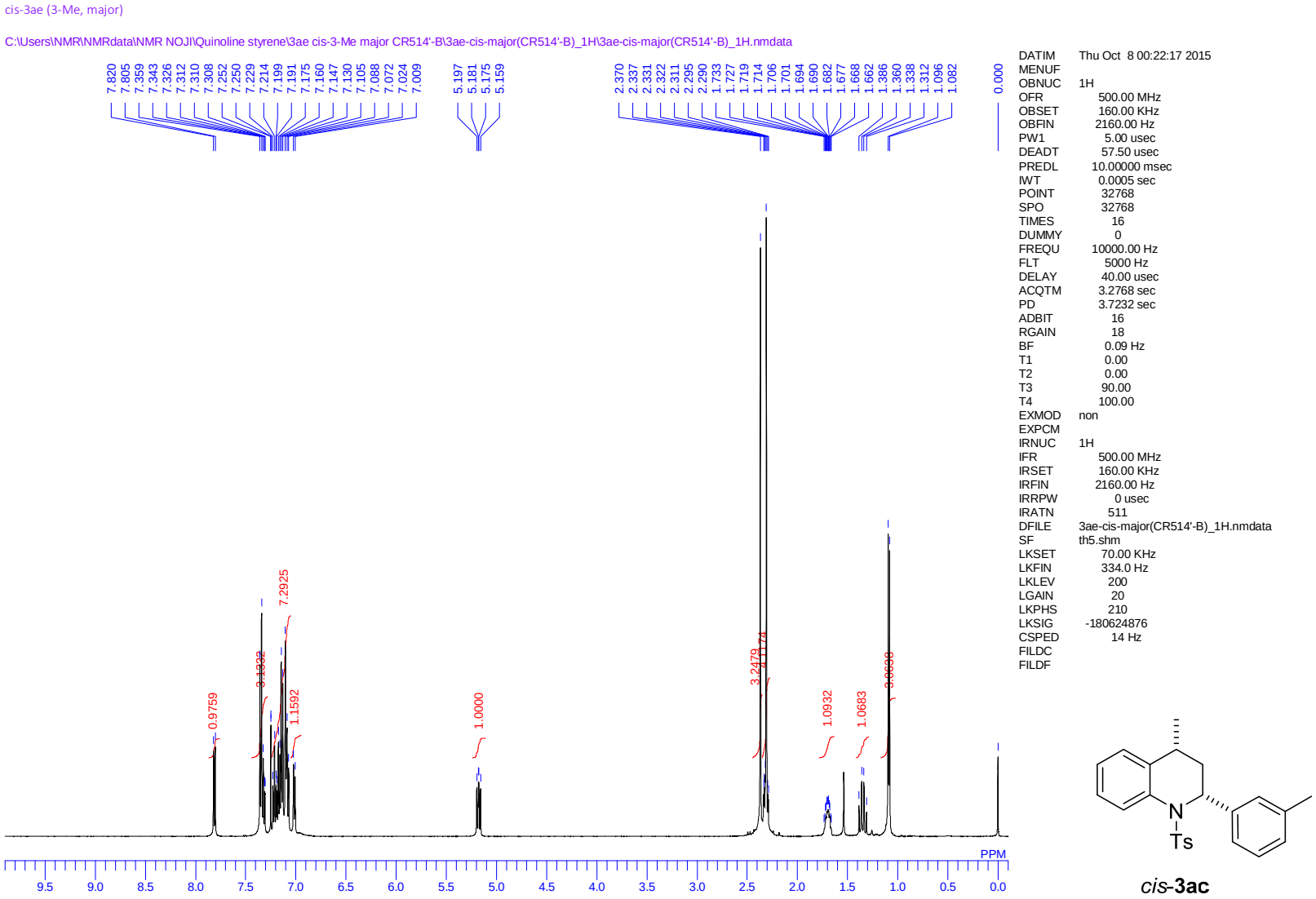


DATIM	Mon Jan 19 01:58:49 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1600
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.01 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	RO15(3-Me)dsmix_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	16764
CSPED	11 Hz
FILDC	
FILDF	

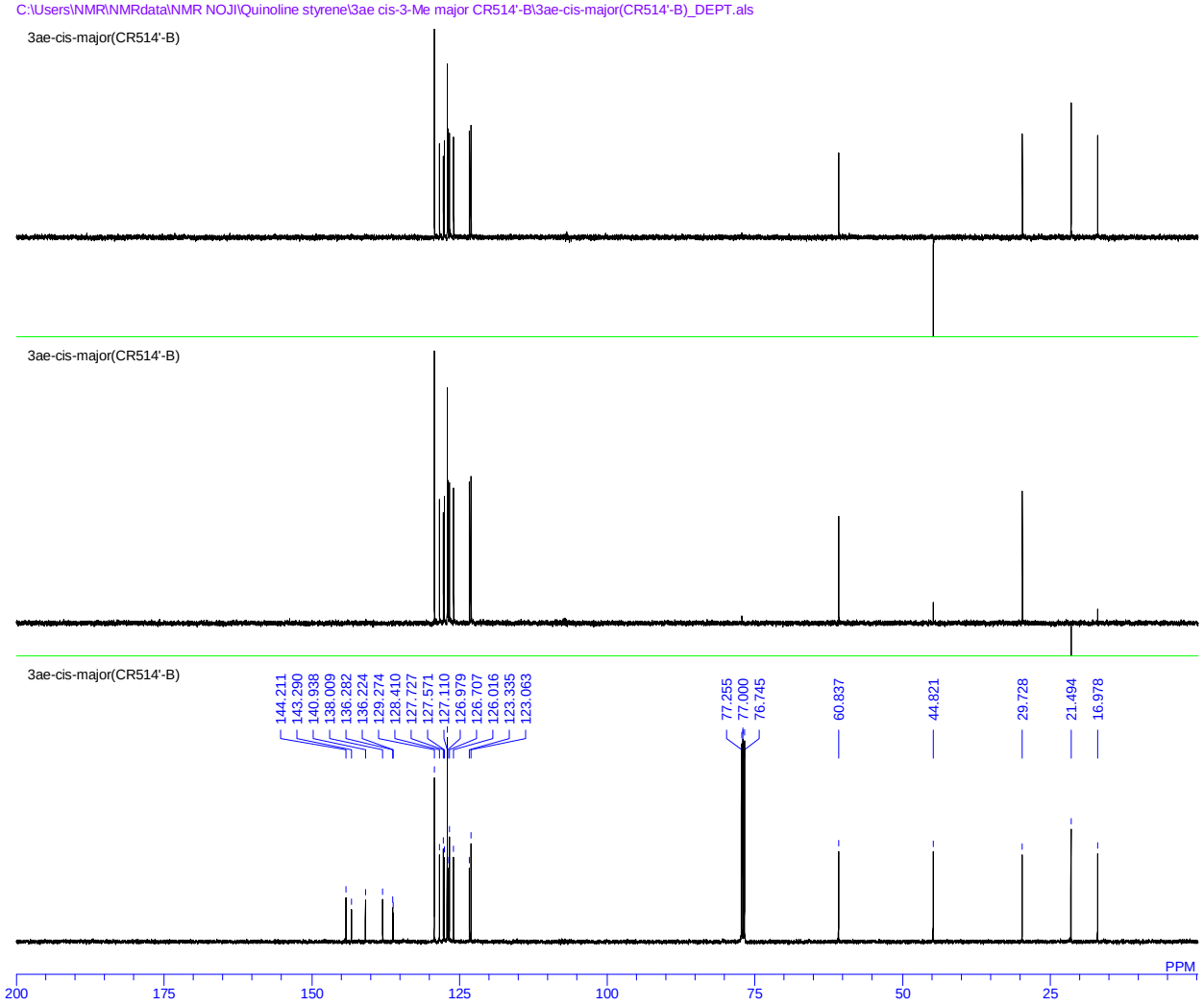


cis-**3ac** (major)

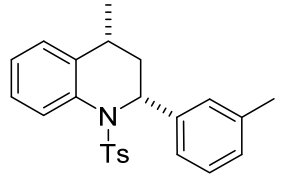
^{1}H NMR spectrum of *cis*-3ac (major)



^{13}C NMR spectrum of *cis*-3ac (major)

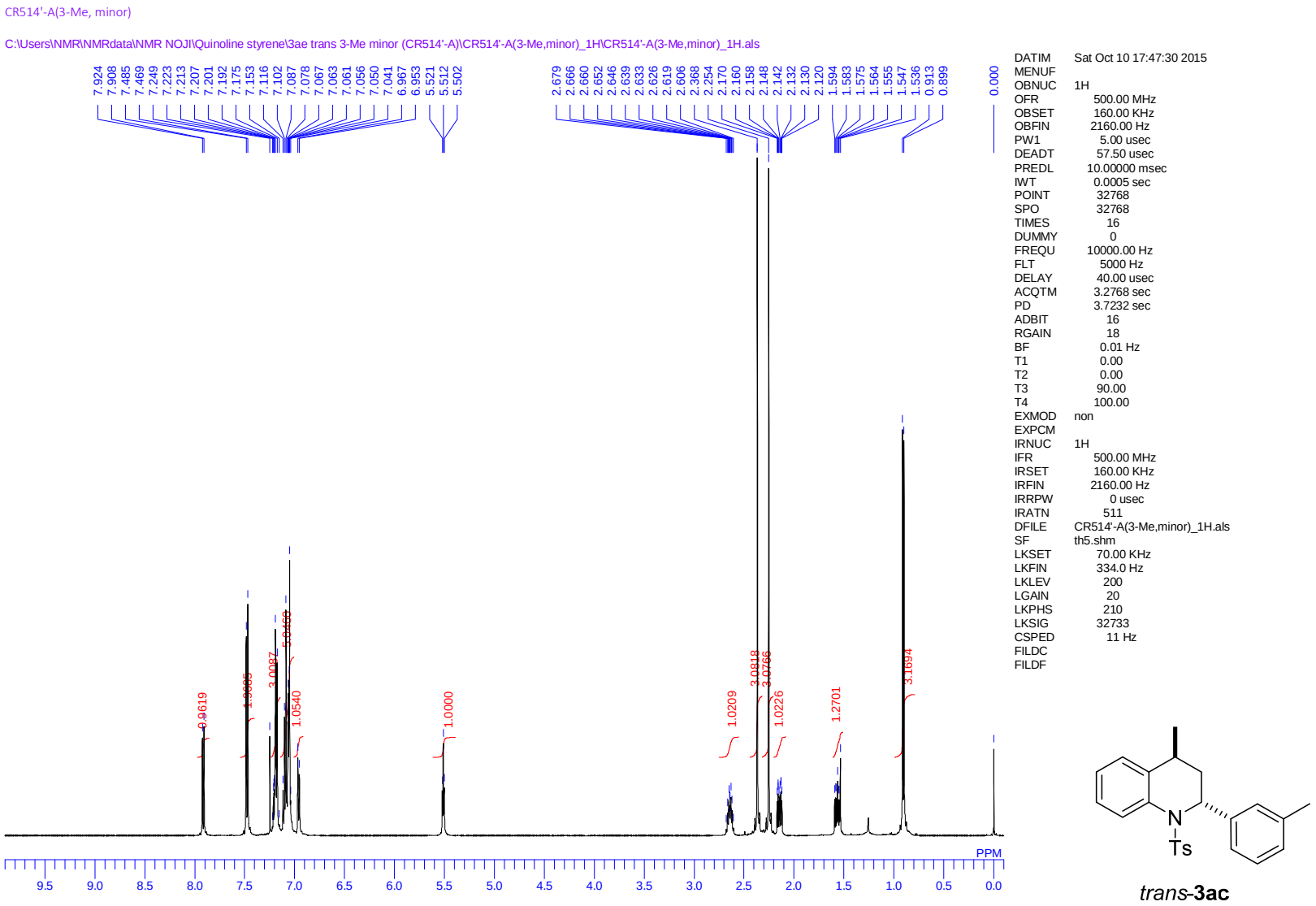


DATIM	Thu Oct 8 01:14:48 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3ae-cis-major(CR514'-B)_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-96584901
CSPED	11 Hz
FILDC	
FILDF	



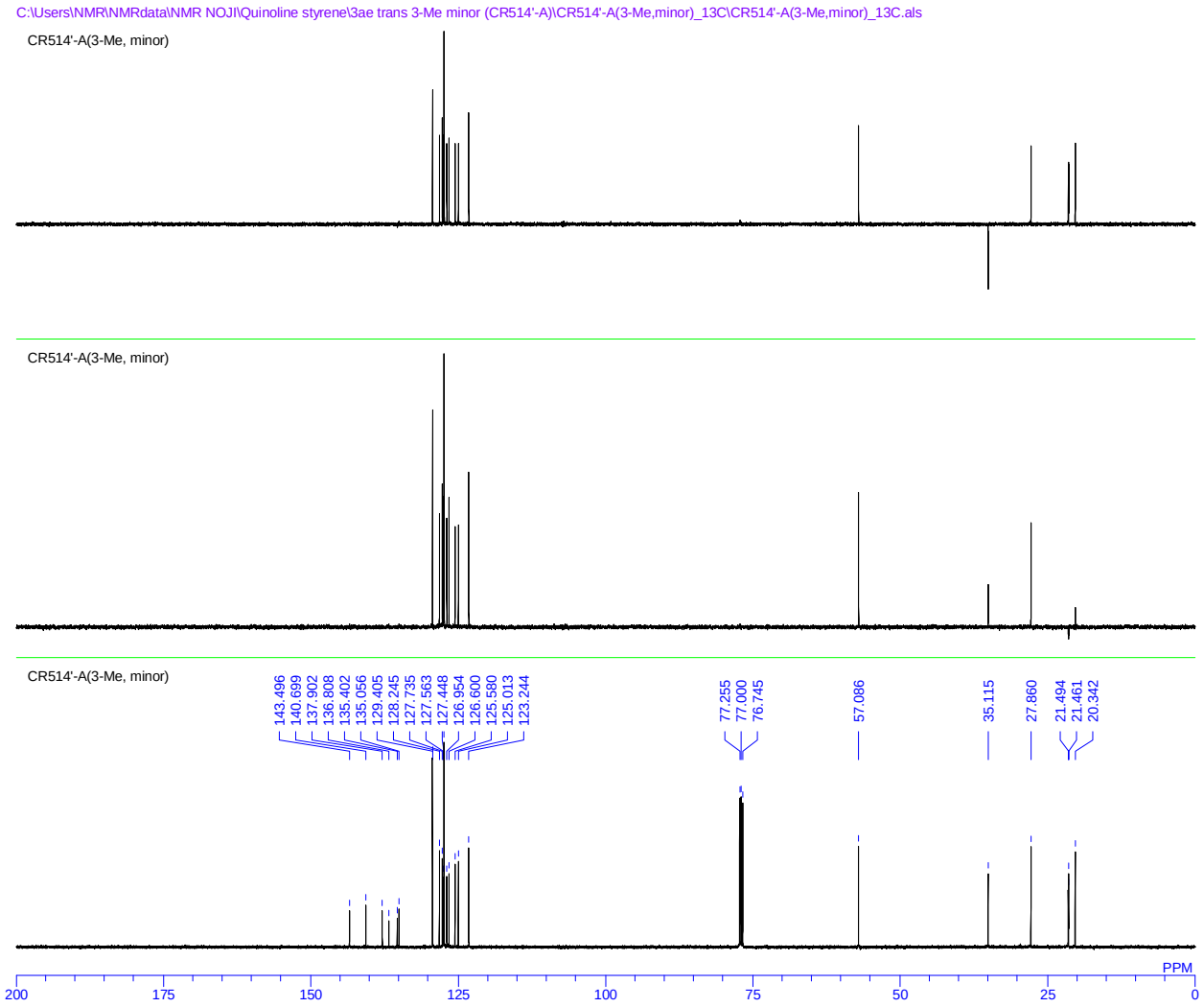
cis-**3ac**

^{1}H NMR spectrum of *trans*-3ac (minor)

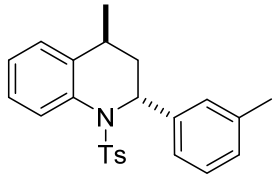


trans-**3ac**

^{13}C NMR spectrum of *trans*-3ac (minor)

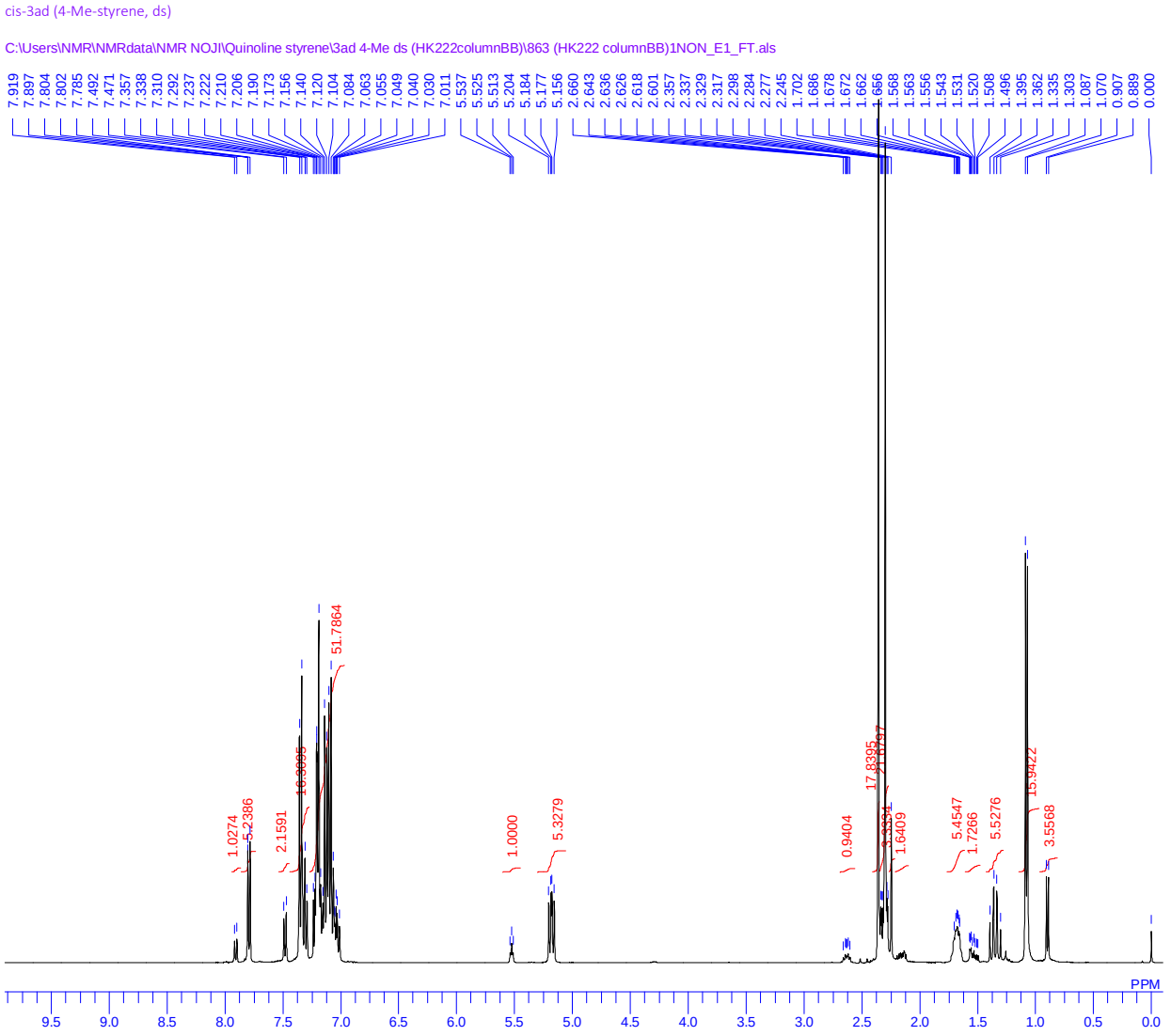


DATIM	Sat Oct 10 18:28:49 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.01 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR514'-A(3-Me,minor)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	12794
CSPED	12 Hz
FILDC	
FILDF	

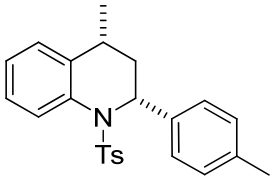


trans-**3ac**

^{1}H NMR spectrum of diastereomixture-3ad (*cis*-major)

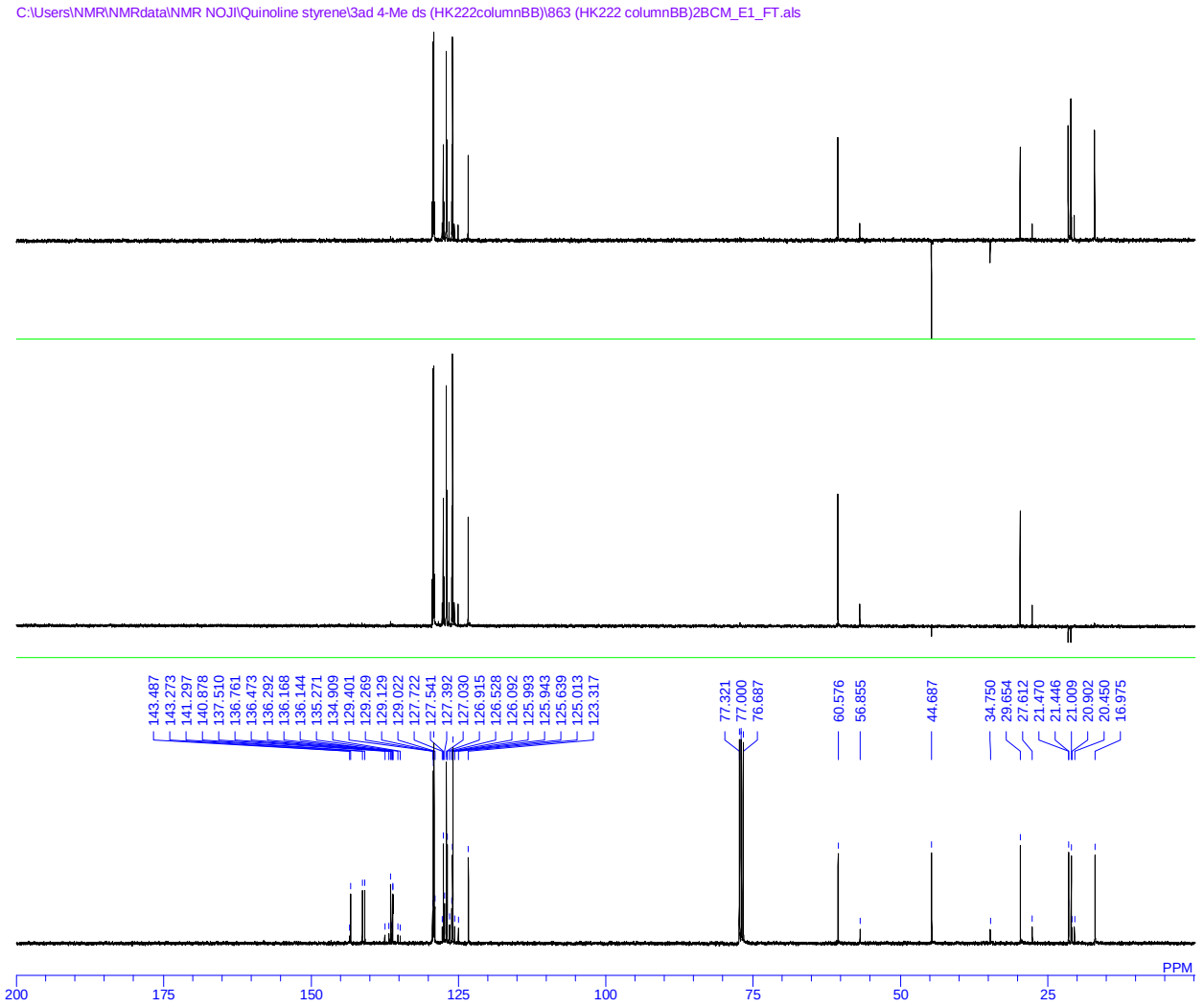


DATIM	Fri Jan 11 11:04:12 2013
MENUF	NON
OBNUC	1H
OFR	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.00 Hz
PW1	5.80 usec
DEADT	72.10 usec
PREDL	0.20000 msec
IWT	1.0000 sec
POINT	16384
SPO	16384
TIMES	16
DUMMY	1
FREQU	7992.01 Hz
FLT	4000 Hz
DELAY	50.00 usec
ACQTM	2.0500 sec
PD	4.9500 sec
ADBIT	16
RGAIN	12
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	NON
EXPCM	NON:Single.coupled:PW1_ACQTM_PD:1H,13C,1
IRNUC	1H
IFR	399.65 MHz
IRSET	124.00 KHz
IRFIN	10500.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	863 (HK222 columnBB)1NON_E1_FT.als
SF	TH5FG2
LKSET	61.60 KHz
LKFIN	79.0 Hz
LKLEV	180
LGAIN	20
LKPHS	330
LKSIG	587
CSPED	15 Hz
FILDC	
FILDF	

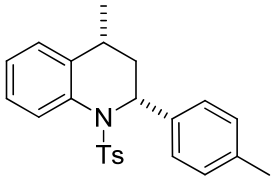


cis-**3ad** (major)

^{13}C NMR spectrum of diastereomixture-3ad (*cis*-major)

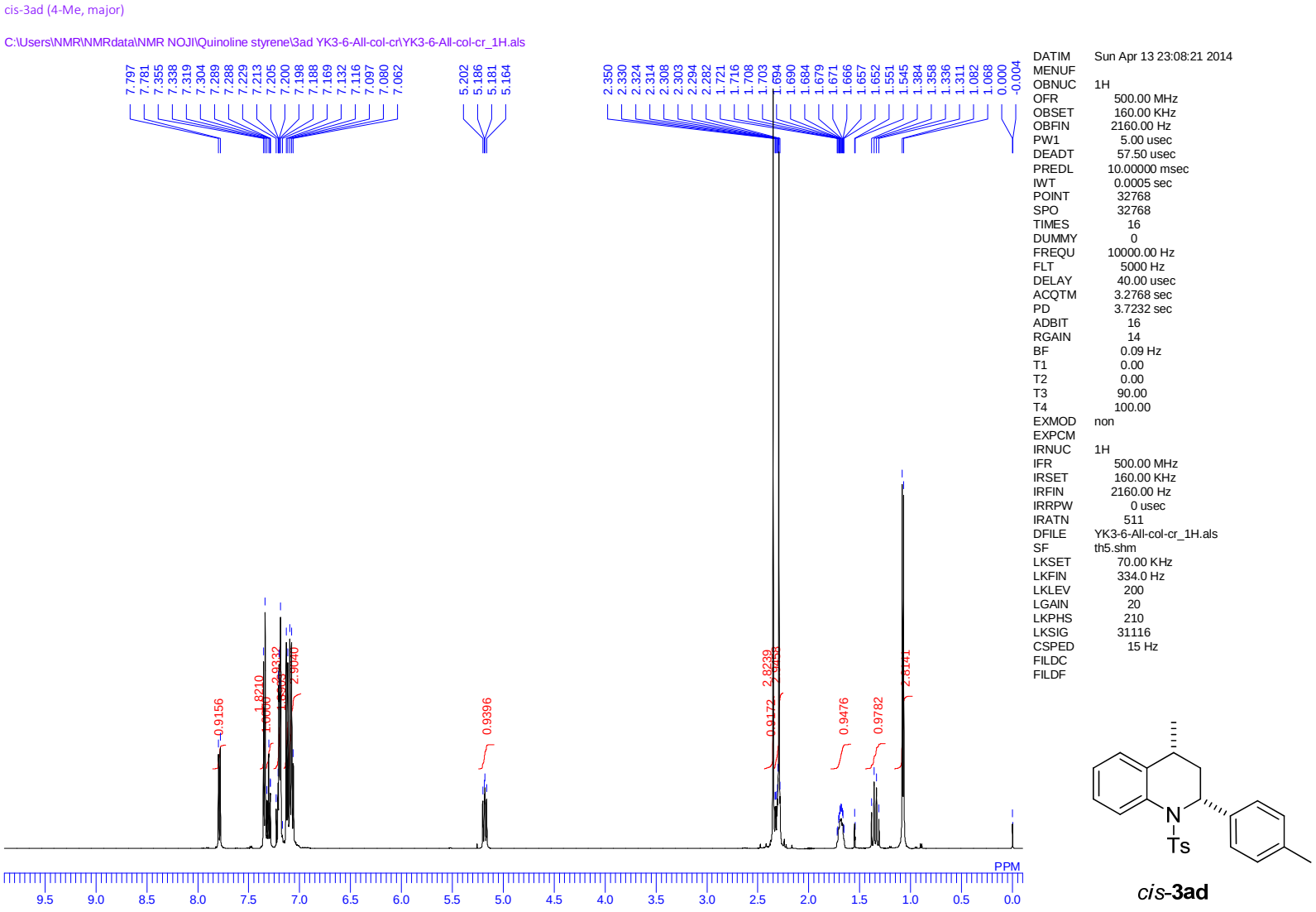


DATIM	Fri Jan 11 11:44:41 2013
MENUF	BCM
OBNUC	13C
OFR	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
PW1	6.00 usec
DEADT	19.14 usec
PREDL	0.20000 msec
IWT	1.0000 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	27118.64 Hz
FLT	13550 Hz
DELAY	14.76 usec
ACQTM	1.2083 sec
PD	1.7920 sec
ADBIT	16
RGAIN	25
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	BCM
EXPCM	Bilevel.complete.decoupling:Set_IRRPW
IRNUC	1H
IFR	399.65 MHz
IRSET	124.00 KHz
IRFIN	10500.00 Hz
IRRPW	50 usec
IRATN	511
DFILE	863 (HK222 columnBB)2BCM_E1_FT.als
SF	TH5FG2
LKSET	61.60 KHz
LKFIN	79.0 Hz
LKLEV	180
LGAIN	20
LKPHS	330
LKSIG	568
CSPED	19 Hz
FILDC	
FILDF	

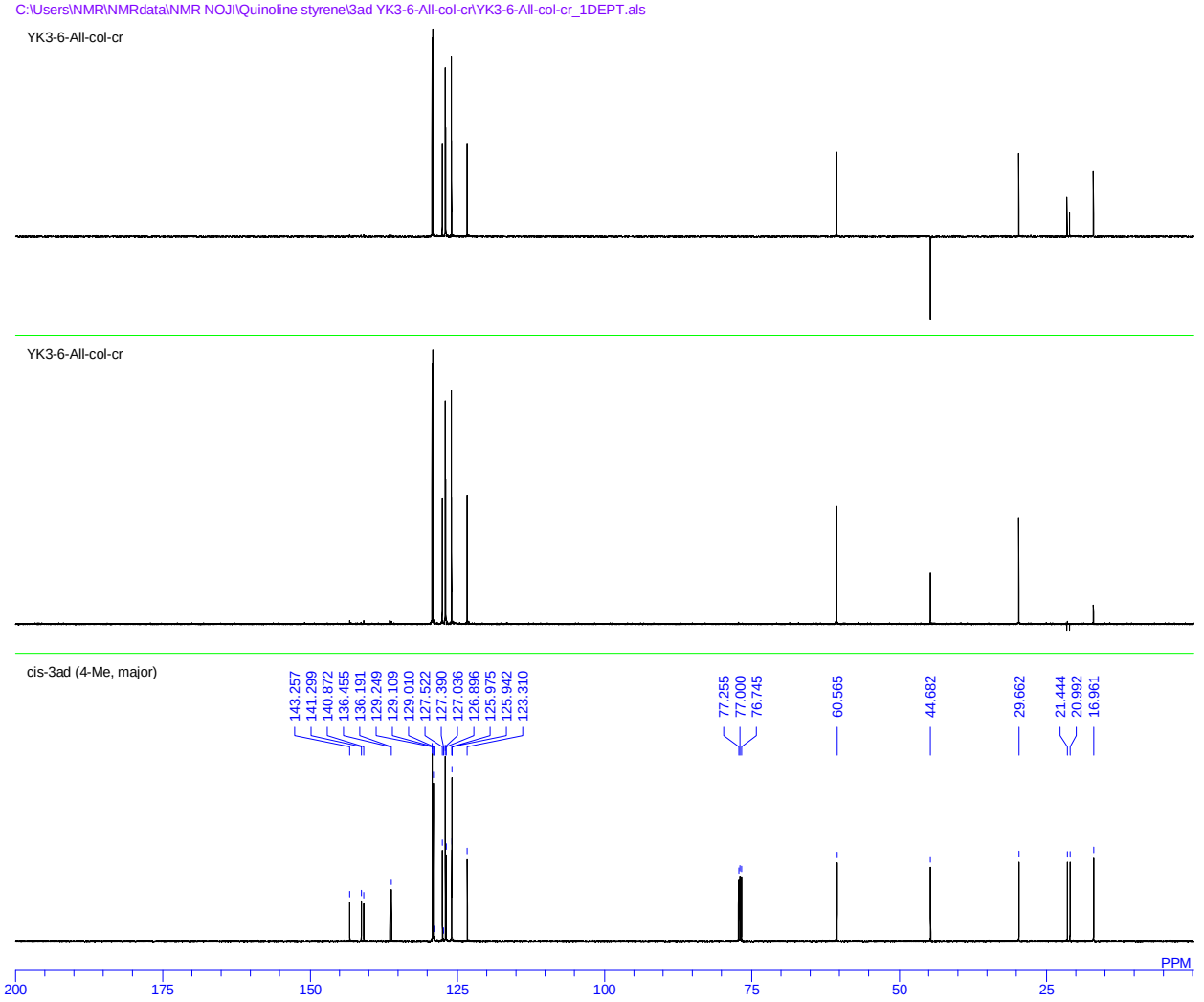


cis-**3ad** (major)

^{1}H NMR spectrum of *cis*-3ad (major)



^{13}C NMR spectrum of *cis*-3ad (major)



DATIM	Mon Apr 14 00:00:52 2014
MENUF	
OBNUC	13C
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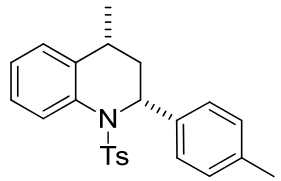
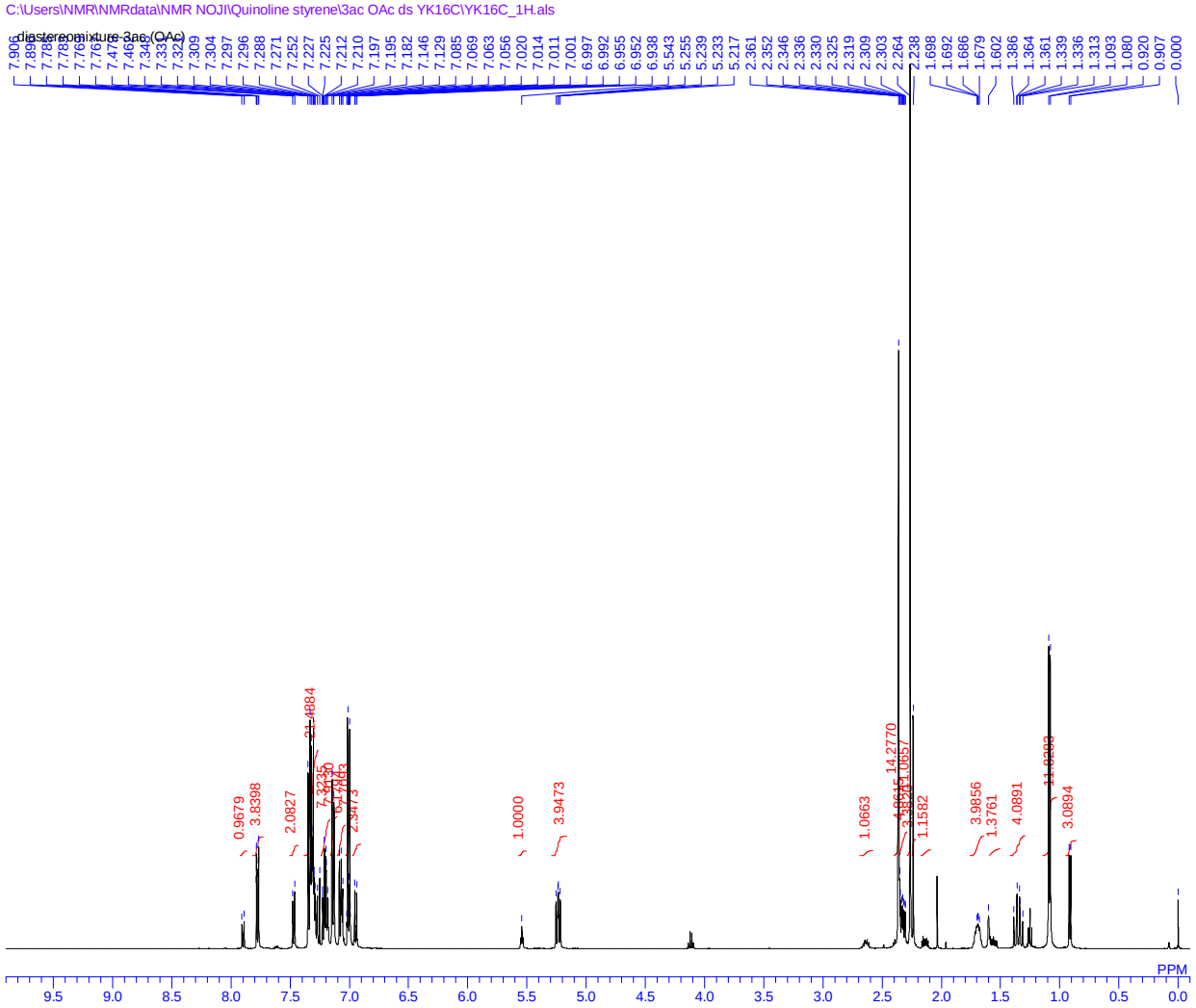
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	YK3-6-All-col-cr_1DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	60838
CSPED	11 Hz
FILDC	
FILDF	

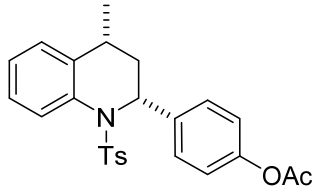


cis-**3ad**

^{1}H NMR spectrum of diastereomixture-3ae (*cis*-major)

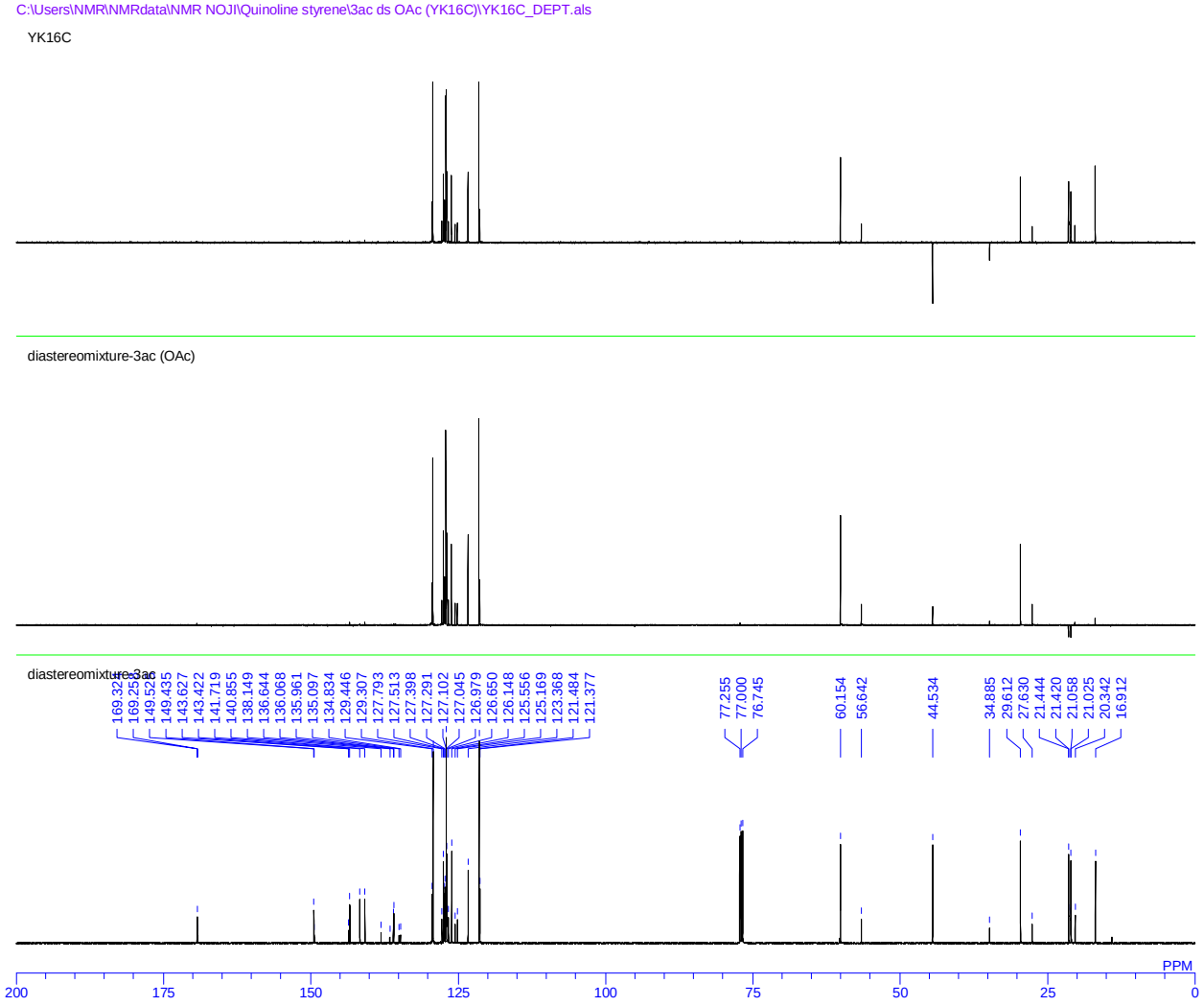


DATIM	Wed Sep 17 20:44:02 2014
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	32
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	14
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	YK16C_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	33536
CSPED	14 Hz
FILDC	
FILDF	

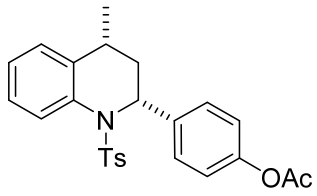


cis-**3ae** (major)

^{13}C NMR spectrum of diastereomixture-3ae (*cis*-major)

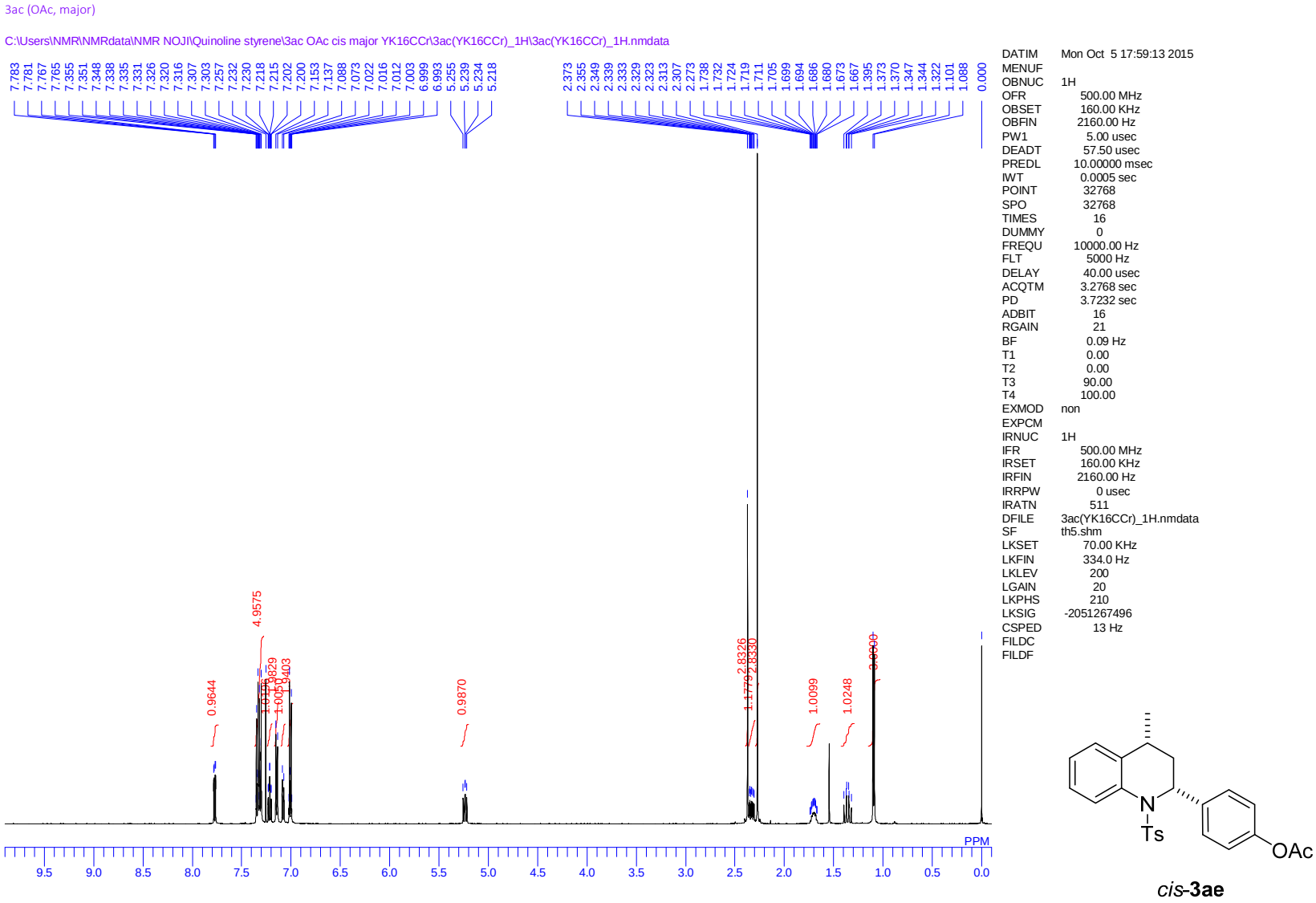


DATIM	Wed Sep 17 22:27:51 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	YK16C_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	56418
CSPED	14 Hz
FILDC	
FILDF	



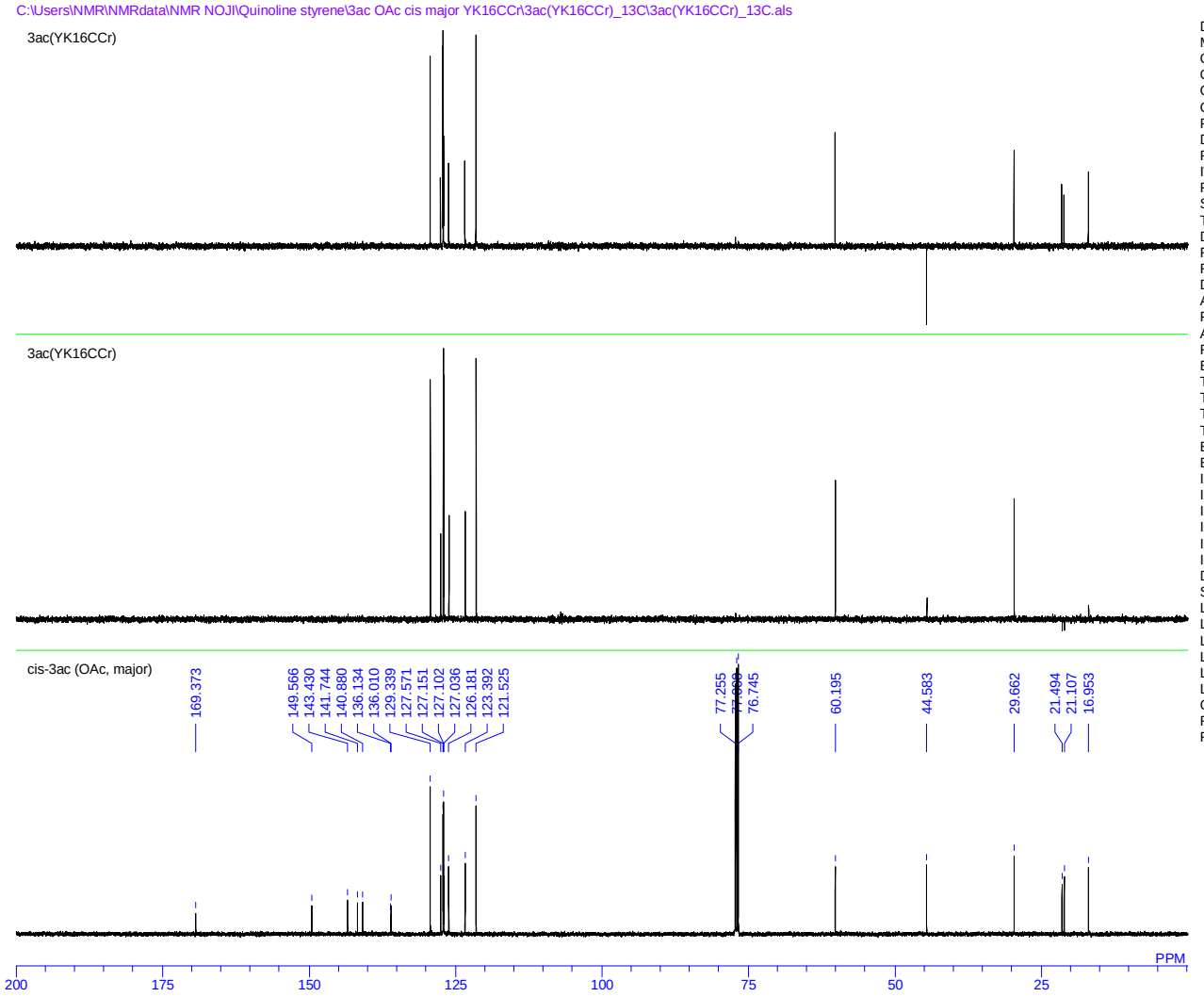
cis-**3ae** (major)

^{1}H NMR spectrum of *cis*-3ae (major)

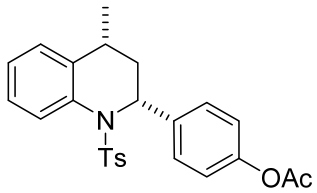


cis-**3ae**

^{13}C NMR spectrum of *cis*-3ae (major)

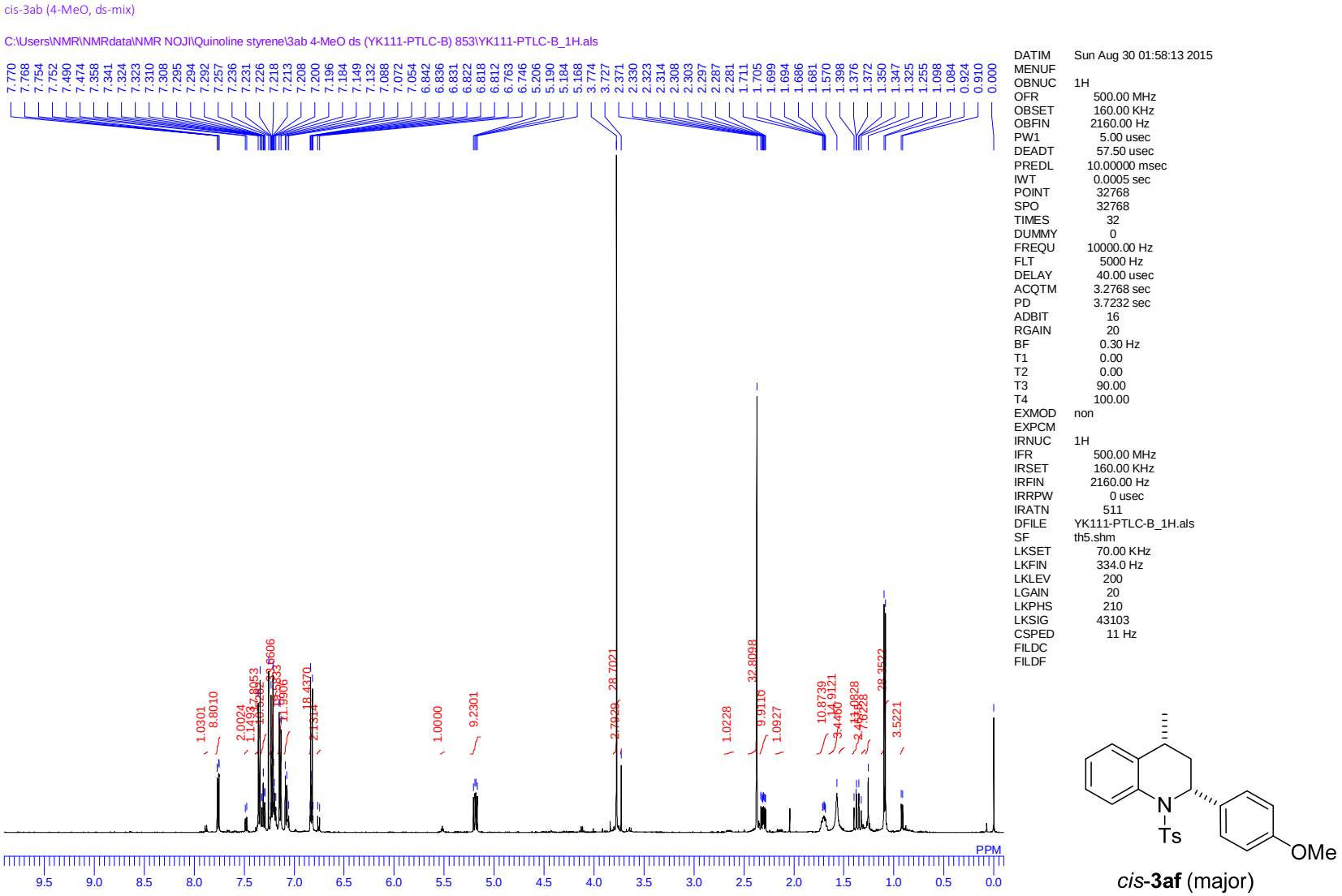


DATIM	Mon Oct 5 18:51:44 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3ac(YK16CCr)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-281069051
CSPED	12 Hz
FILDC	
FILDF	



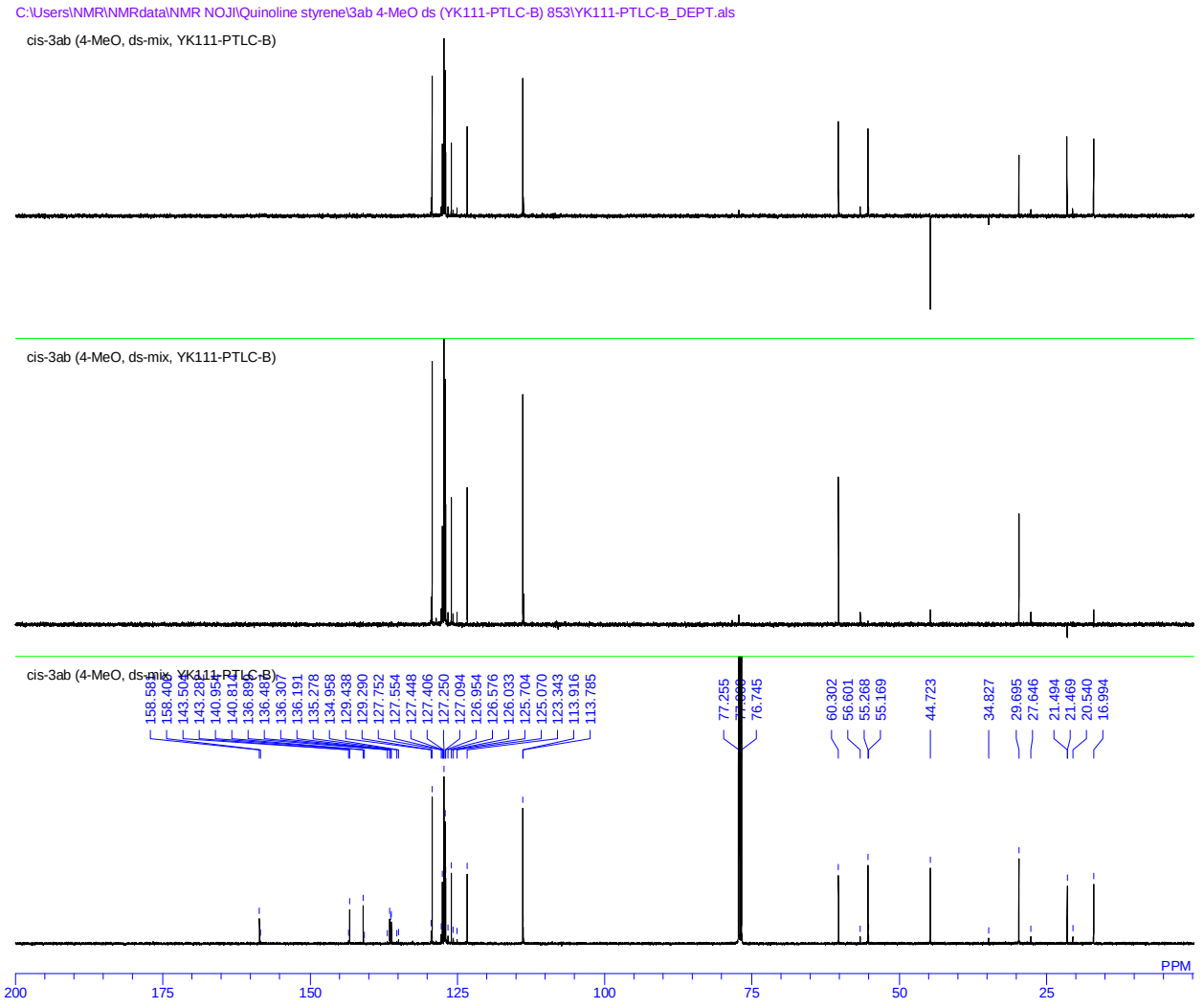
cis-**3ae**

^{1}H NMR spectrum of diastereomixture-3af (*cis*-major)

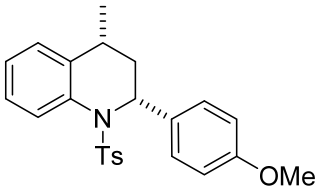


cis-**3af** (major)

^{13}C NMR spectrum of diastereomixture-3af (*cis*-major)

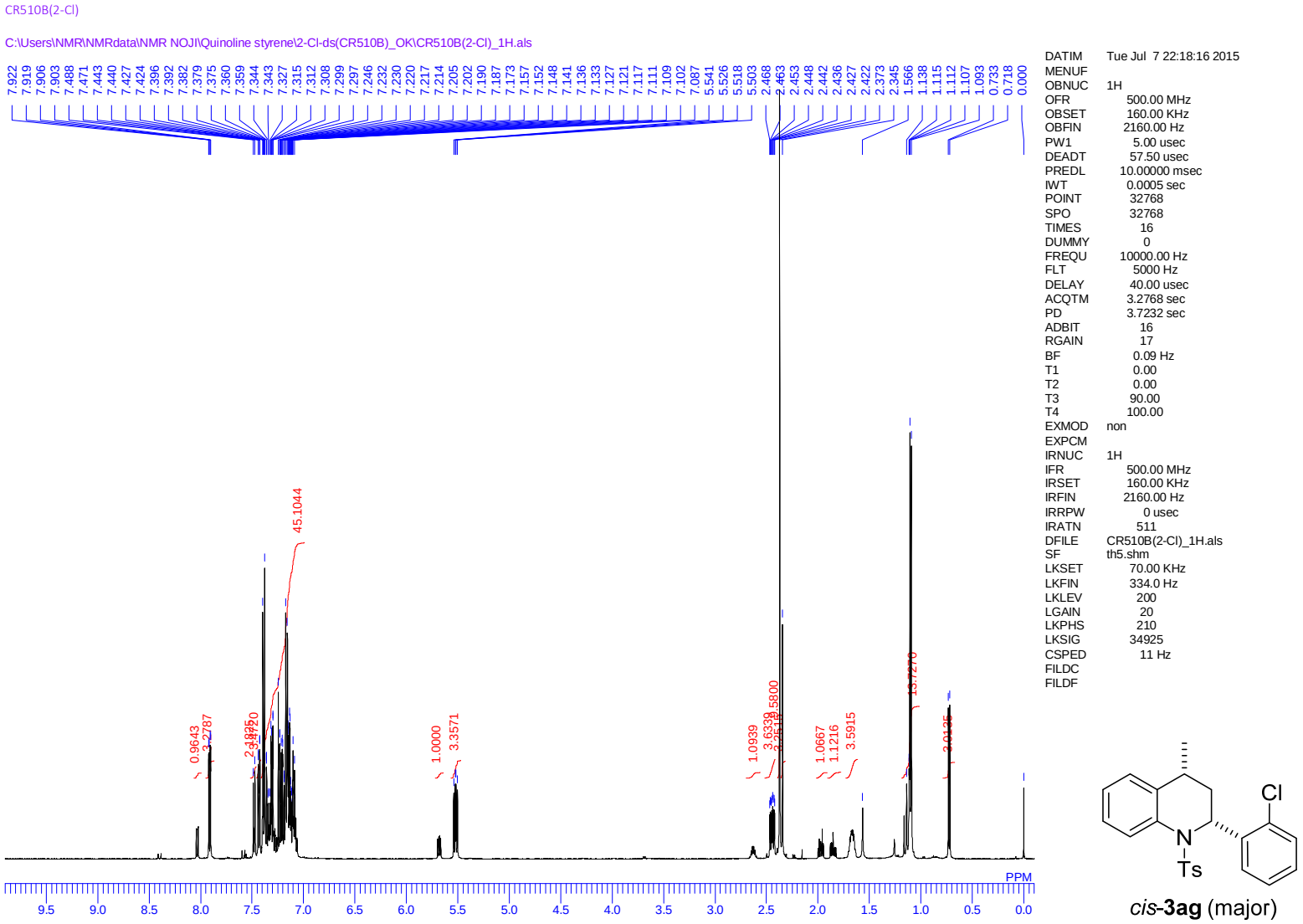


DATIM	Sun Aug 30 05:24:15 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	4096
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.30 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	YK111-PTLC-B_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	21913
CSPED	12 Hz
FILDC	
FILDF	



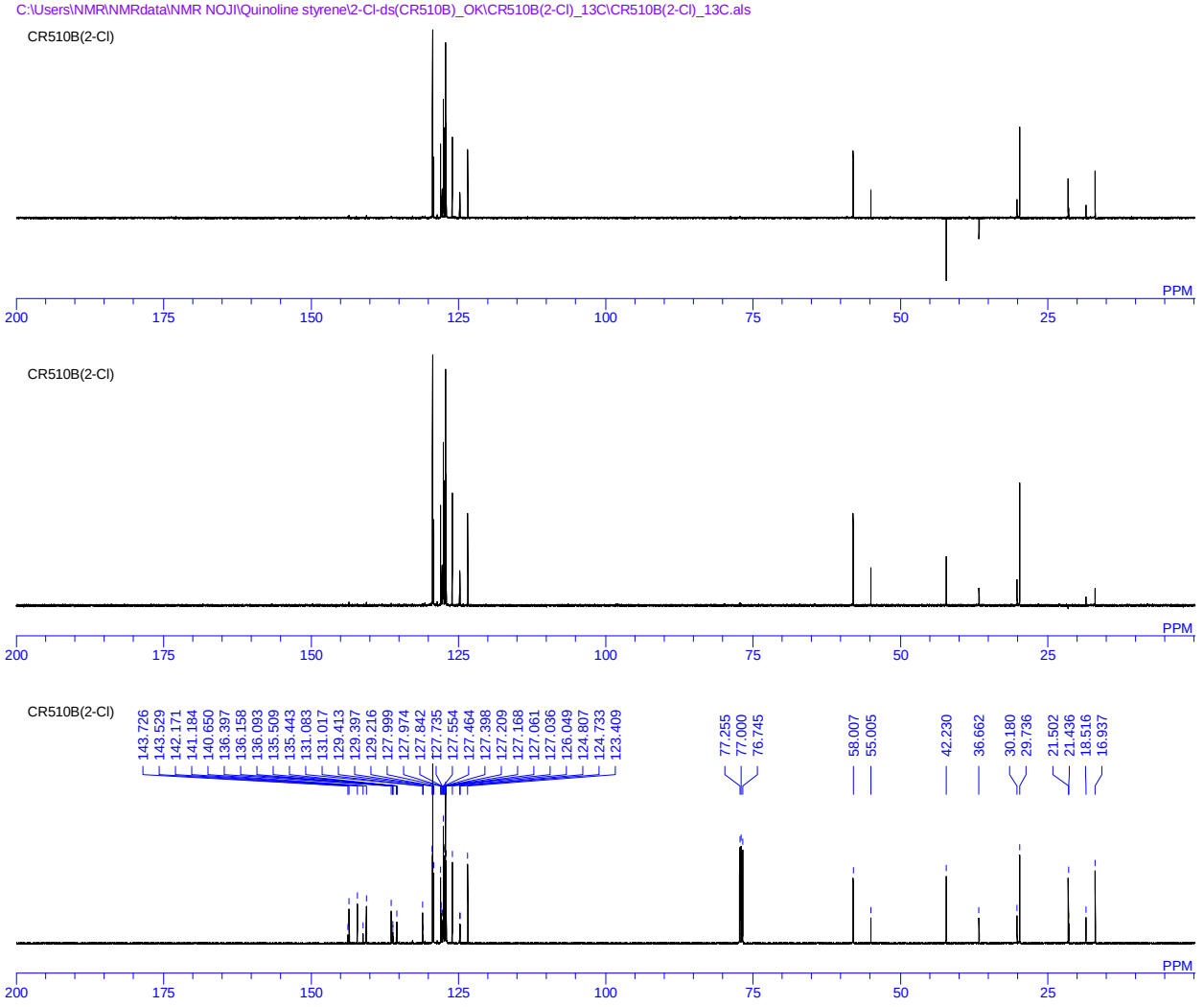
cis-**3af** (major)

^{1}H NMR spectrum of diastereomixture-3ag (*cis*-major)

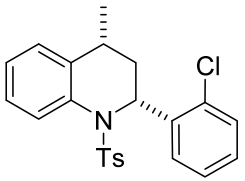


cis-**3ag** (major)

^{13}C NMR spectrum of diastereomixture-3ag (*cis*-major)

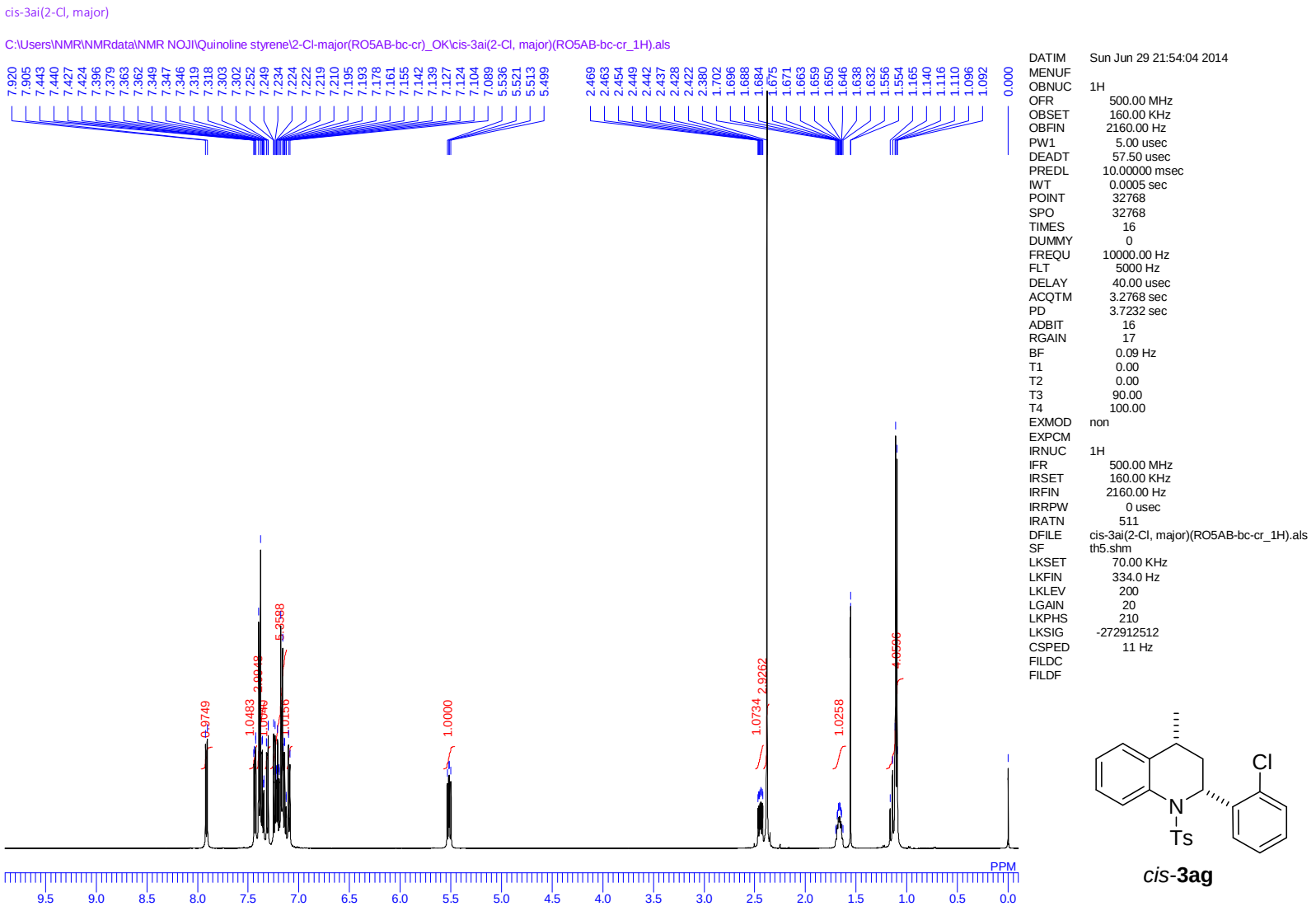


DATIM	Tue Jul 7 23:10:54 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR510B(2-Cl)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	50011
CSPED	10 Hz
FILDC	
FILDF	

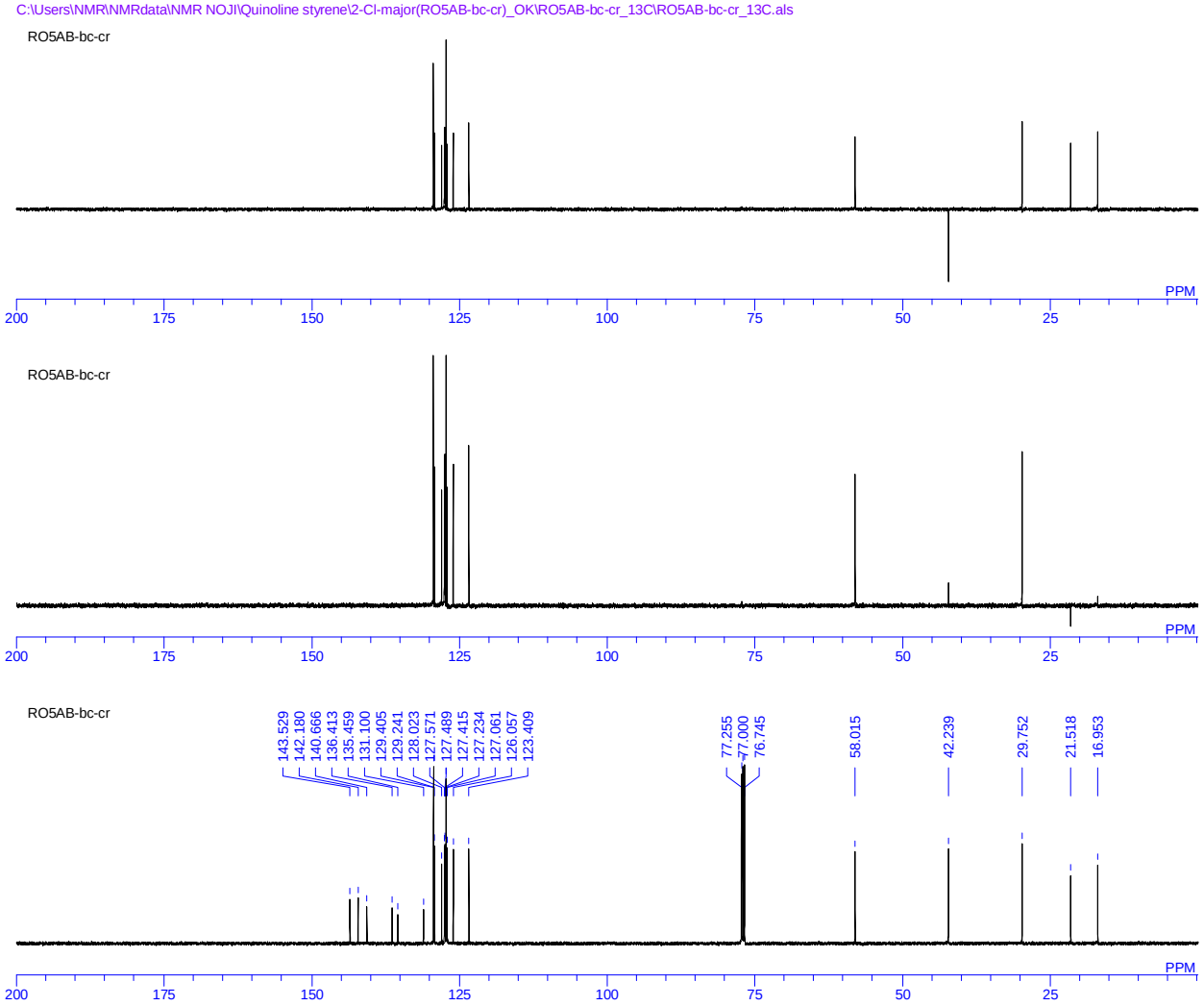


cis-**3ag** (major)

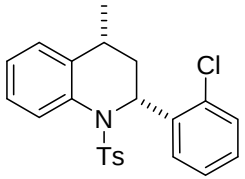
^{1}H NMR spectrum of *cis*-3ag (major)



^{13}C NMR spectrum of *cis*-3ag (major)

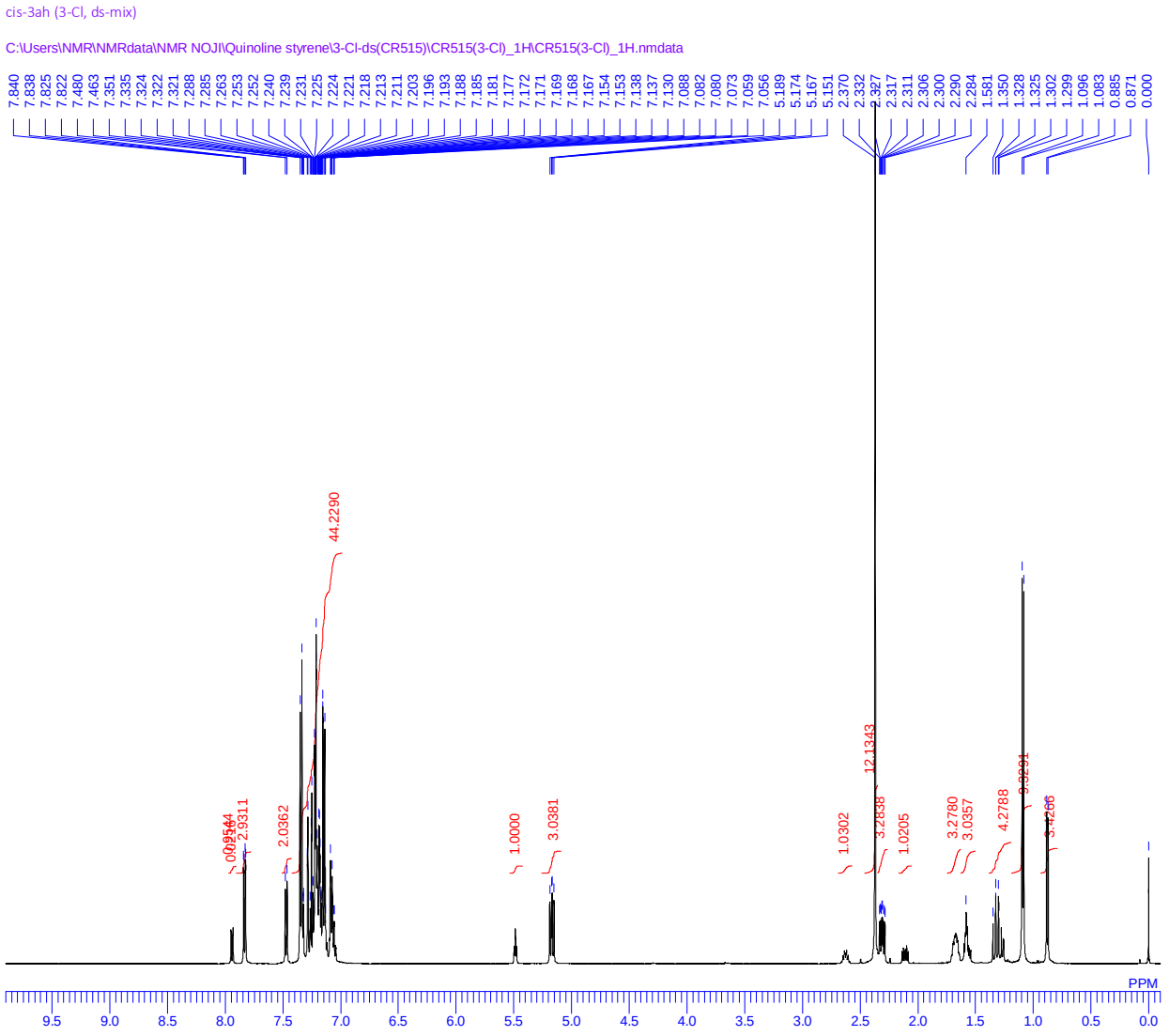


DATIM	Sun Jun 29 22:46:38 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	RO5AB-bc-cr_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-457269566
CSPED	11 Hz
FILDC	
FILDF	

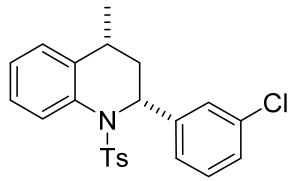


cis-**3ag**

^{1}H NMR spectrum of diastereomixture-3ah (*cis*-major)

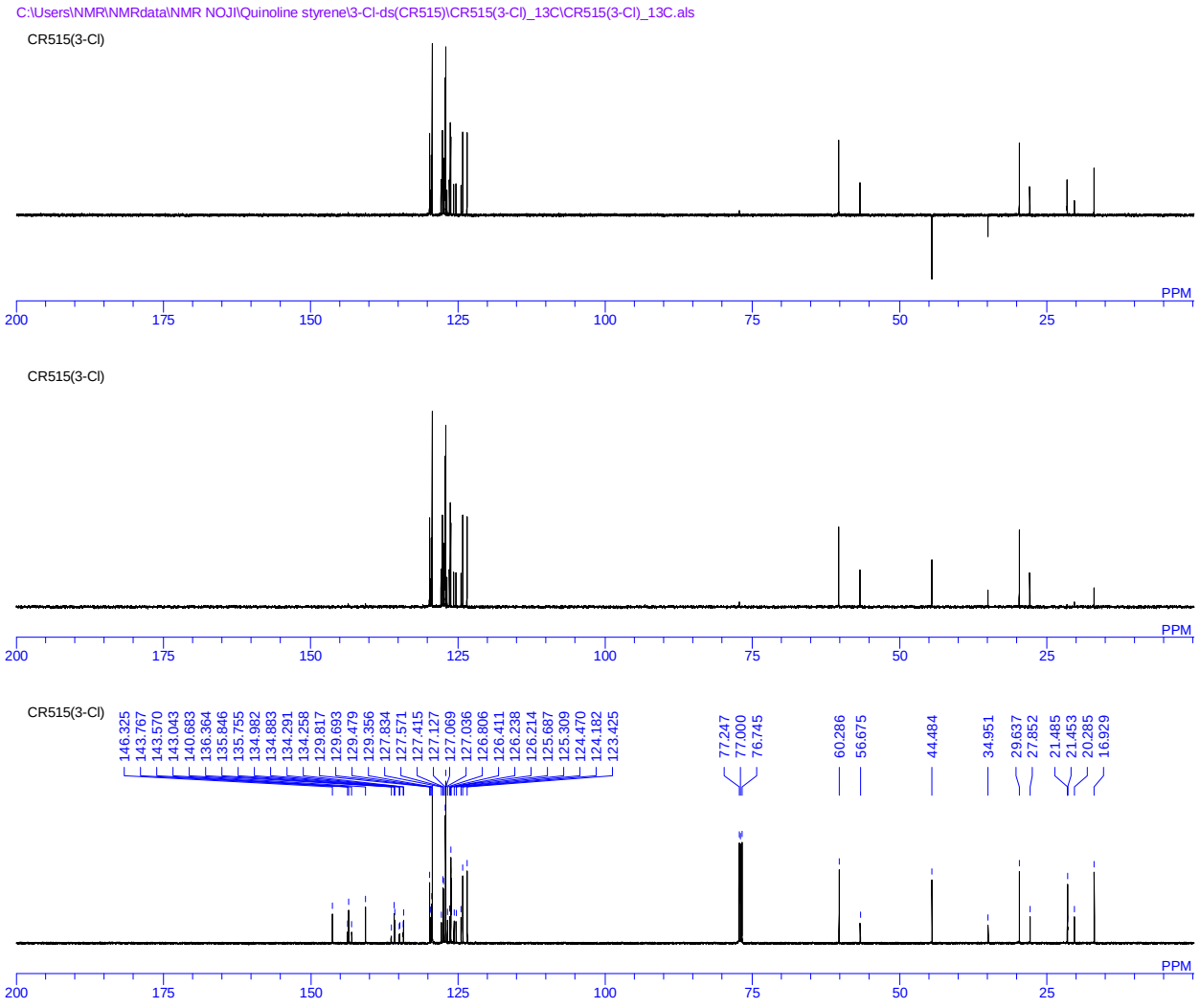


DATIM	Sat Jul 18 19:07:20 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR515(3-Cl)_1H.nmdata
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-1229183320
CSPED	11 Hz
FILDC	
FILDF	

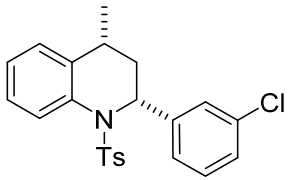


cis-**3ah** (major)

^{13}C NMR spectrum of diastereomixture-3ah (*cis*-major)

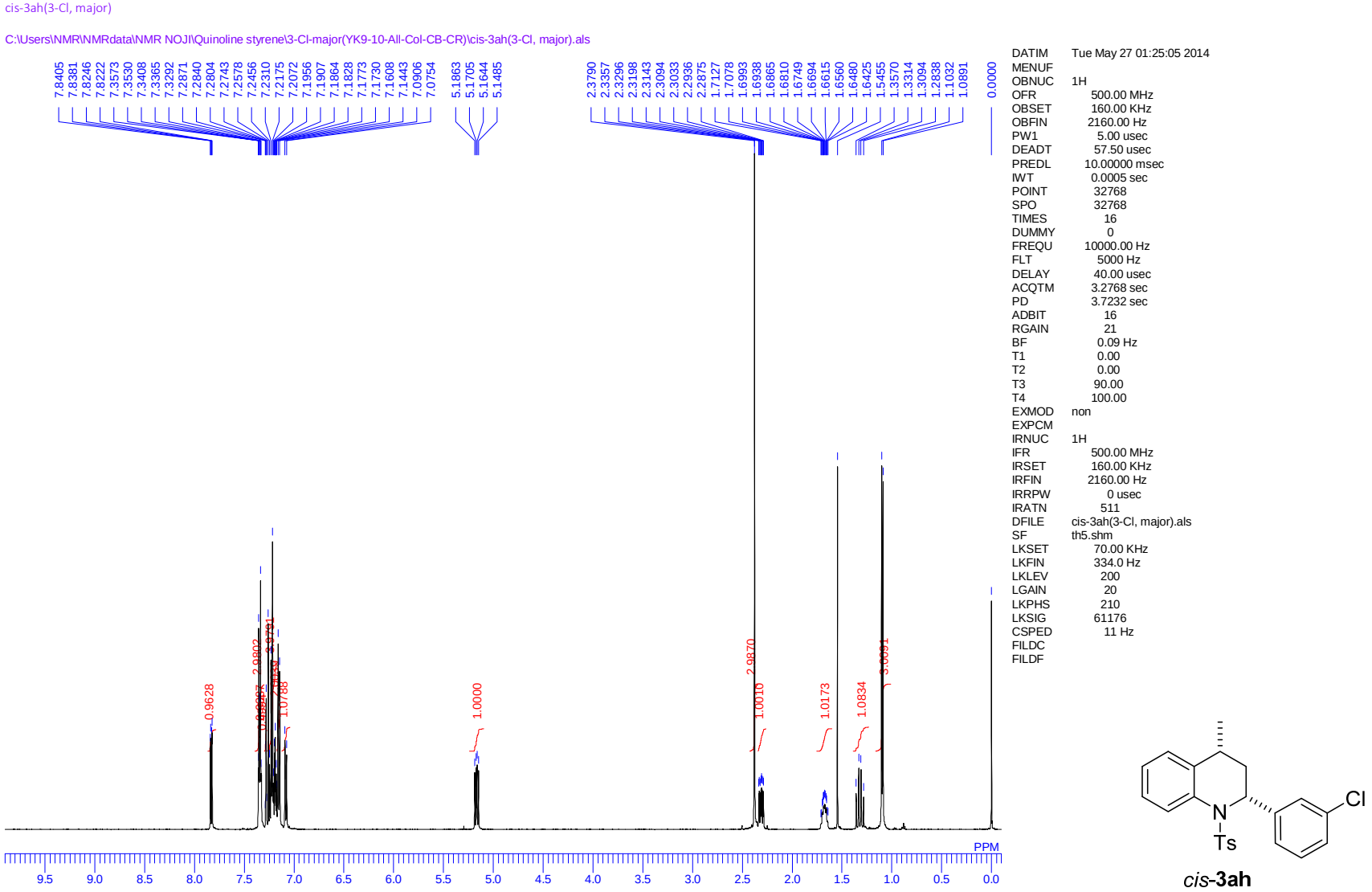


DATIM	Sat Jul 18 19:59:48 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	27
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR515(3-Cl)_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-901893360
CSPED	11 Hz
FILDC	
FILDF	



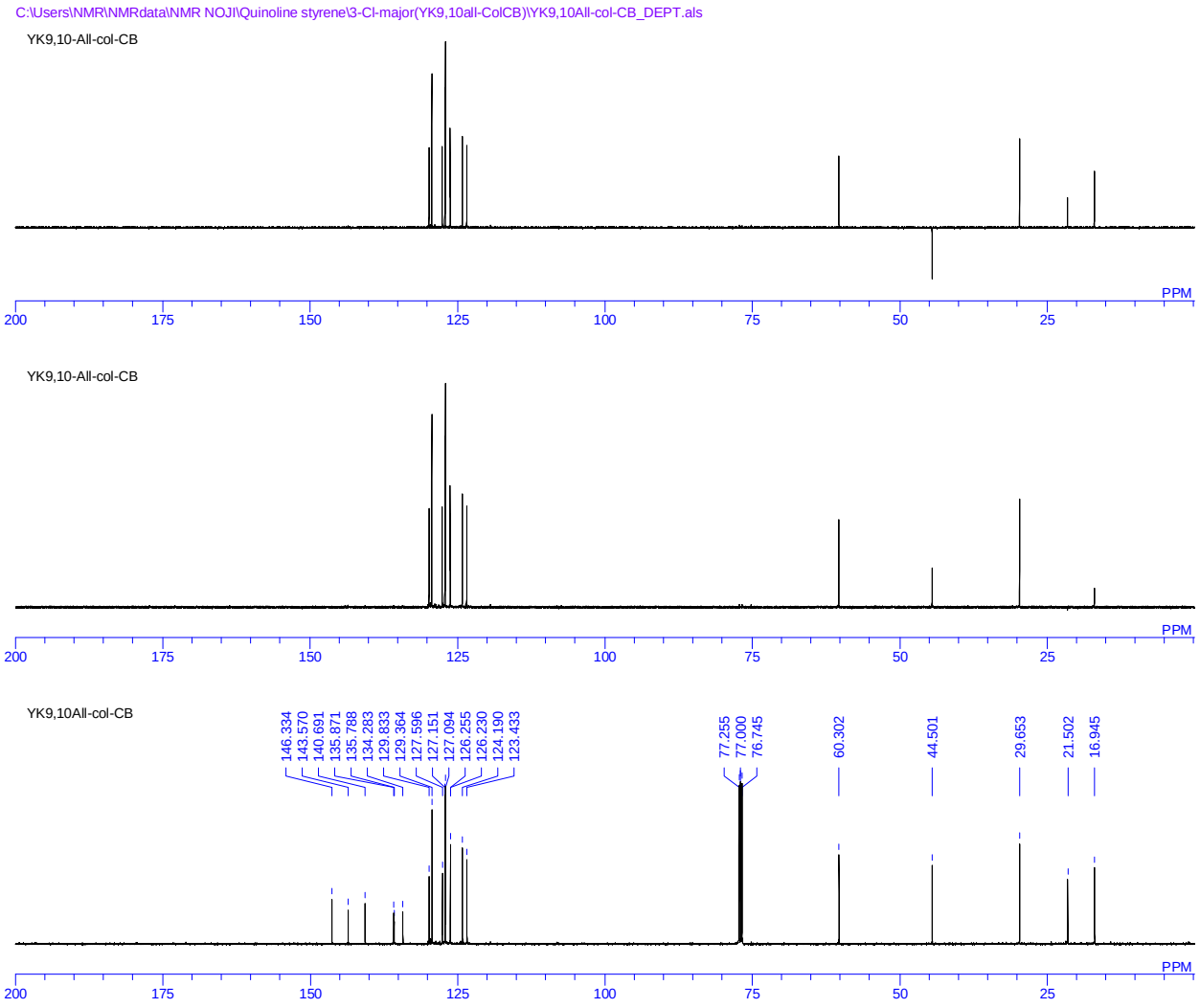
cis-**3ah** (major)

^{1}H NMR spectrum of *cis*-3ah (major)

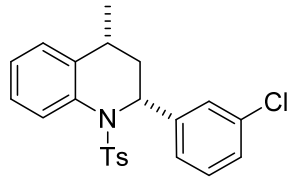


cis-**3ah**

^{13}C NMR spectrum of *cis*-3ah (major)

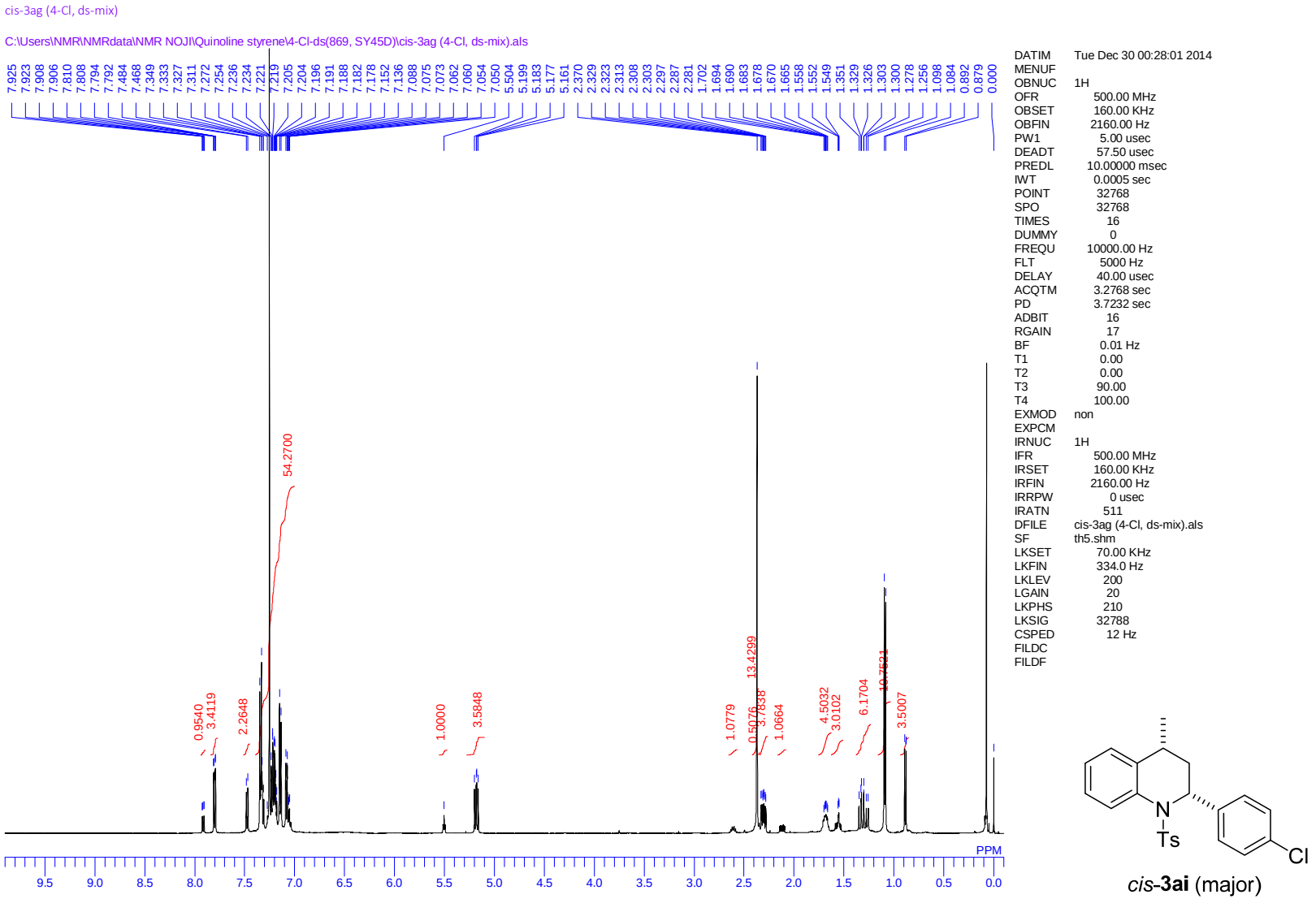


DATIM	Sat May 24 20:07:43 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.01 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	YK9,10All-col-CB_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	45193
CSPED	12 Hz
FILDC	
FILDF	



cis-3ah

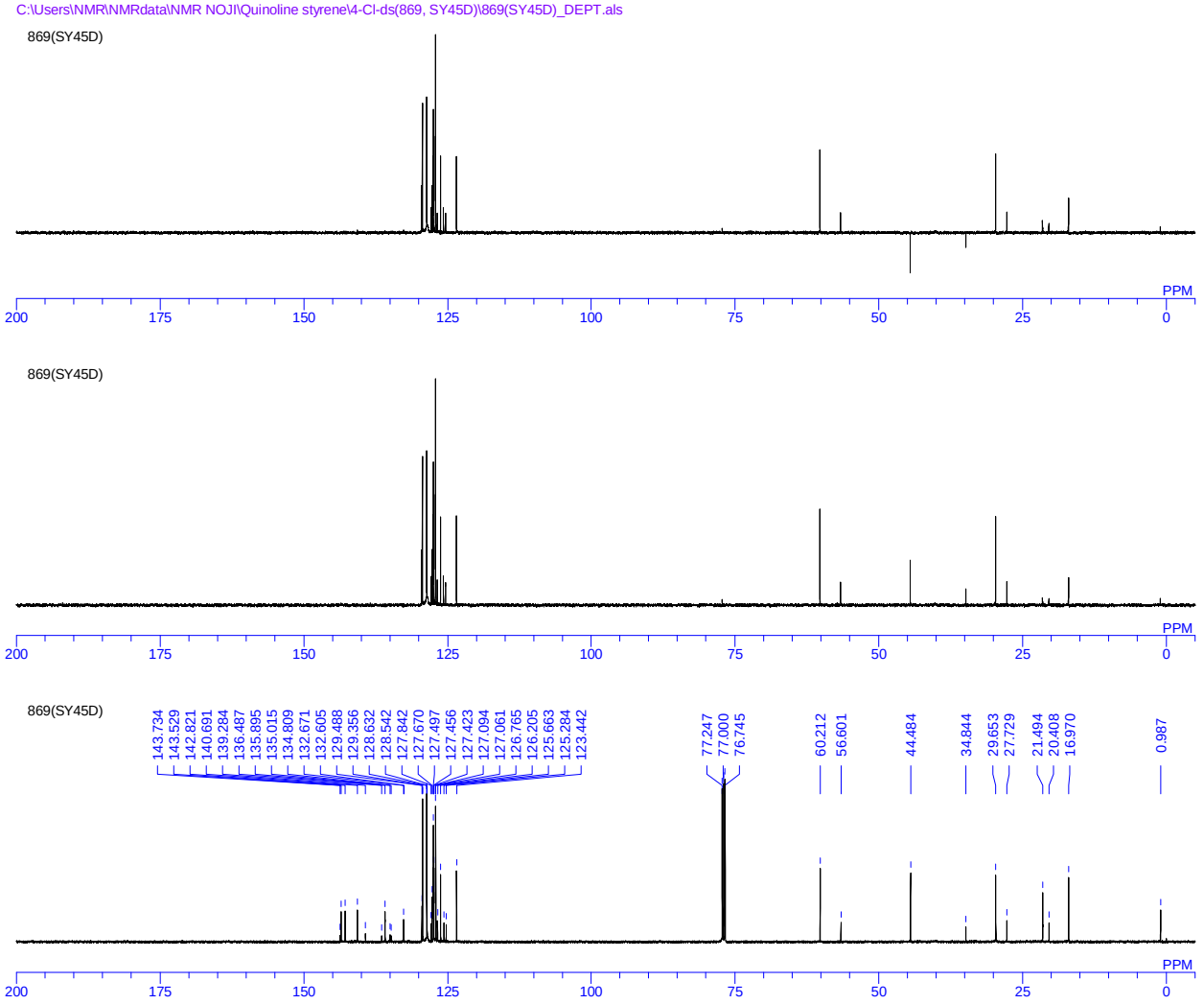
^{1}H NMR spectrum of diastereomixture-3ai (*cis*-major)



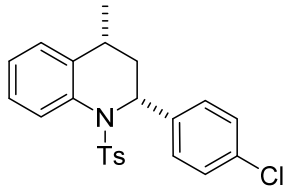
DATIM	Tue Dec 30 00:28:01 2014
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	17
BF	0.01 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	cis-3ag (4-Cl, ds-mix).als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	32788
CSPED	12 Hz
FILDC	
FILDF	

cis-**3ai** (major)

^{13}C NMR spectrum of diastereomixture-3ai (*cis*-major)

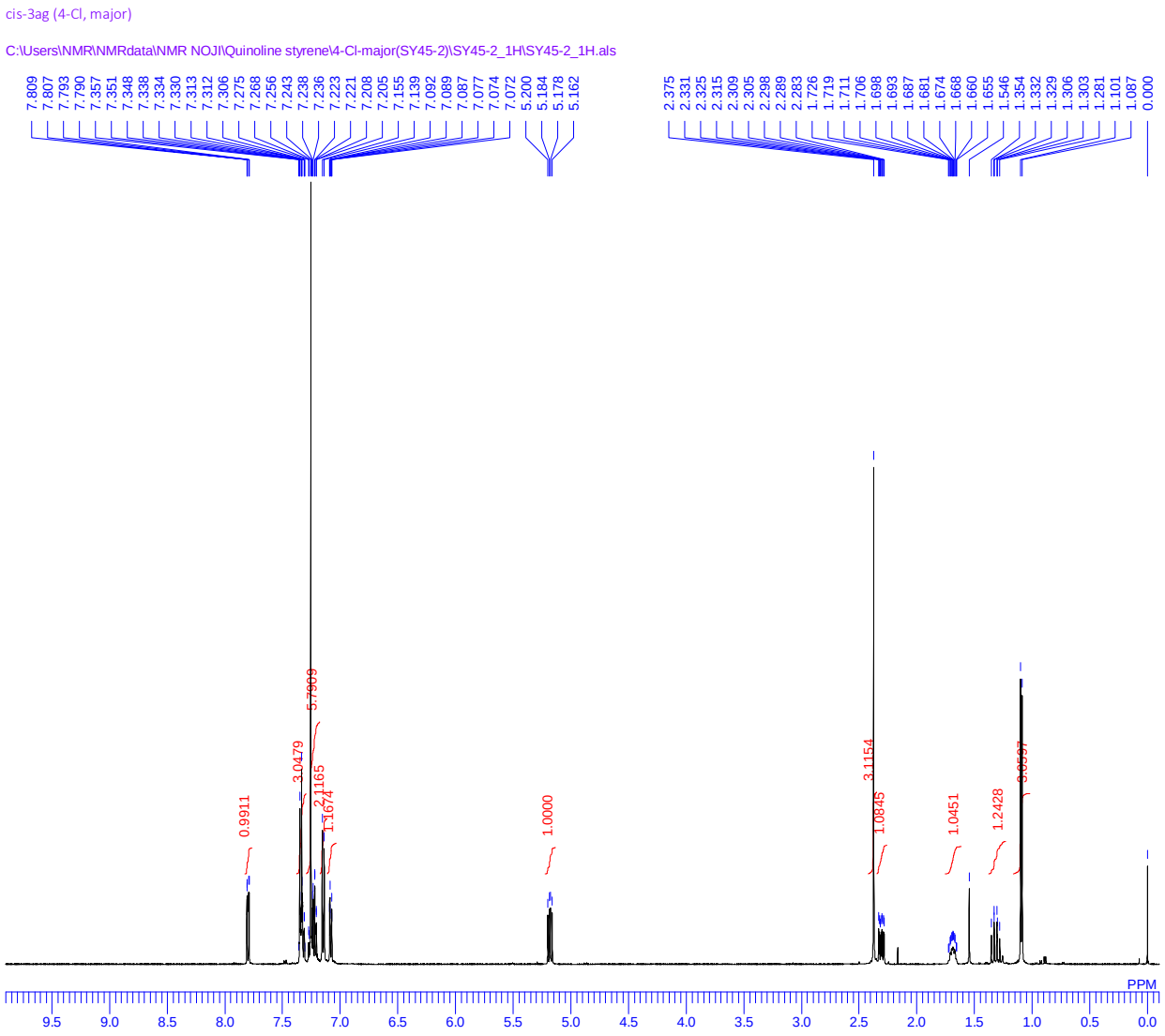


DATIM	Tue Dec 30 01:49:26 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1600
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.01 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	869(SY45D)_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	44792
CSPED	14 Hz
FILDC	
FILDF	

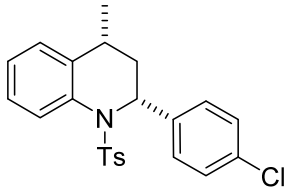


cis-**3ai** (major)

^{1}H NMR spectrum of *cis*-3ai (major)

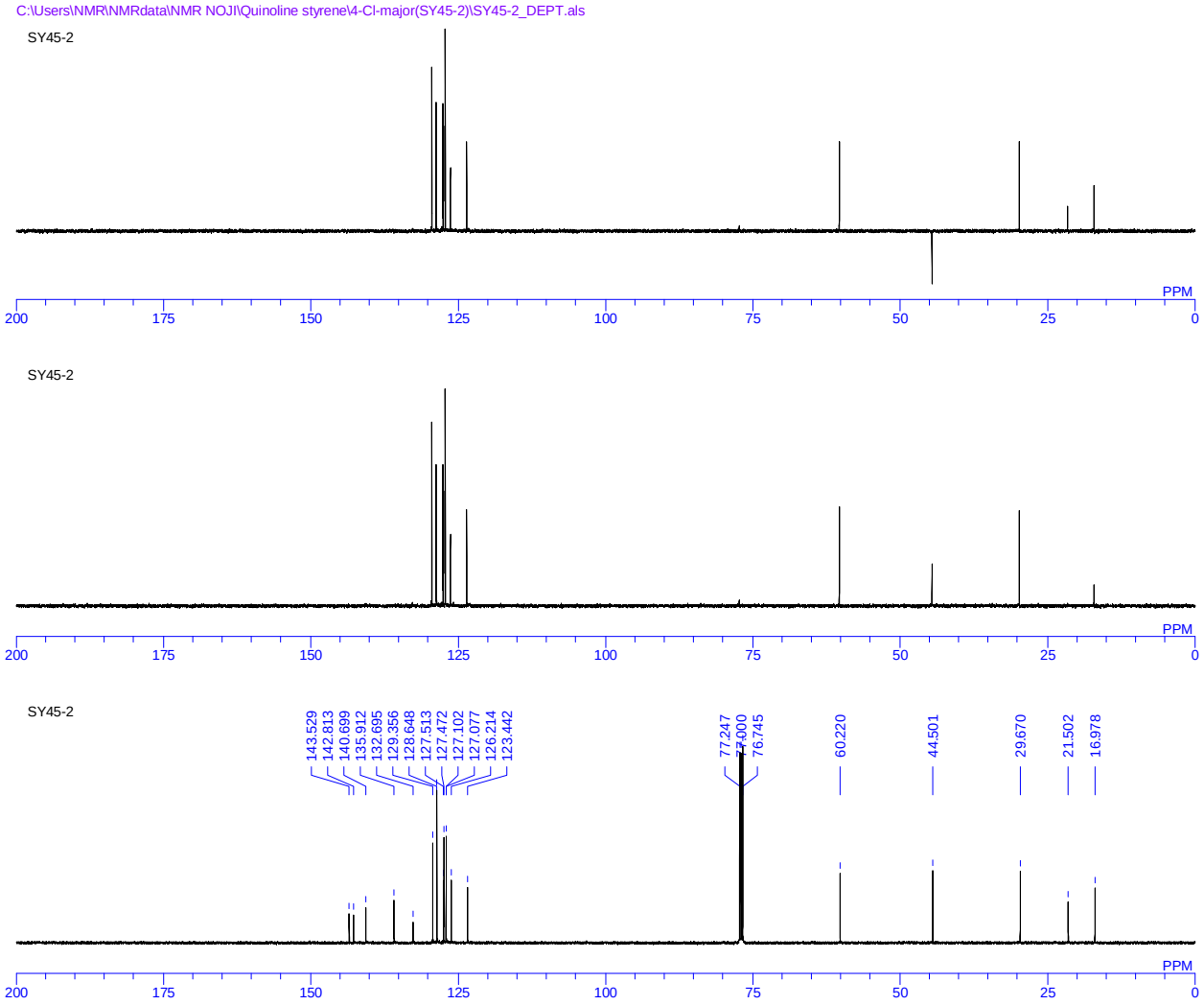


DATIM	Sat Jan 10 02:01:21 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	20
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	SY45-2_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	53110
CSPED	12 Hz
FILDC	
FILDF	

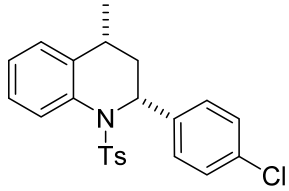


cis-**3ai**

^{13}C NMR spectrum of *cis*-3ai (major)

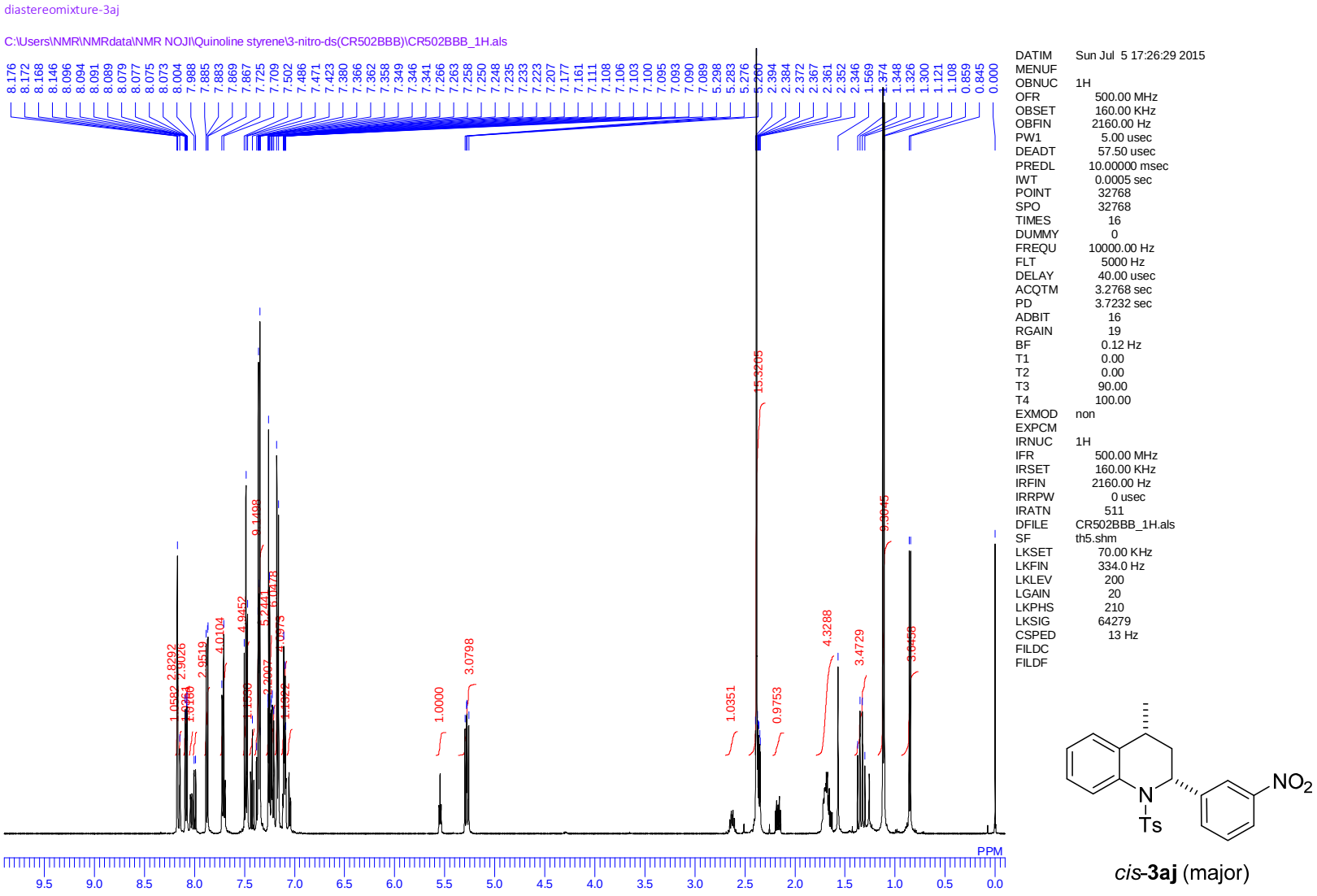


DATIM	Sat Jan 10 03:22:40 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1600
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	SY45-2_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	32151
CSPED	11 Hz
FILDC	
FILDF	



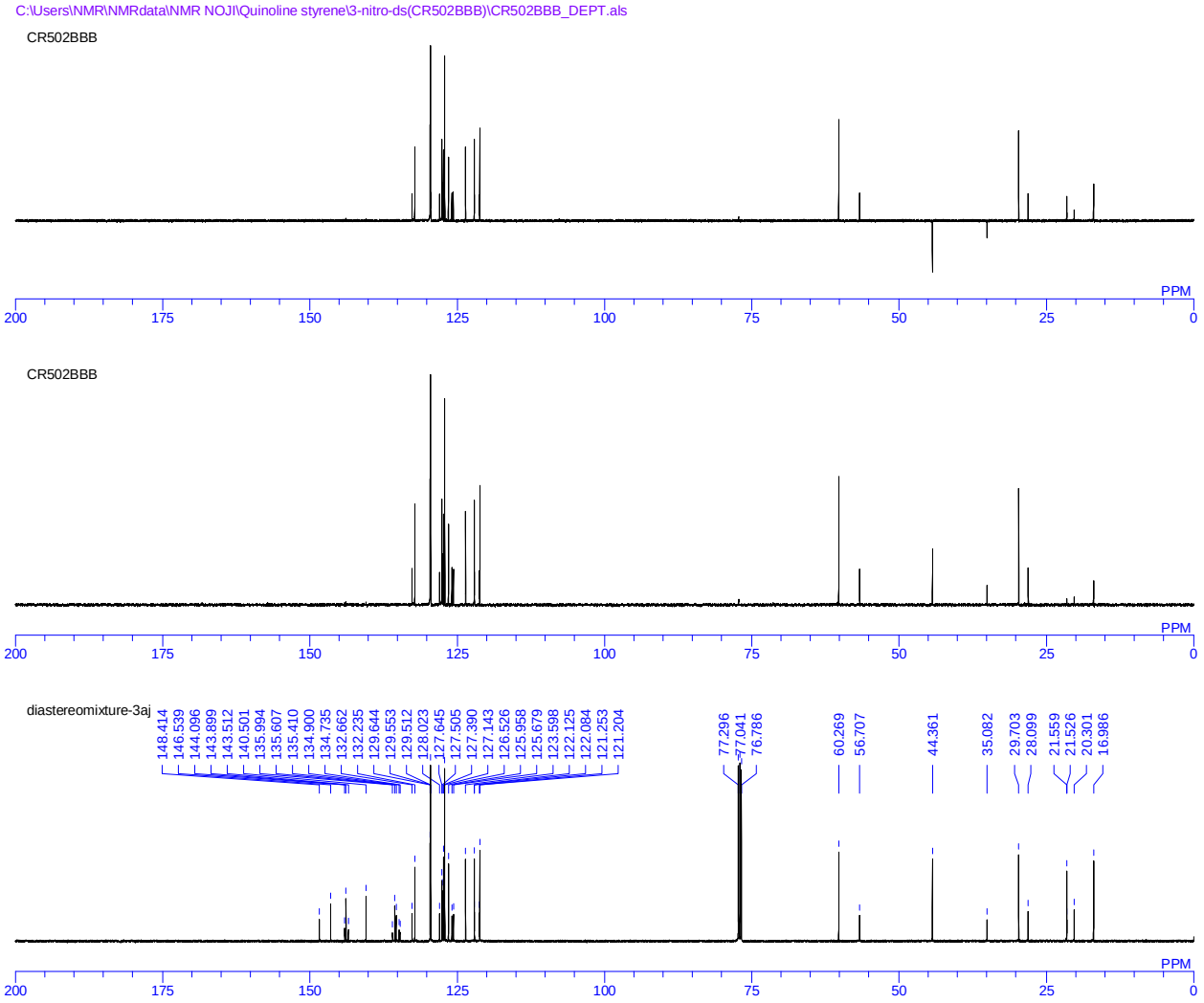
cis-**3ai**

^{1}H NMR spectrum of diastereomixture-3aj (*cis*-major)

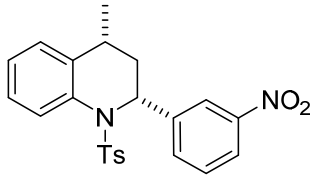


cis-**3aj** (major)

^{13}C NMR spectrum of diastereomixture-3aj (*cis*-major)

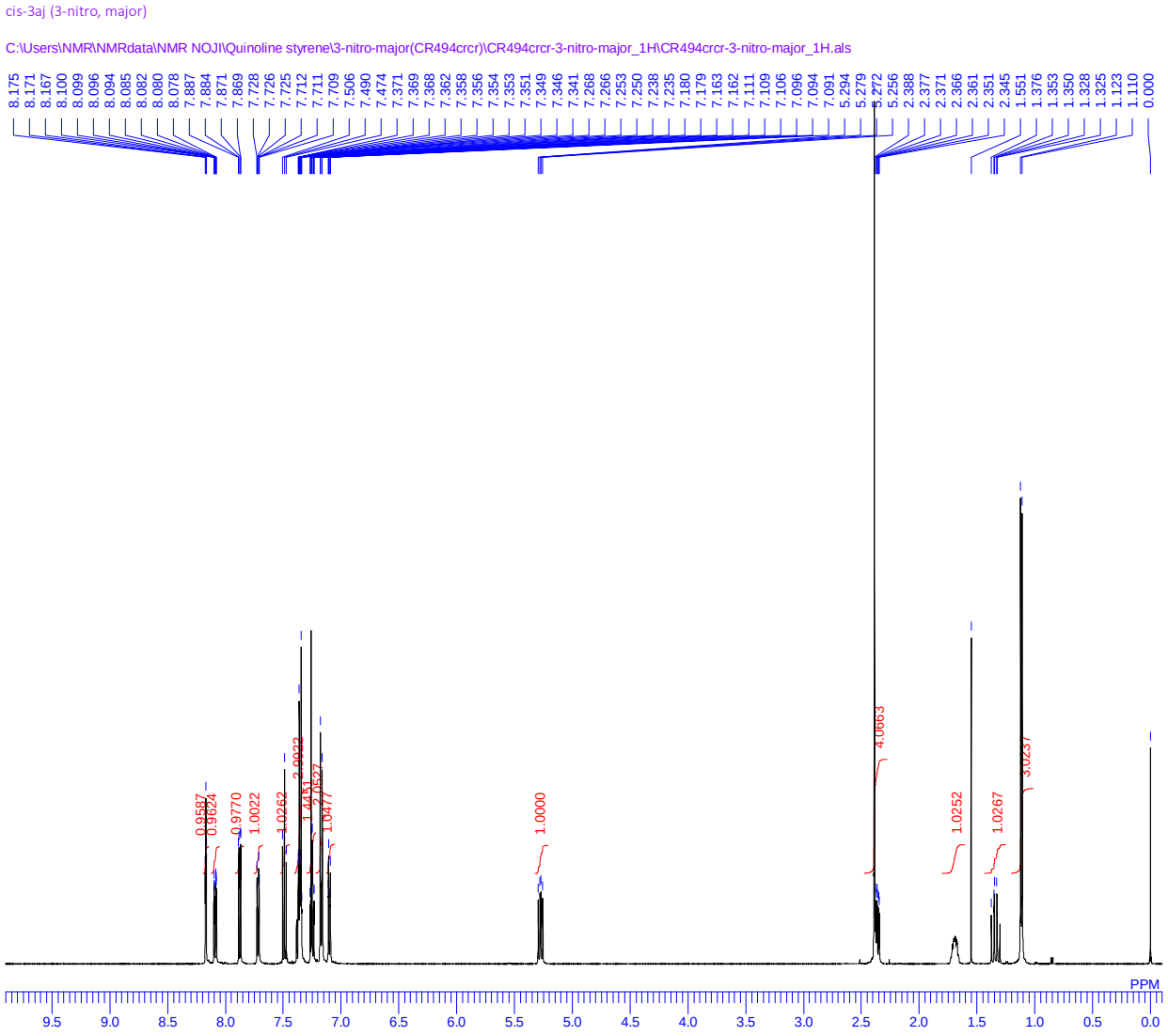


DATIM	Sun Jul 5 19:10:13 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR502BBB_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	38489
CSPED	13 Hz
FILDC	
FILDF	

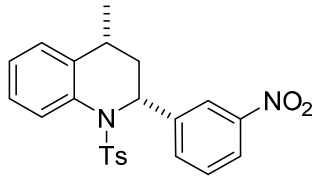


cis-**3aj** (major)

^{1}H NMR spectrum of *cis*-3aj (major)

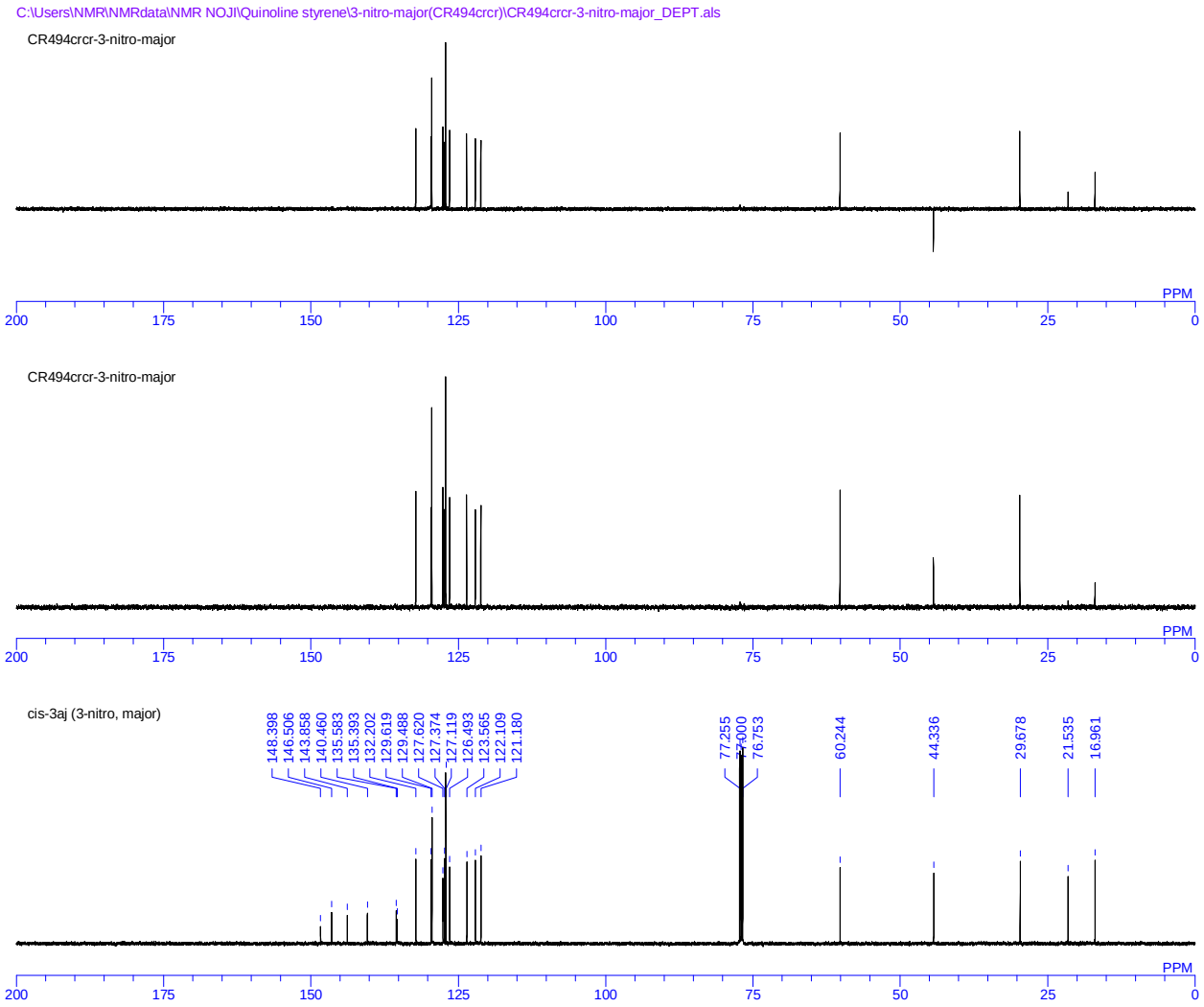


DATIM	Mon Jul 6 02:29:52 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	20
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR494crcr-3-nitro-major_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	45772
CSPED	11 Hz
FILDC	
FILDF	

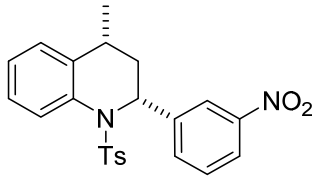


cis-**3aj**

^{13}C NMR spectrum of *cis*-3aj (major)

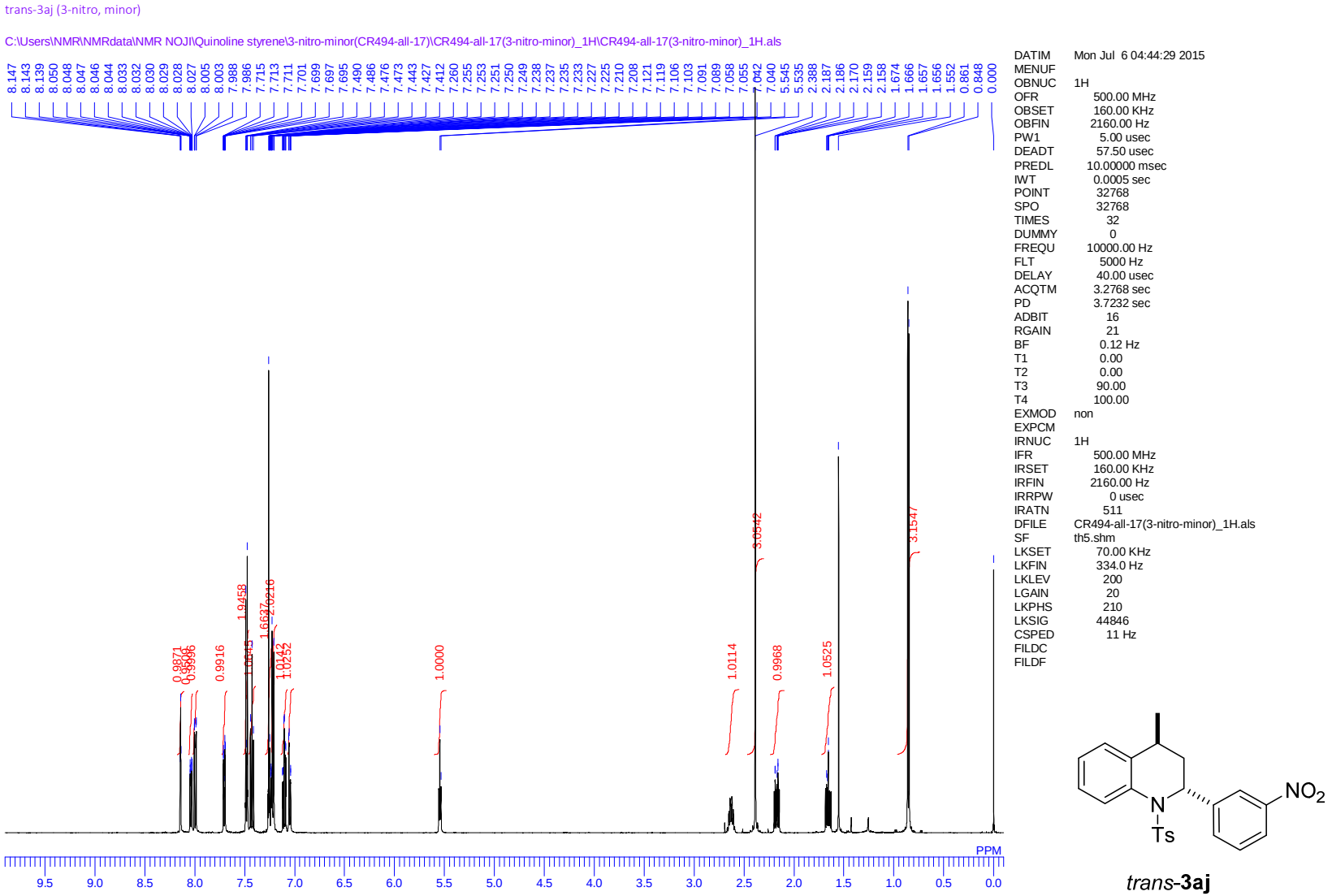


DATIM	Mon Jul 6 03:22:27 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR494crcr-3-nitro-major_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	10252
CSPED	14 Hz
FILDC	
FILDF	



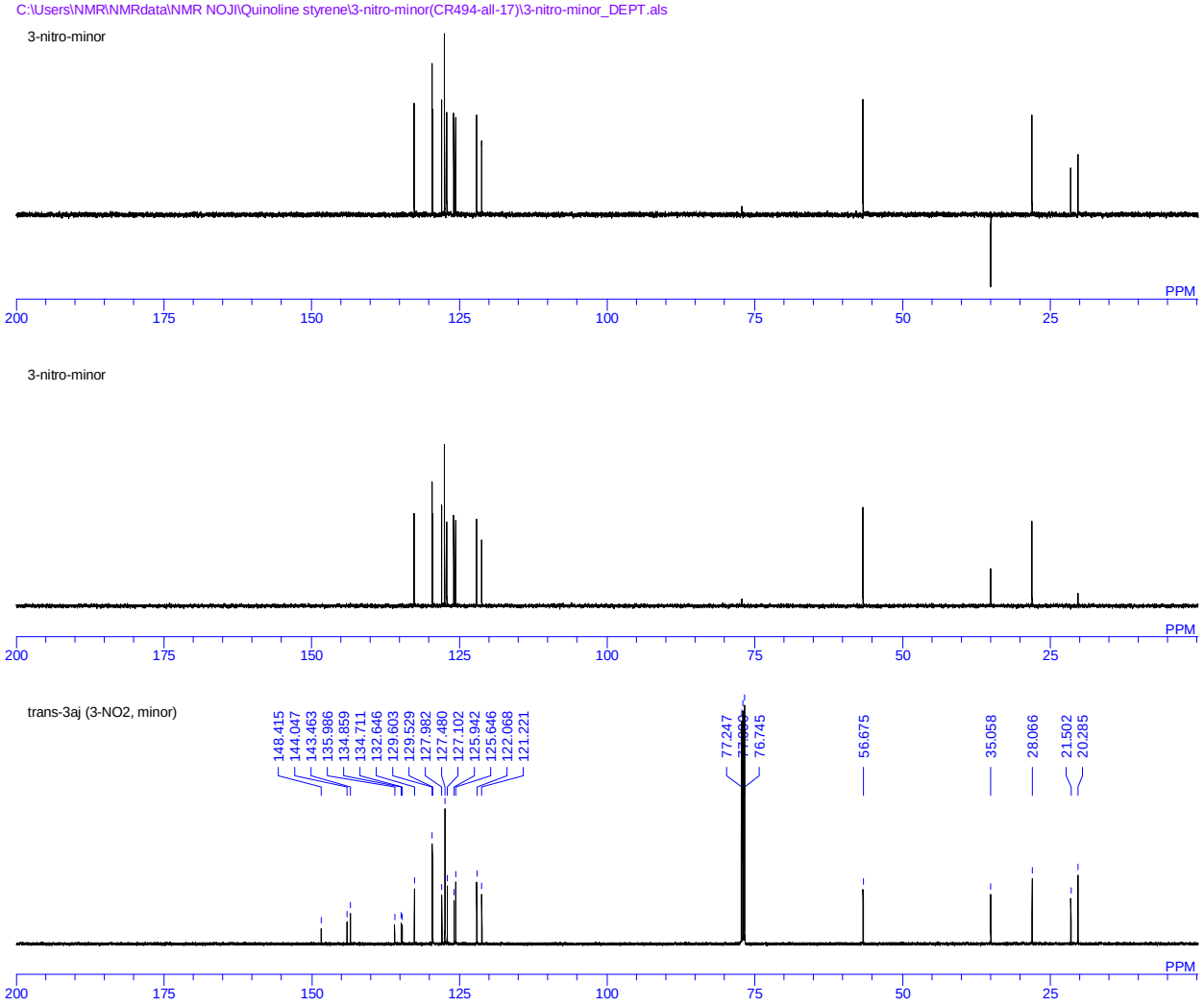
cis-**3aj**

^{1}H NMR spectrum of *trans*-3aj (minor)

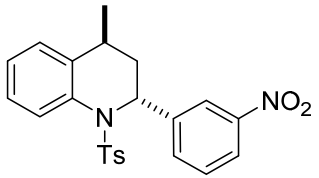


trans-**3aj**

^{13}C NMR spectrum of *trans*-3aj (minor)

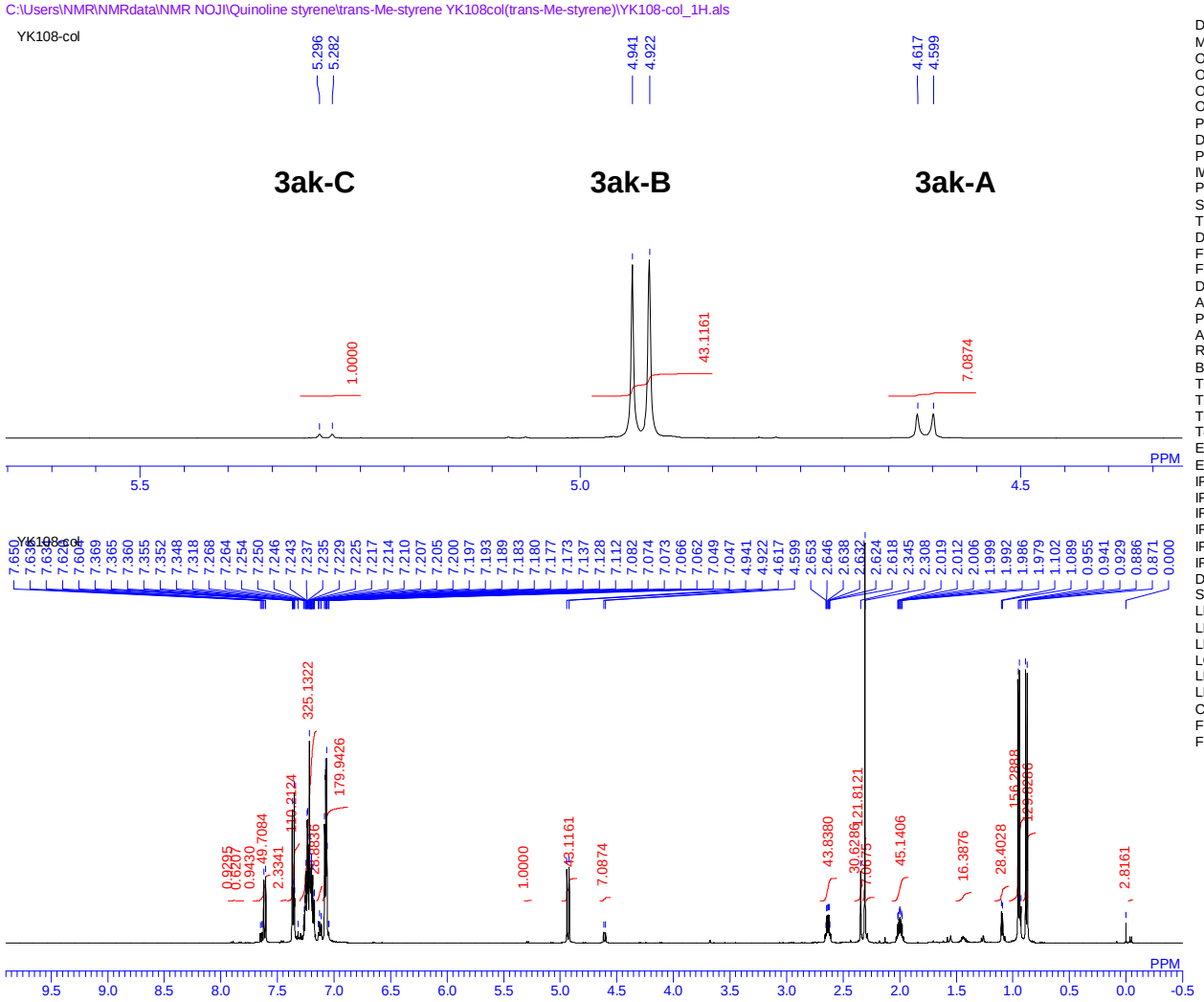


DATIM	Mon Jul 6 06:28:12 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	2048
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.12 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	3-nitro-minor_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	39450
CSPED	13 Hz
FILDC	
FILDF	

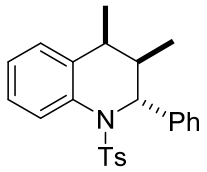


trans-**3aj**

^{1}H NMR spectrum of diastereomixture-3ak-B major (from *trans*-methylstyrene)

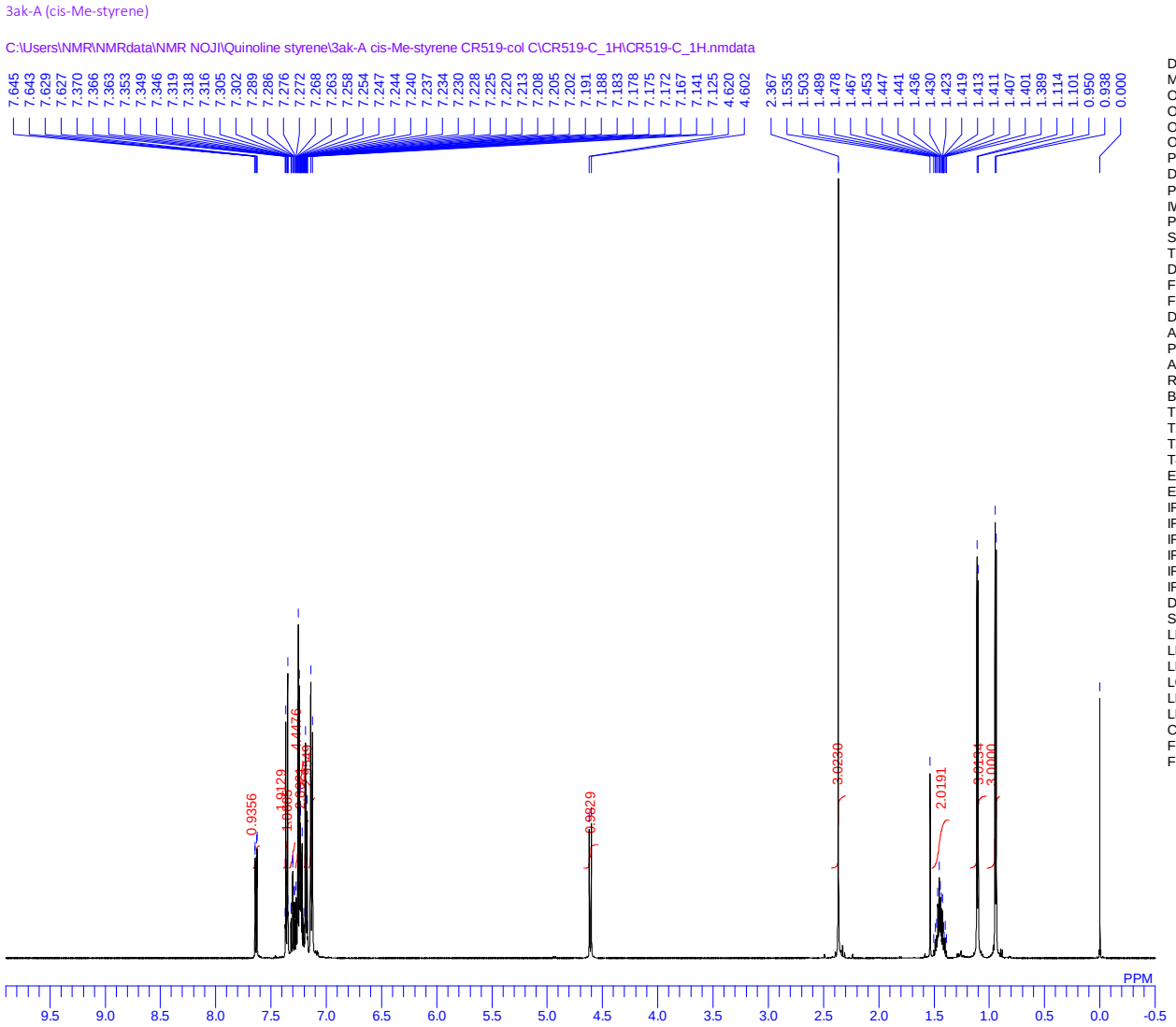


DATIM	Tue Aug 11 01:31:56 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	13
BF	0.00 Hz
T1	0.00
T2	0.00
T3	100.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	YK108-col_1H.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-751119492
CSPED	14 Hz
FILDC	
FILDF	

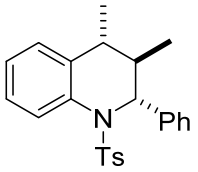


3ak-B (major)

^{1}H NMR spectrum of 3ak-A

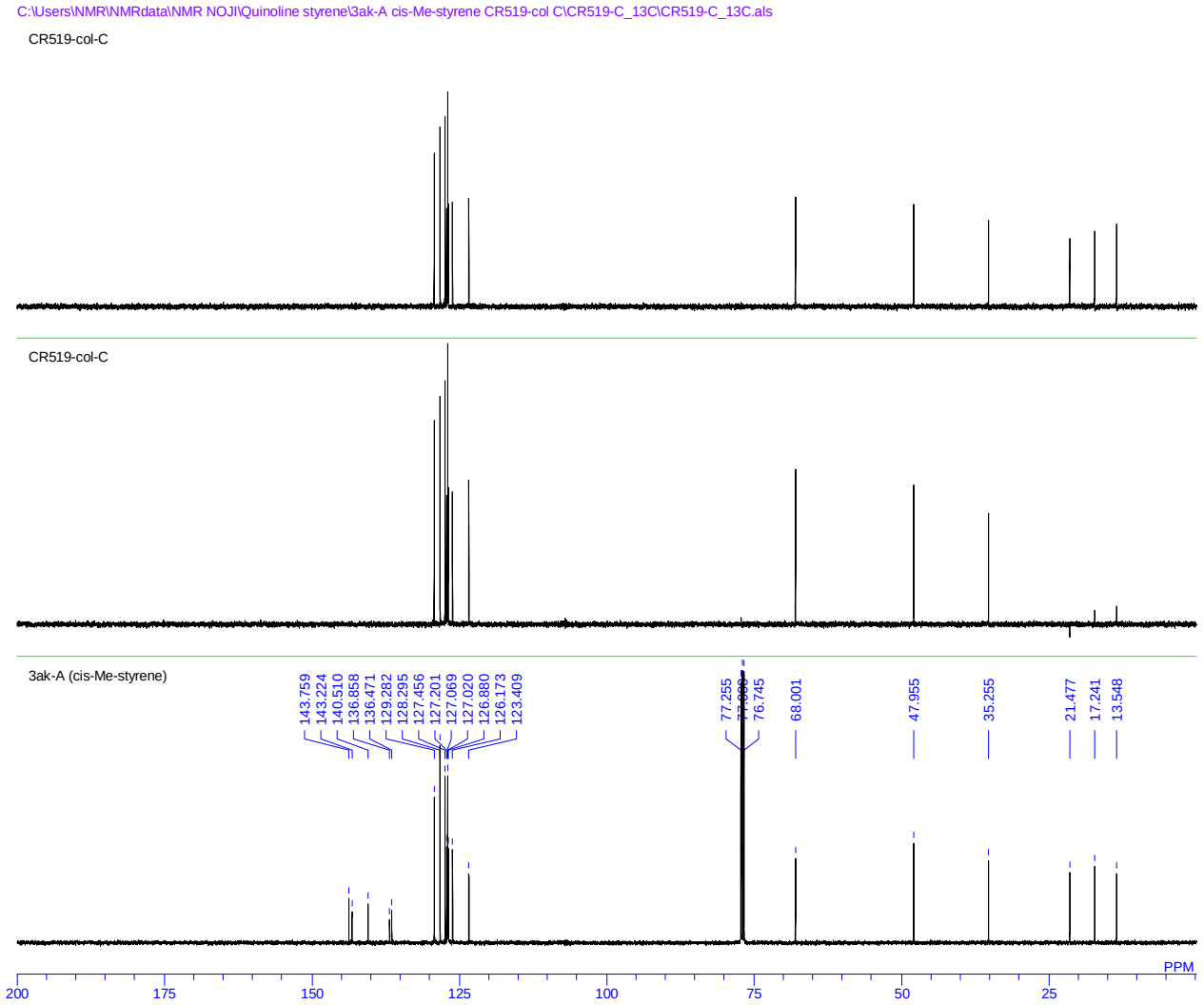


DATIM	Mon Oct 5 22:57:42 2015
MENUF	
OBNUC	1H
OFR	500.00 MHz
OBSET	160.00 KHz
OBFIN	2160.00 Hz
PW1	5.00 usec
DEADT	57.50 usec
PREDL	10.00000 msec
IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	19
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR519-C_1H.nmdata
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	-88284379
CSPED	13 Hz
FILDC	
FILDF	

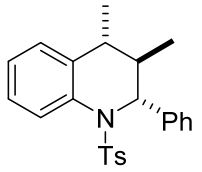


3ak-A (major)

^{13}C NMR spectrum of 3ak-A

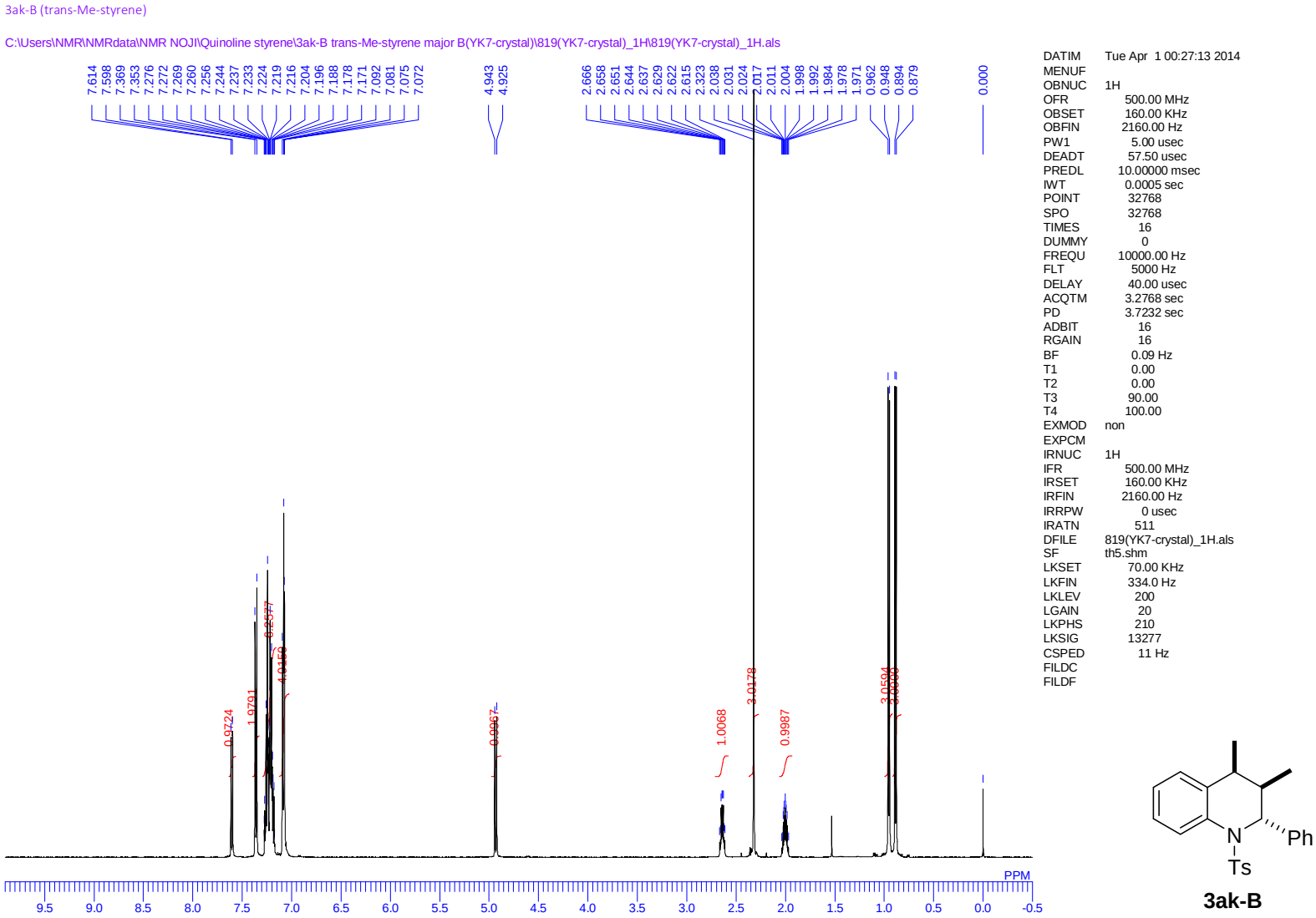


DATIM	Mon Oct 5 23:50:13 2015
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR519-C_13C.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	264087868
CSPED	12 Hz
FILDC	
FILDF	

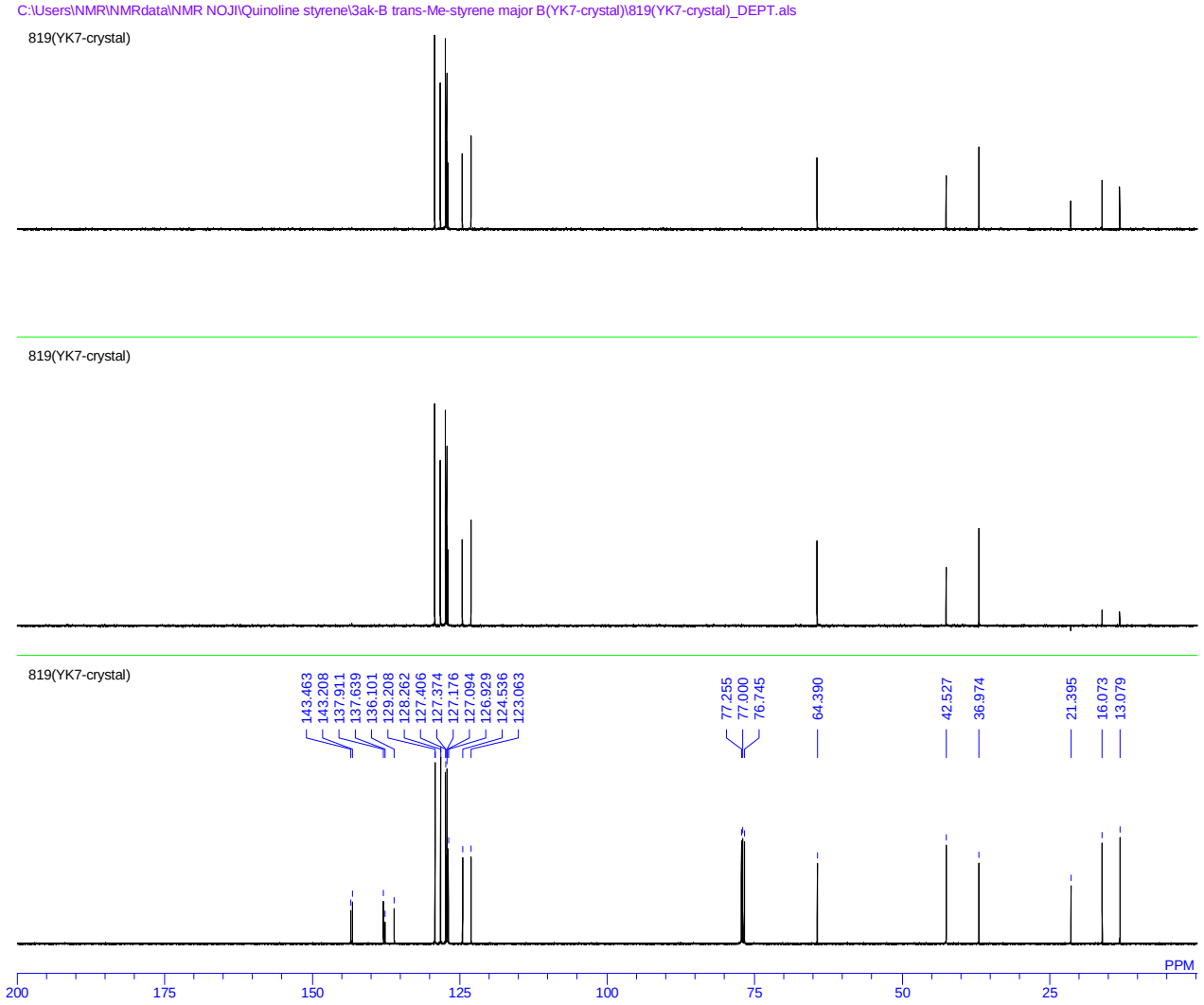


3ak-A (major)

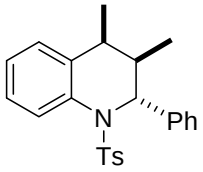
^{1}H NMR spectrum of 3ak-B



^{13}C NMR spectrum of 3ak-B

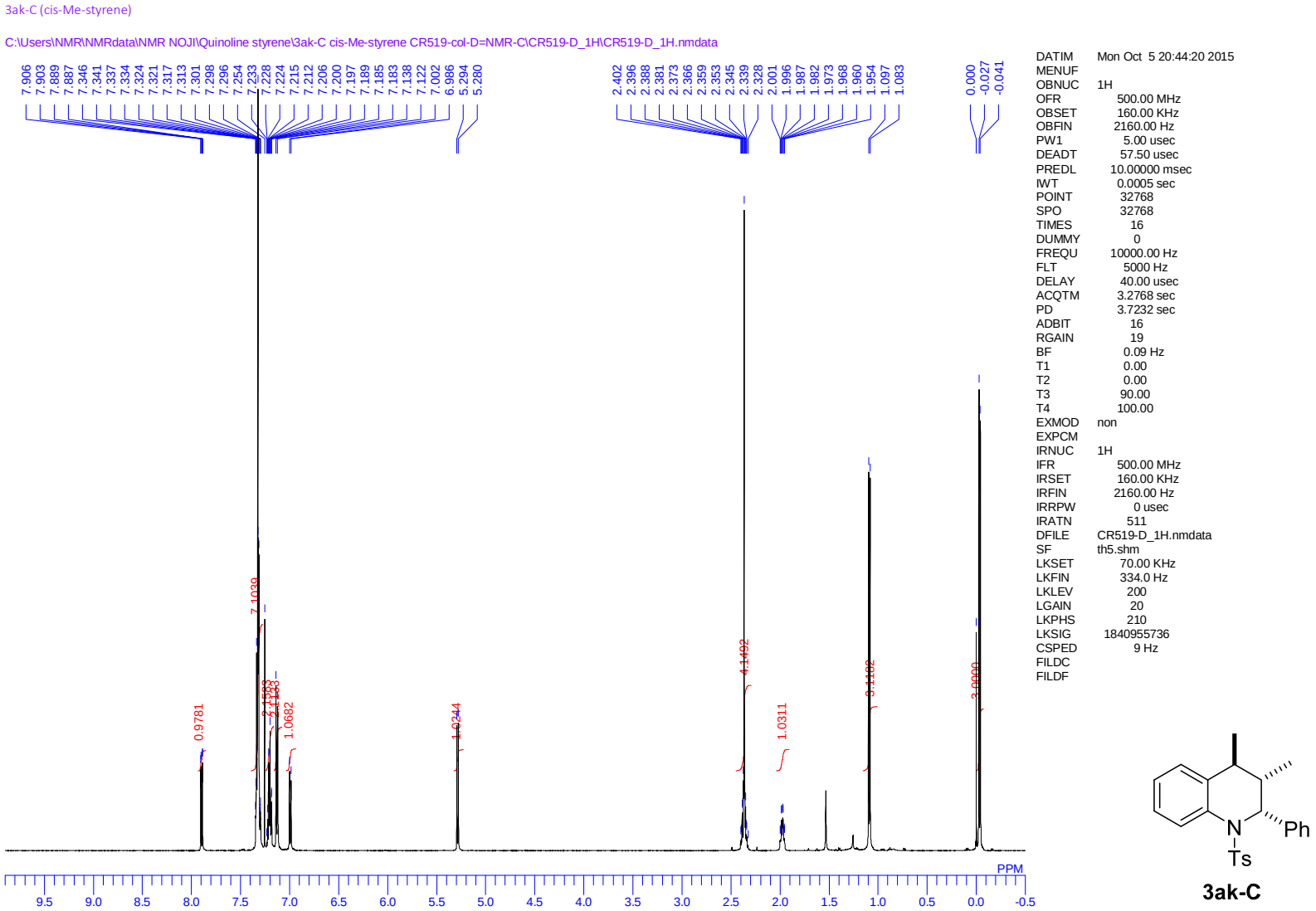


DATIM	Tue Apr 1 01:08:37 2014
MENUF	
OBNUC	13C
OFR	125.65 MHz
OBSET	120.00 KHz
OBFIN	7958.00 Hz
PW1	4.40 usec
DEADT	15.50 usec
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	800
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	819(YK7-crystal)_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	39820
CSPED	11 Hz
FILDC	
FILDF	

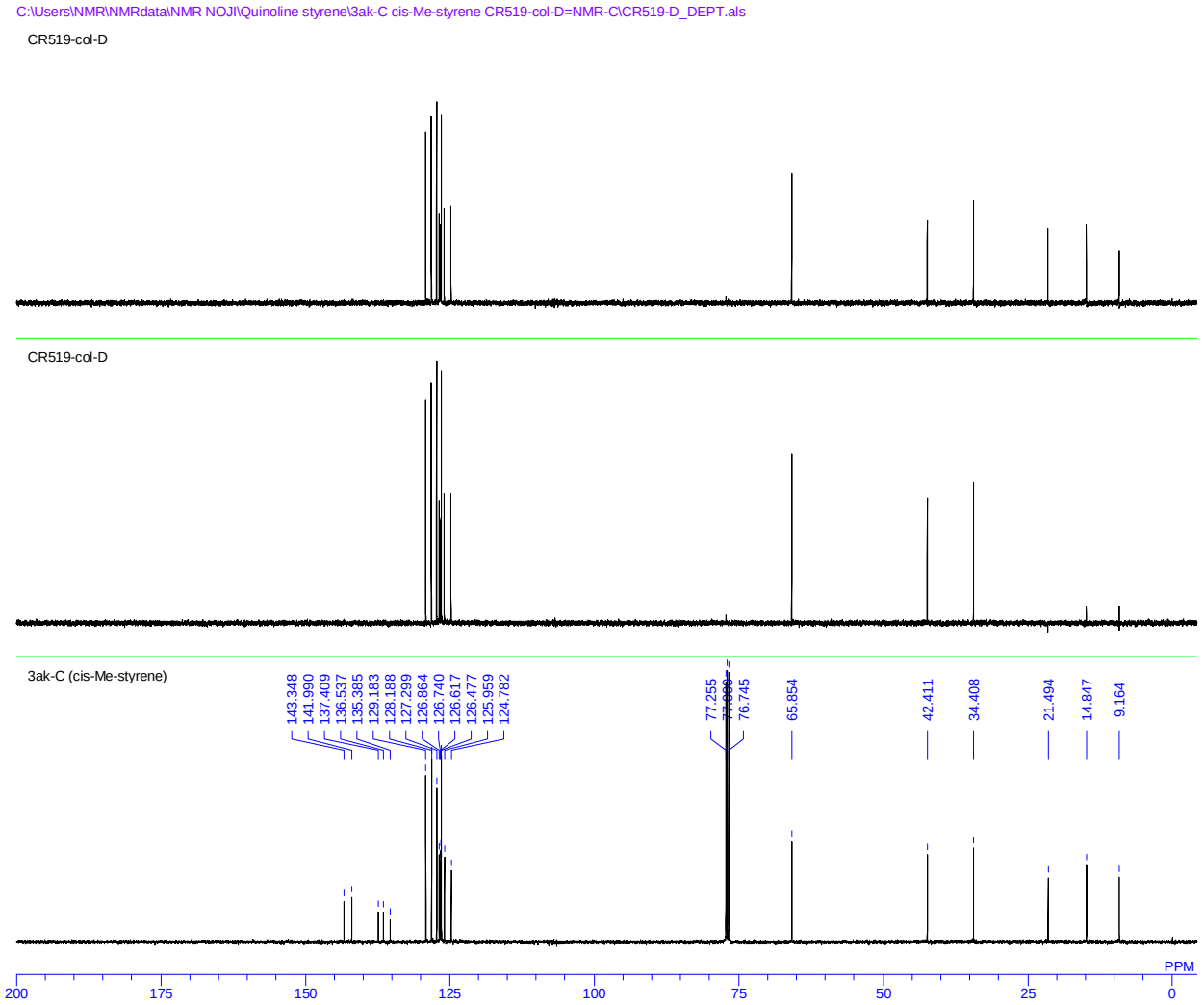


3ak-B

^{1}H NMR spectrum of 3ak-C



^{13}C NMR spectrum of 3ak-C



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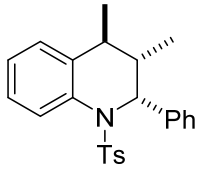
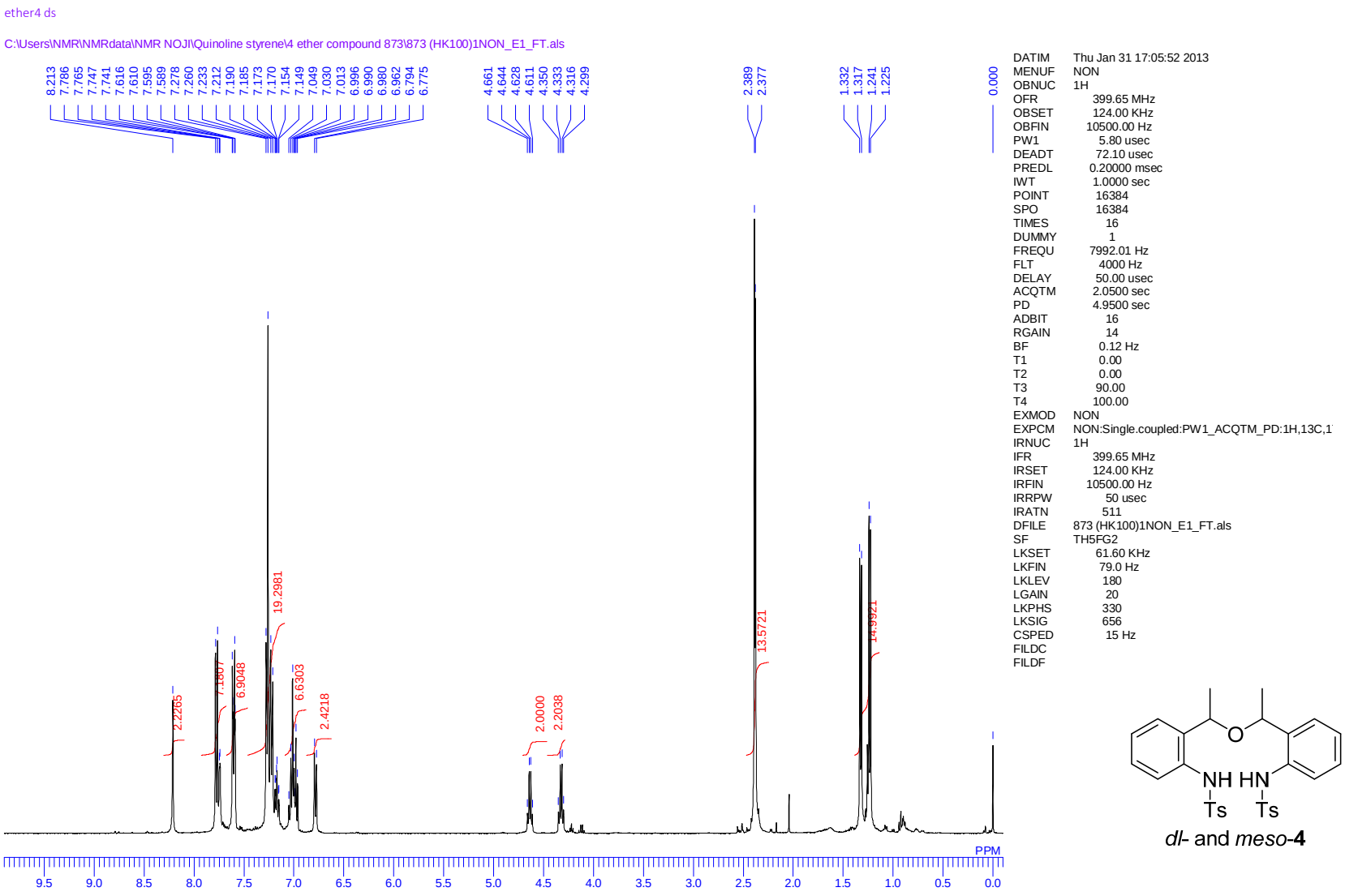
PREDL	10.00000 msec
IWT	0.0100 sec
POINT	32768
SPO	32768
TIMES	1024
DUMMY	1
FREQU	33898.30 Hz
FLT	16950 Hz
DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR519-D_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
LKFIN	334.0 Hz
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	2126368407
CSPED	12 Hz
FILDC	
FILDF	



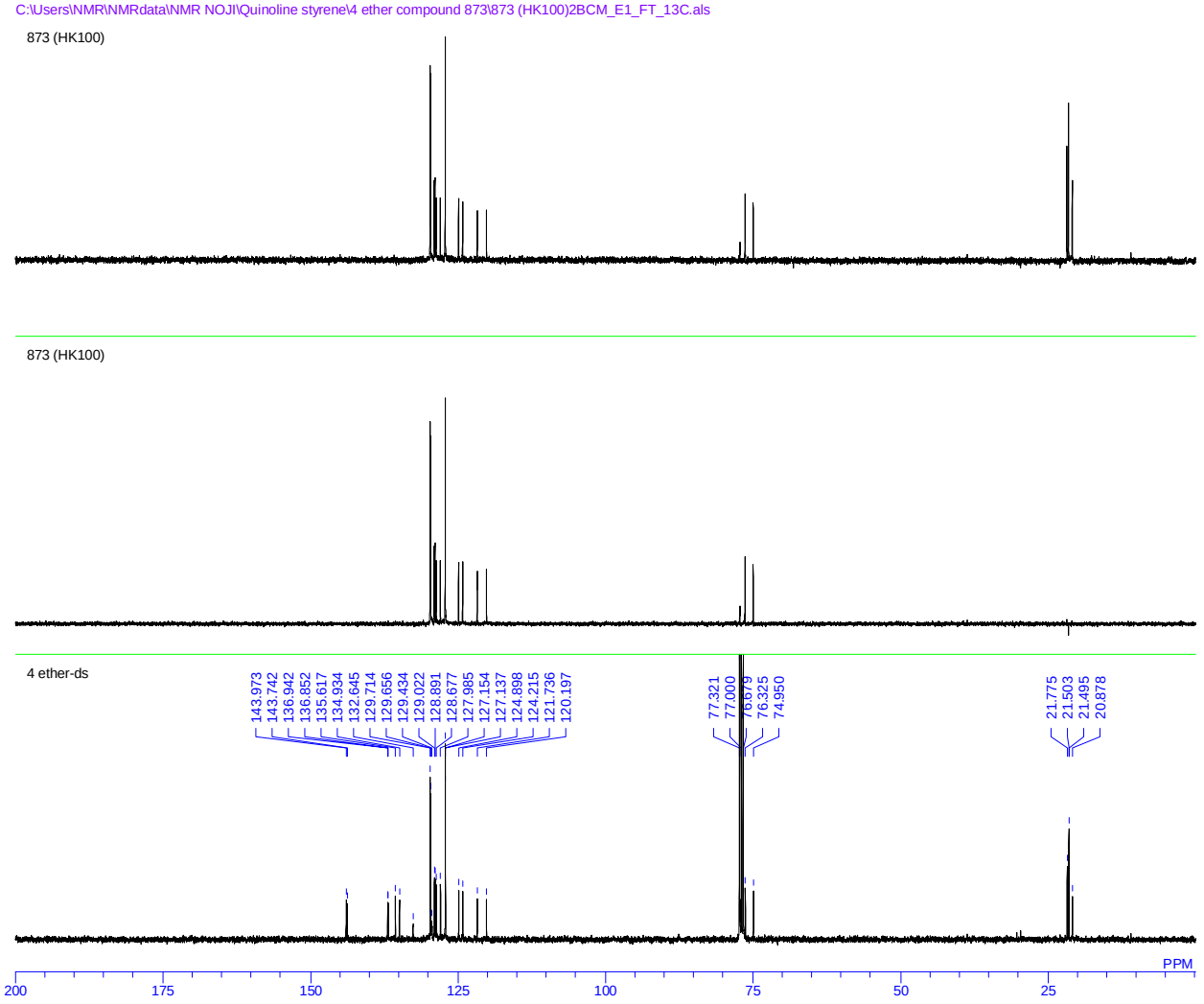
3ak-C

^{1}H NMR spectrum of 4, diastereomixture



dl- and *meso*-**4**

^{13}C NMR spectrum of 4, diastereomixture



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IWT	1.0000 sec
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SPO	32768
TIMES	800
DUMMY	1
FREQU	27118.64 Hz
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DELAY	14.76 usec
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PD	1.7920 sec
ADBIT	16
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BF	1.20 Hz
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T3	90.00
T4	100.00
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EXPCM	Bilevel.complete.decoupling:Set_IRRPW
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IRRPW	50 usec
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LKSIG	650
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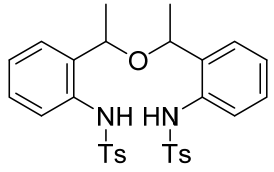
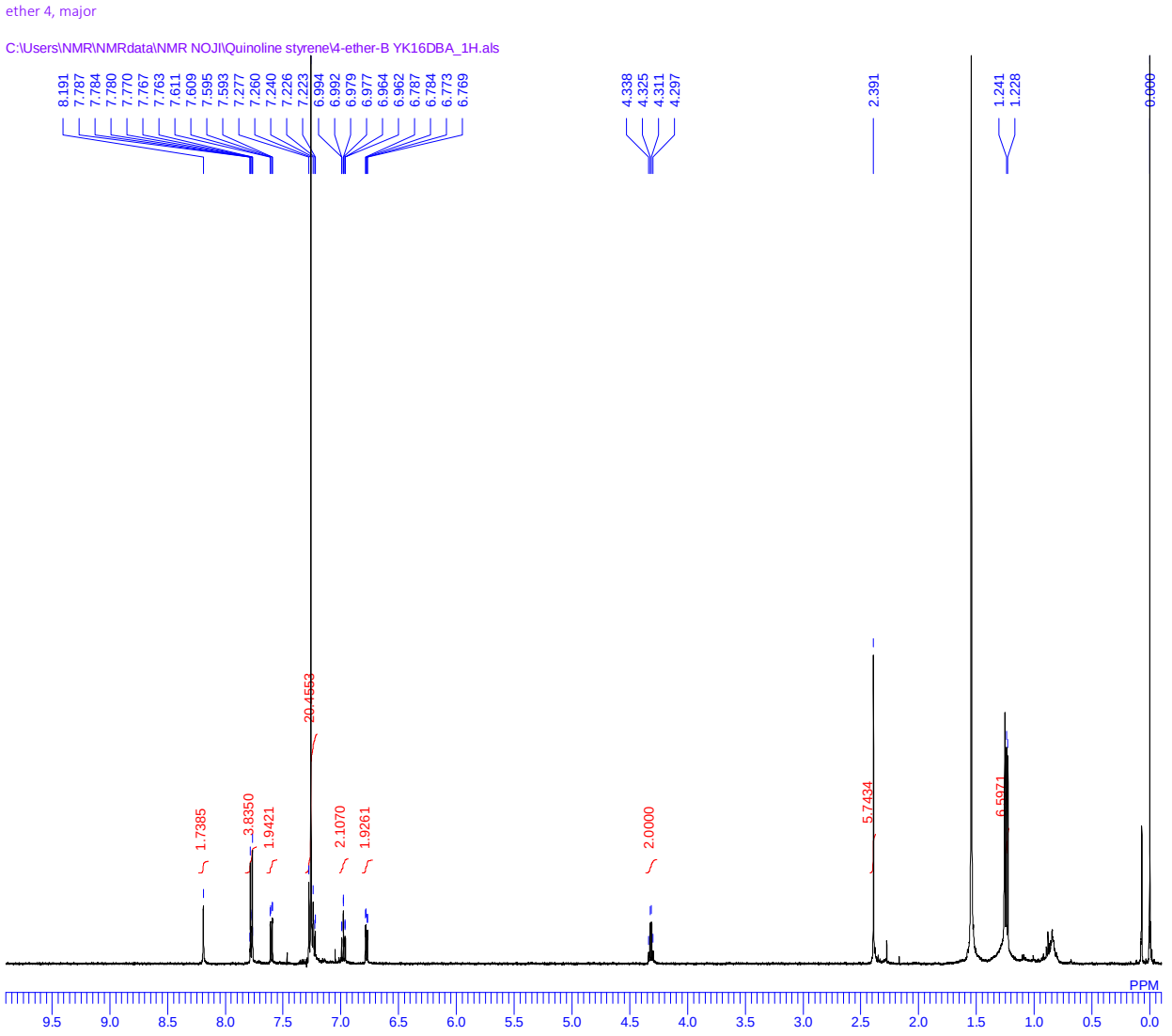
FILDC	
FILDF	



dl- and *meso*-**4**

^{1}H NMR spectrum of 4, major



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SPO	32768
TIMES	16
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FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	25
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
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LKSET	70.00 KHz
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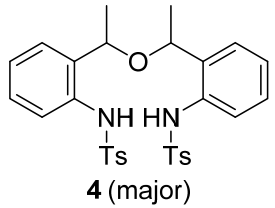
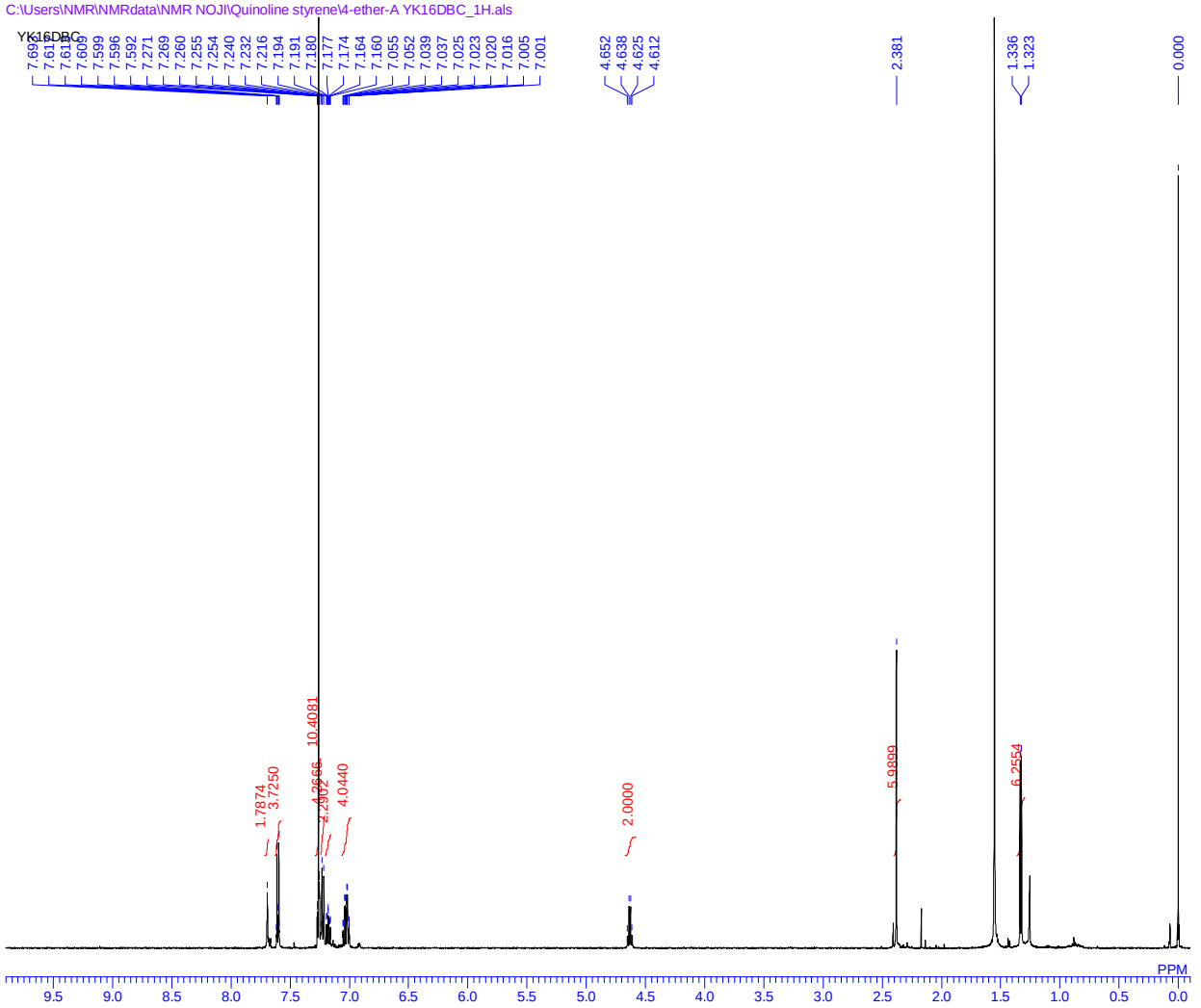
LKLEV	200
LGAIN	20
LKPHS	210
LKSIG	21342
CSPED	9 Hz
FILDC	
FILDF	



4 (major)

^{1}H NMR spectrum of 4, major



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IWT	0.0005 sec
POINT	32768
SPO	32768
TIMES	16
DUMMY	0
FREQU	10000.00 Hz
FLT	5000 Hz
DELAY	40.00 usec
ACQTM	3.2768 sec
PD	3.7232 sec
ADBIT	16
RGAIN	24
BF	1.20 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	non
EXPCM	
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
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LKSET	70.00 KHz
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LKPHS	210
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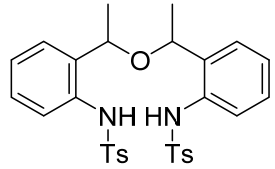
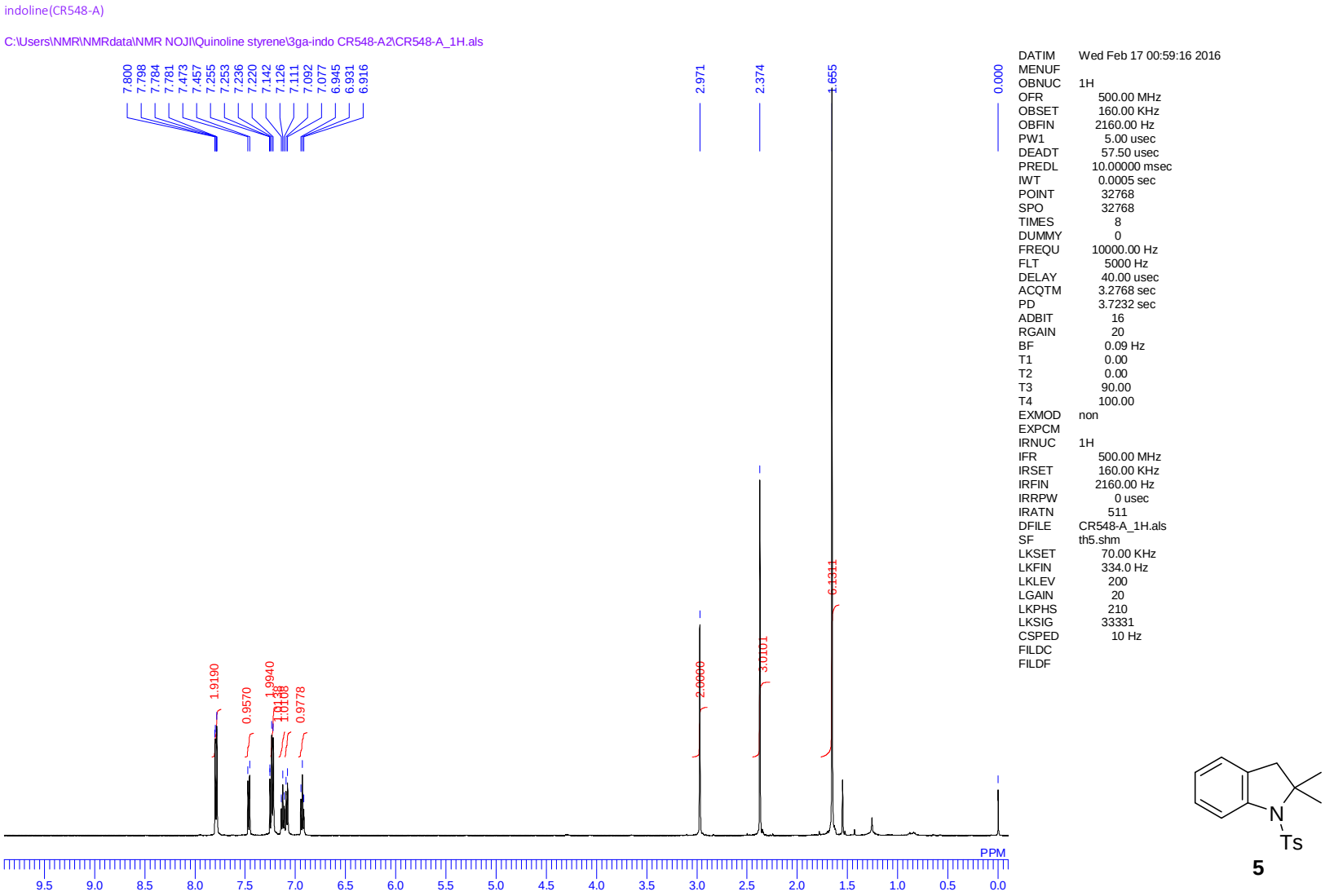
CSPED	12 Hz
FILDC	
FILDF	



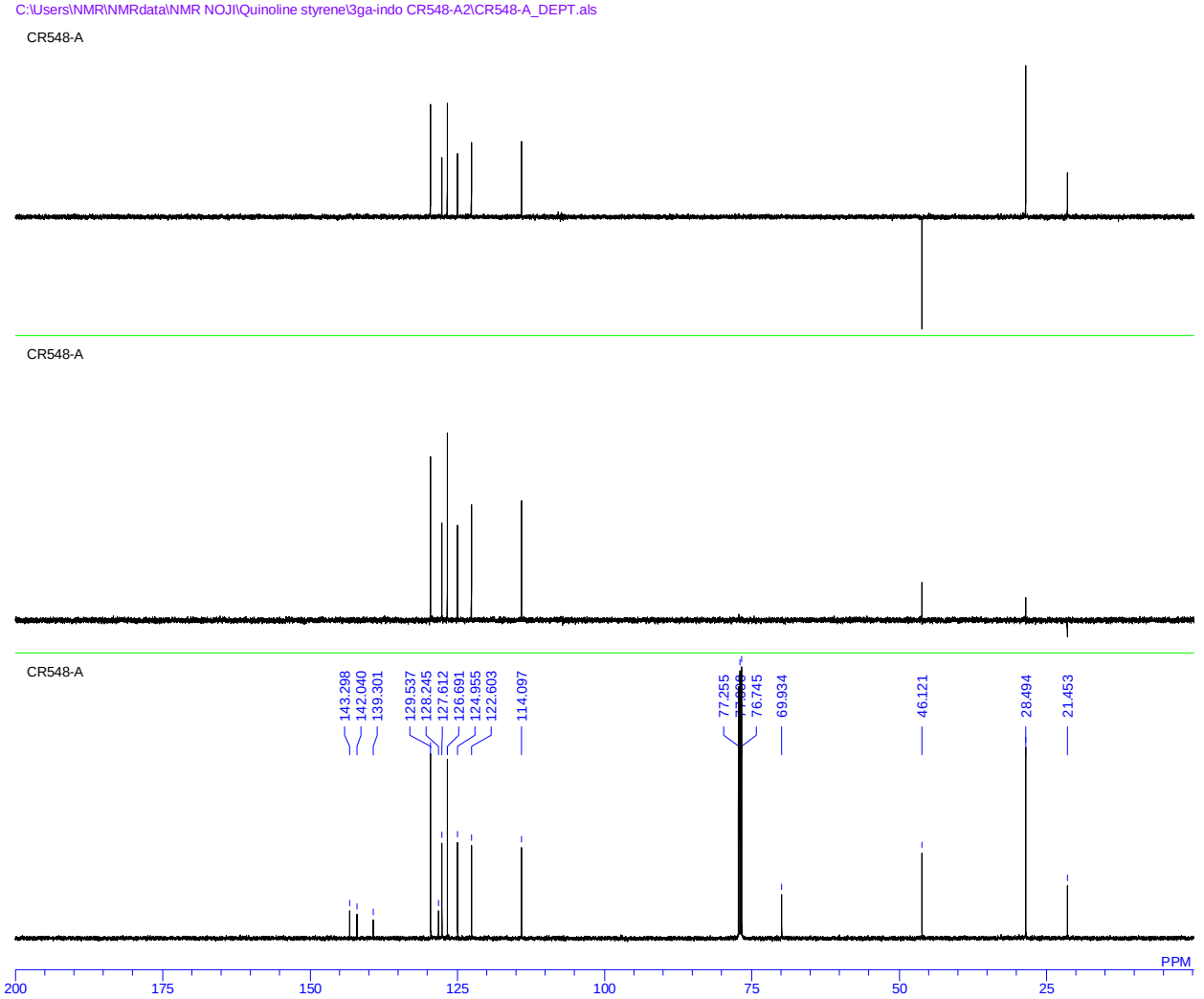
4 (minor)

^{1}H NMR spectrum of 2,2-Dimethyl-1-tosylindoline



5

^{13}C NMR spectrum of 2,2-Dimethyl-1-tosylindoline



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SPO	32768
TIMES	1024
DUMMY	1
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DELAY	11.80 usec
ACQTM	0.9667 sec
PD	2.0333 sec
ADBIT	16
RGAIN	28
BF	0.09 Hz
T1	0.00
T2	0.00
T3	90.00
T4	100.00
EXMOD	bcm
EXPCM	error_expcm
IRNUC	1H
IFR	500.00 MHz
IRSET	160.00 KHz
IRFIN	2160.00 Hz
IRRPW	0 usec
IRATN	511
DFILE	CR548-A_DEPT.als
SF	th5.shm
LKSET	70.00 KHz
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LKPHS	210
LKSIG	5746
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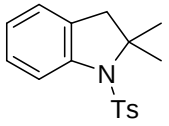
FILDC	
FILDF	



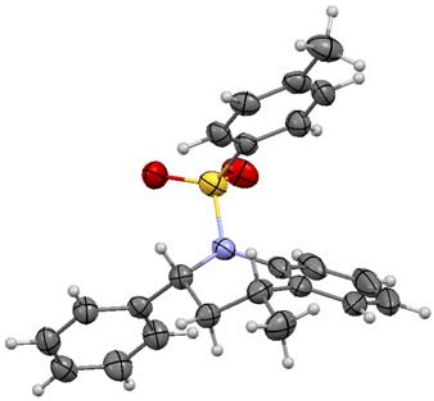
5

X-ray crystallographic Analysis

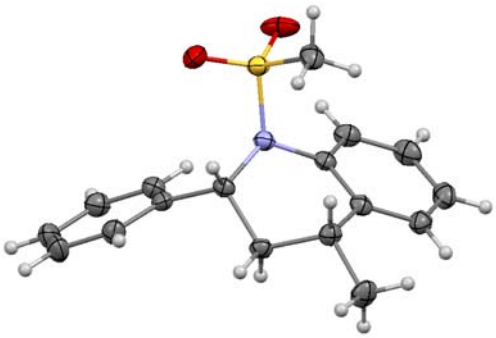
Single crystals of tetrahydroquinolines **3** were mounted on a MicroMount® or MicroMesh® polyimide tip with a paraffin oil. All measurements were made on a Rigaku R-AXIS RAPID imaging plate diffractometer using filtered Cu-Kα radiation. The data were corrected for Lorentz and polarization effects and numerical absorption. The structures were solved by direct methods[1] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms of **2a** and **2b** were refined using the riding model. All calculations were performed using the CrystalStructure[2] crystallographic software package except for refinement, which was performed using SHELXL 2014.[3]

Table S1. Experimental Data for the X-ray Crystallography of *cis*-**3aa**, *cis*-**3ba**, *cis*-**3da**, *cis*-**3fa**

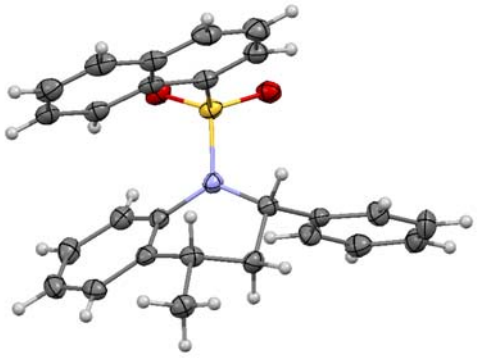
parameter	*cis*-**3aa**	*cis*-**3ba**	*cis*-**3da**	*cis*-**3fa**
formula	$C_{46}H_{46}N_2O_4S_2$	$C_{46}H_{46}N_2O_4S_2$	$C_{26}H_{23}NO_2S$	$C_{28}H_{25}NO_2S$
Mw	644.77	301.40	413.53	439.57
crystal size/mm	0.230 x 0.210 x 0.210	0.270 X 0.230 X 0.140	0.285 X 0.203 X 0.188	0.226 X 0.176 X 0.102
crystal system	triclinic	monoclinic	orthorhombic	triclinic
a/Å	13.4592(4)	9.31361(17)	10.76106(19)	10.7020(2)
b/Å	13.7532(4)	17.0717(3)	12.6449(2)	10.8460(2)
c/Å	13.8380(3)	10.31691(19)	15.1251(3)	10.8473(2)
α/deg	60.5530(13)	90	90	61.637(4)
β/deg	66.5791(14)	111.3479(8)	90	87.161(6)
γ/deg	71.0600(15)	90	90	86.133(6)
V/Å^3	2019.90(10)	1527.83(5)	2058.11(6)	1105.20(6)
space group	*P*-1 (#2)	$P2_1/n$ (#14)	$P2_12_12_1$ (#19)	*P*-1 (#2)
Z	2	4	4	2
g/cm	1.241	1.310	1.334	1.321
μ (Cu Kα)/cm^{-1}	15.515	19.092	15.751	14.994
T/K	113	93	93	93
no. of measured reflections	21597	27343	23345	13011
no. of unique reflections	7203	2796	3646	3949
R_{int}	0.0984	0.0396	0.0225	0.0264
goodness of fit	0.974	1.063	1.062	1.049
R_1	0.0606	0.0353	0.0285	0.0361
wR_2	0.1422	0.0952	0.0779	0.0935
Flack parameter	-	-	0.028(5)	-
Structure solv	SIR2008	SIR2008	SIR2011	SIR92
Refinement	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7
CCDC Number	CCDC 1503781	CCDC 1503788	CCDC 1503797	CCDC 1503786



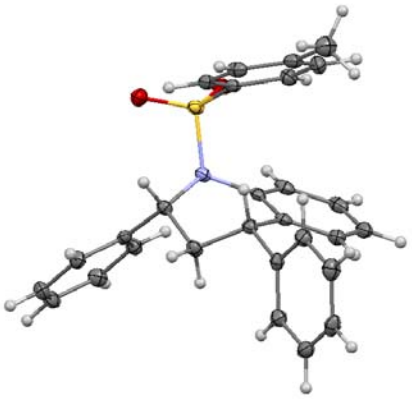
(a) *cis*-**3aa**



(b) *cis*-**3ba**



(c) *cis*-**3da**

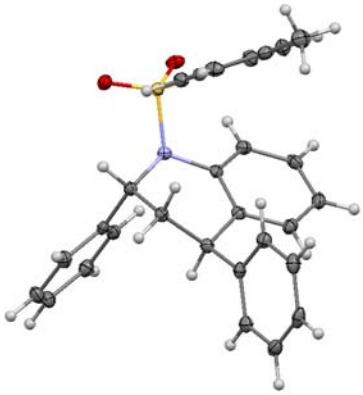


(d) *cis*-**3fa**

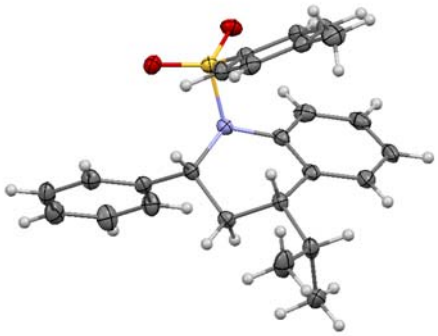
Figure S1. Crystal structure of (a) *cis*-**3aa**, (b) *cis*-**3ba**, (c) *cis*-**3da**, (d) *cis*-**3fa**; atomic thermal ellipsoids are drawn at the 50% probability level for non-hydrogen atoms.

Table S2. Experimental Data for the X-ray Crystallography of *trans*-**3fa**, *cis*-**3ga**, *cis*-**3ha**, *trans*-**3ha**

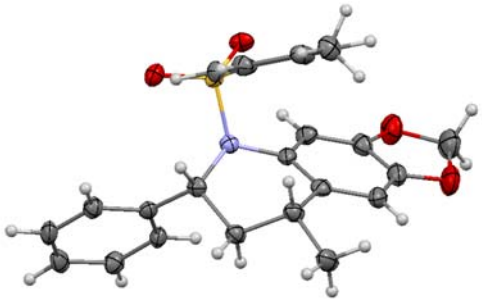
parameter	*trans*-**3fa**	*cis*-**3ga**	*cis*-**3ha**	*trans*-**3ha**
formula	$C_{28}H_{25}NO_2S$	$C_{50}H_{54}N_2O_4S_2$	$C_{24}H_{23}NO_4S$	$C_{24}H_{23}NO_4S$
Mw	439.57	811.11	421.51	421.51
crystal size/mm	0.254 X 0.210 X 0.046	0.315 X 0.179 X 0.120	0.270 X 0.230 X 0.120	0.270 X 0.240 X 0.083
crystal system	triclinic	triclinic	monoclinic	monoclinic
a/Å	10.44551(19)	10.38081(19)	10.1672(2)	25.9376(7)
b/Å	10.56013(19)	14.6860(3)	17.7370(4)	10.5259(3)
c/Å	10.9713(2)	15.5780(3)	11.8622(3)	15.1628(6)
α/deg	87.346(6)	81.5557(11)	90	90
β/deg	65.296(5)	88.3312(11)	93.7758(16)	96.397(2)
γ/deg	85.087(6)	67.6755(10)	90	90
V/Å^3	1095.33(5)	2172.17(7)	2134.54(9)	4113.9(2)
space group	*P*-1 (#2)	*P*-1 (#2)	$P2_1/n$ (#14)	C_2/c (#15)
Z	2	2	4	8
g/cm	1.333	1.240	1.312	1.361
μ (Cu Kα)/cm^{-1}	15.129	14.763	15.995	16.598
T/K	93	93	93	93
no. of measured reflections	17943	23339	21717	20876
no. of unique reflections	3914	7797	3857	3774
R_{int}	0.0223	0.0599	0.0893	0.1309
goodness of fit	1.053	1.049	1.193	1.035
R_1	0.0396	0.0493	0.0627	0.0746
wR_2	0.1046	0.1432	0.1494	0.1658
Structure solv	SIR2011	SIR2008	SIR2008	SIR2008
Refinement	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7
CCDC Number	CCDC 1503787	CCDC 1503792	CCDC 1503790	CCDC 1503791



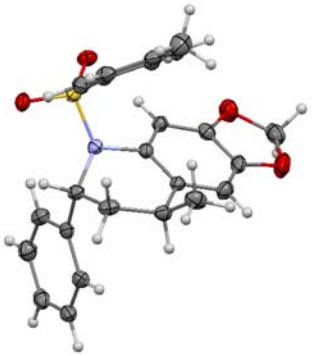
(a) *trans*-**3fa**



(b) *cis*-**3ga**



(c) *cis*-**3ha**

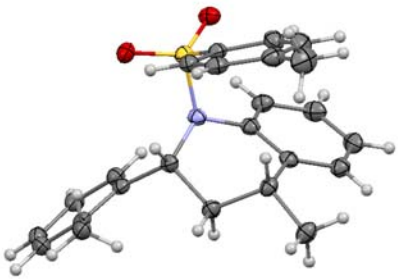


(d) *trans*-**3ha**

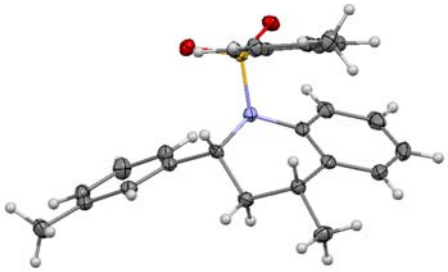
Figure S2. Crystal structure of (a) *trans*-**3fa**, (b) *cis*-**3ga**, (c) *cis*-**3ha**, (d) *trans*-**3ha**; atomic thermal ellipsoids are drawn at the 50% probability level for non-hydrogen atoms.

Table S3. Experimental Data for the X-ray Crystallography of *cis*-**3ac**, *cis*-**3ad**, *cis*-**3ae**, *trans*-**3ae**

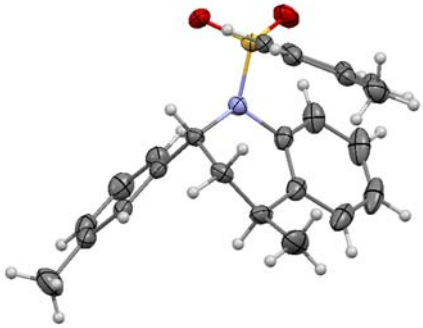
parameter	*cis*-**3ab**	*cis*-**3ac**	*trans*-**3ac**	*cis*-**3ad**
formula	$C_{24}H_{25}NO_2S$	$C_{24}H_{25}NO_2S$	$C_{24}H_{25}NO_2S$	$C_{48}H_{50}N_2O_4S_2$
Mw	391.53	391.53	391.53	783.05
crystal size/mm	0.241 X 0.171 X 0.124	0.312 X 0.109 X 0.024	0.215 X 0.206 X 0.111	0.269 X 0.241 X 0.165
crystal system	triclinic	monoclinic	monoclinic	triclinic
a/Å	8.05213(15)	19.8146(4)	13.8968(6)	12.4194(2)
b/Å	11.1171(2)	11.0383(2)	7.9542(3)	12.6505(2)
c/Å	11.9245(2)	11.3171(2)	18.7882(7)	15.0345(3)
α/deg	100.4325(10)	90	90	69.9775(9)
β/deg	92.1642(10	125.947(9)	94.222(7)	83.3540(9)
γ/deg	102.6609(10)	90	90	70.5639(9)
V/Å^3	1020.93(3)	2003.9(2)	2071.16(14)	2092.85(7)
space group	*P*-1 (#2)	*Cc* (#9)	$P2_1/c$ (#14)	*P*-1 (#2)
Z	2	4	4	2
g/cm	1.274	1.298	1.256	1.243
μ (Cu Kα)/cm^{-1}	15.526	15.821	15.307	15.148
T/K	93	93	93	93
no. of measured reflections	17595	11294	22597	22333
no. of unique reflections	3682	3294	3719	7480
R_{int}	0.0693	0.0257	0.0308	0.0605
goodness of fit	0.976	1.057	1.193	1.174
R_1	0.0490	0.0333	0.0466	0.0548
wR_2	0.1369	0.0888	0.1303	0.1416
Flack parameter	-	0.034(6)	-	-
Structure solv	SIR2008	SIR2011	SIR2011	SIR2008
Refinement	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7
CCDC Number	CCDC 1503782	CCDC 1503777	CCDC 1503780	CCDC 1503779



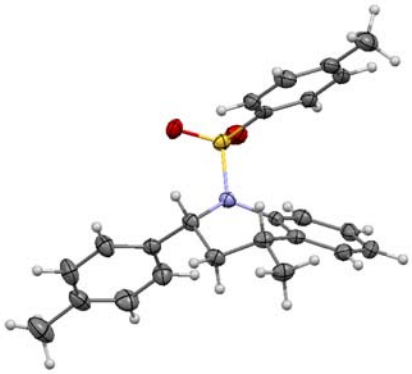
(a) *cis*-**3ab**



(b) *cis*-**3ac**



(c) *trans*-**3ac**

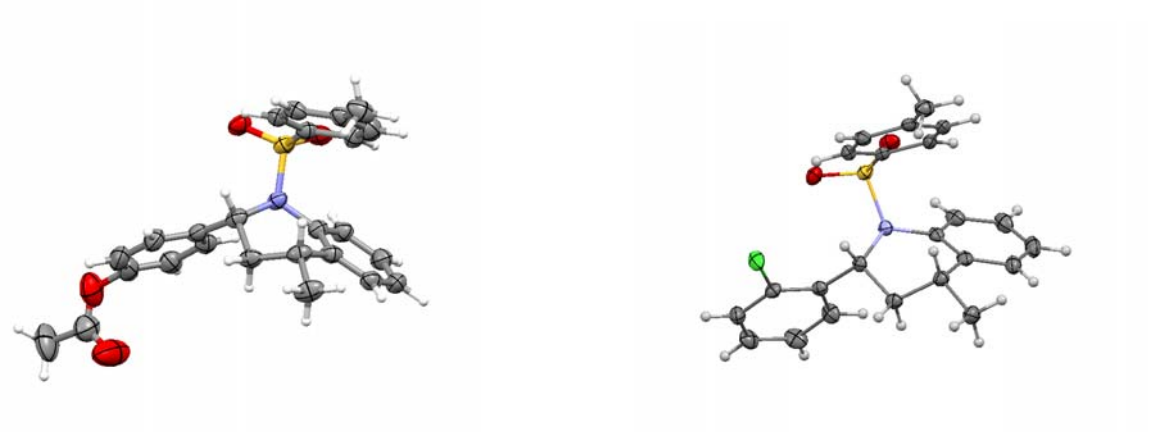


(d) *cis*-**3ad**

Figure S3. Crystal structure of (a) *cis*-**3ab**, (b) *cis*-**3ac**, (c) *trans*-**3ac**, (d) *cis*-**3ad**; atomic thermal ellipsoids are drawn at the 50% probability level for non-hydrogen atoms.

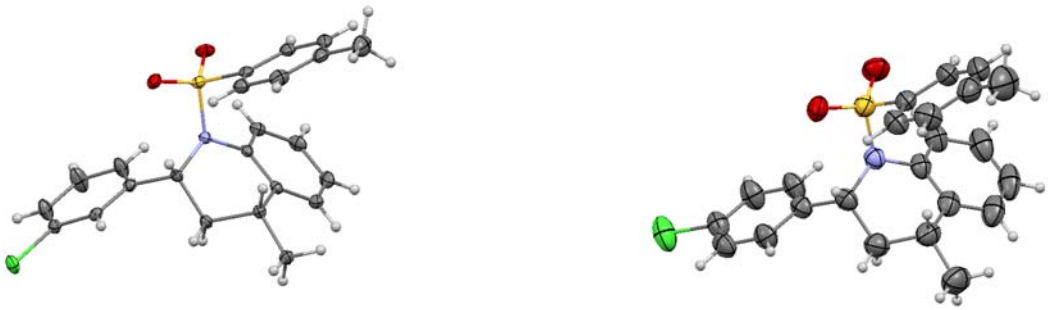
Table S4. Experimental Data for the X-ray Crystallography of *cis*-**3af**, *cis*-**3ag**, *cis*-**3ah**, *cis*-**3ai**

parameter	*cis*-**3ae**	*cis*-**3ag**	*cis*-**3ah**	*cis*-**3ai**
formula	$C_{50}H_{50}N_2O_8S_2$	$C_{46}H_{44}N_2O_4S_2Cl_2$	$C_{23}H_{22}NO_2SCl$	$C_{46}H_{44}N_2O_4S_2Cl_2$
Mw	871.07	823.89	411.95	823.89
crystal size/mm	0.261 X 0.189 X 0.070	0.273 X 0.253 X 0.182	0.322 X 0.176 X 0.11	0.209 X 0.203 X 0.058
crystal system	triclinic	monoclinic	monoclinic	triclinic
a/Å	9.1775(2)	9.44882(17)	10.8276(2)	12.8311(2)
b/Å	13.7711(3)	13.9220(3)	9.64645(19)	13.4491(3)
c/Å	18.9720(4)	30.4243(6)	19.2261(4)	13.7483(3)
α/deg	68.731(5)	90	90	64.3587(8)
β/deg	88.243(6)	95.2278(7	92.599(7)	85.9065(8)
γ/deg	87.680(6)	90	90	77.6964(9)
V/Å^3	2232.27(11)	3985.56(12)	2006.07(7)	2089.15(7)
space group	*P*-1 (#2)	$P2_1/c$ (#14)	$P2_1/c$ (#14)	*P*-1 (#2)
Z	2	4	4	2
g/cm	1.296	1.373	1.364	1.310
μ (Cu Kα)/cm^{-1}	15.458	28.249	28.062	26.946
T/K	93	93	93	173
no. of measured reflections	26289	44335	22671	23497
no. of unique reflections	7995	7300	3658	7404
R_{int}	0.1109	0.0444	0.0237	0.0427
goodness of fit	1.099	1.108	1.104	1.085
R_1	0.0737	0.0454	0.0316	0.0415
wR_2	0.2346	0.1185	0.0843	0.1200
Structure solv	SIR2011	SIR2008	SIR2008	SIR2008
Refinement	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7
CCDC Number	CCDC 1503778	CCDC 1503794	CCDC 1503793	CCDC 1503796



(a) *cis*-**3ae** (b) *cis*-**3ag**

Disordered acetoxy group was omitted for clarity.

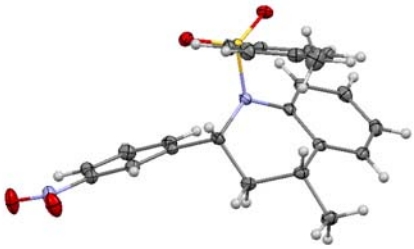


(c) *cis*-**3ah** (d) *cis*-**3ai**

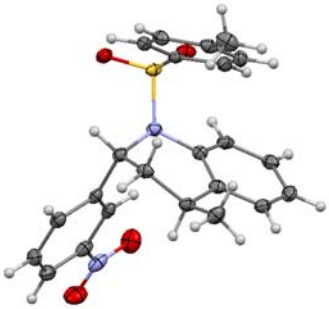
Figure S4. Crystal structure of (a) *cis*-**3ae**, (b) *cis*-**3ag**, (c) *cis*-**3ah**, (d) *cis*-**3ai**; atomic thermal ellipsoids are drawn at the 50% probability level for non-hydrogen atoms.

Table S5. Experimental Data for the X-ray Crystallography of *cis*-**3aj**, *trans*-**3aj**, **3ak-A**, **3ak-B**

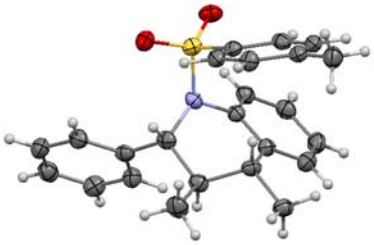
parameter	*cis*-**3aj**	*trans*-**3aj**	**3ak-A**	**3ak-B**
formula	$C_{23}H_{22}N_2O_4S$	$C_{23}H_{22}N_2O_4S$	$C_{48}H_{50}N_2O_4S_2$	$C_{24}H_{25}NO_2S$
Mw	422.50	422.50	783.05	391.53
crystal size/mm	0.356 X 0.217 X 0.130	0.191 X 0.182 X 0.080	0.229 X 0.201 X 0.170	0.318 X 0.307 X 0.125
crystal system	triclinic	monoclinic	monoclinic	monoclinic
a/Å	7.58966(19)	12.0068(3)	9.8930(2)	9.54275(17)
b/Å	11.1047(3)	8.16703(18)	7.98805(16)	12.8177(2)
c/Å	11.8359(3)	20.4719(5)	25.8524(6)	16.5996(3)
α/deg	95.725(7)	90	90	90
β/deg	90.396(6)	97.127(7)	95.040(7)	90.4922(7)
γ/deg	90.747(6)	90	90	90
V/Å^3	992.44(4)	1991.97(8)	2035.12(8)	2030.33(6)
space group	*P*-1 (#2)	$P2_1/c$ (#14)	*Pc* (#7)	$P2_1/n$ (#14)
Z	2	4	2	4
g/cm	1.414	1.409	1.278	1.281
μ (Cu Kα)/cm^{-1}	17.367	17.305	15.578	15.615
T/K	93	93	93	93
no. of measured reflections	10831	21794	22397	20899
no. of unique reflections	3456	3632	6861	3722
R_{int}	0.0294	0.0349	0.0570	0.0754
goodness of fit	1.093	1.185	1.101	1.050
R_1	0.0403	0.0682	0.0402	0.0504
wR_2	0.1084	0.0707	0.1042	0.1190
Structure solv	SIR2011	SIR2011	SIR2011	SIR2008
Refinement	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7	SHELXL 2014/7
CCDC Number	CCDC 1503795	CCDC 1503789	CCDC 1503783	CCDC 1503784



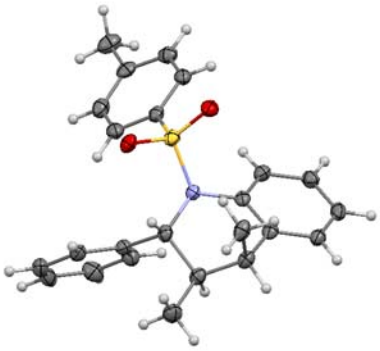
(a) *cis*-**3aj**



(b) *trans*-**3aj**



(c) **3ak-A**

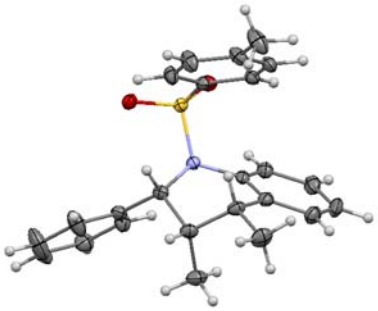


(d) **3ak-B**

Figure S5. Crystal structure of (a) *cis*-**3aj**, (b) *trans*-**3aj**, (c) **3ak-A**, (d) **3ak-B**; atomic thermal ellipsoids are drawn at the 50% probability level for non-hydrogen atoms.

Table S6. Experimental Data for the X-ray Crystallography of **3ak-C**

parameter	**3ak-C**
formula	$C_{24}H_{25}NO_2S$
Mw	391.53
crystal size/mm	0.300 X 0.235 X 0.142
crystal system	monoclinic
a/Å	9.1686(2)
b/Å	11.1342(3)
c/Å	20.5060(5)
α/deg	90
β/deg	100.270(7)
γ/deg	90
V/Å^3	2059.82(9)
space group	$P2_1/c$ (#14)
Z	4
g/cm	1.262
μ (Cu Kα)/cm^{-1}	15.391
T/K	93
no. of measured reflections	22264
no. of unique reflections	3717
R_{int}	0.0282
goodness of fit	1.080
R_1	0.0404
wR_2	0.1147
Structure solv	SIR2011
Refinement	SHELXL 2014/7
CCDC Number	CCDC 1503785



(b) **3ak-C**

Figure S6. Crystal structure of **3ak-C**; atomic thermal ellipsoids are drawn at the 50% probability level for non-hydrogen atoms.

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