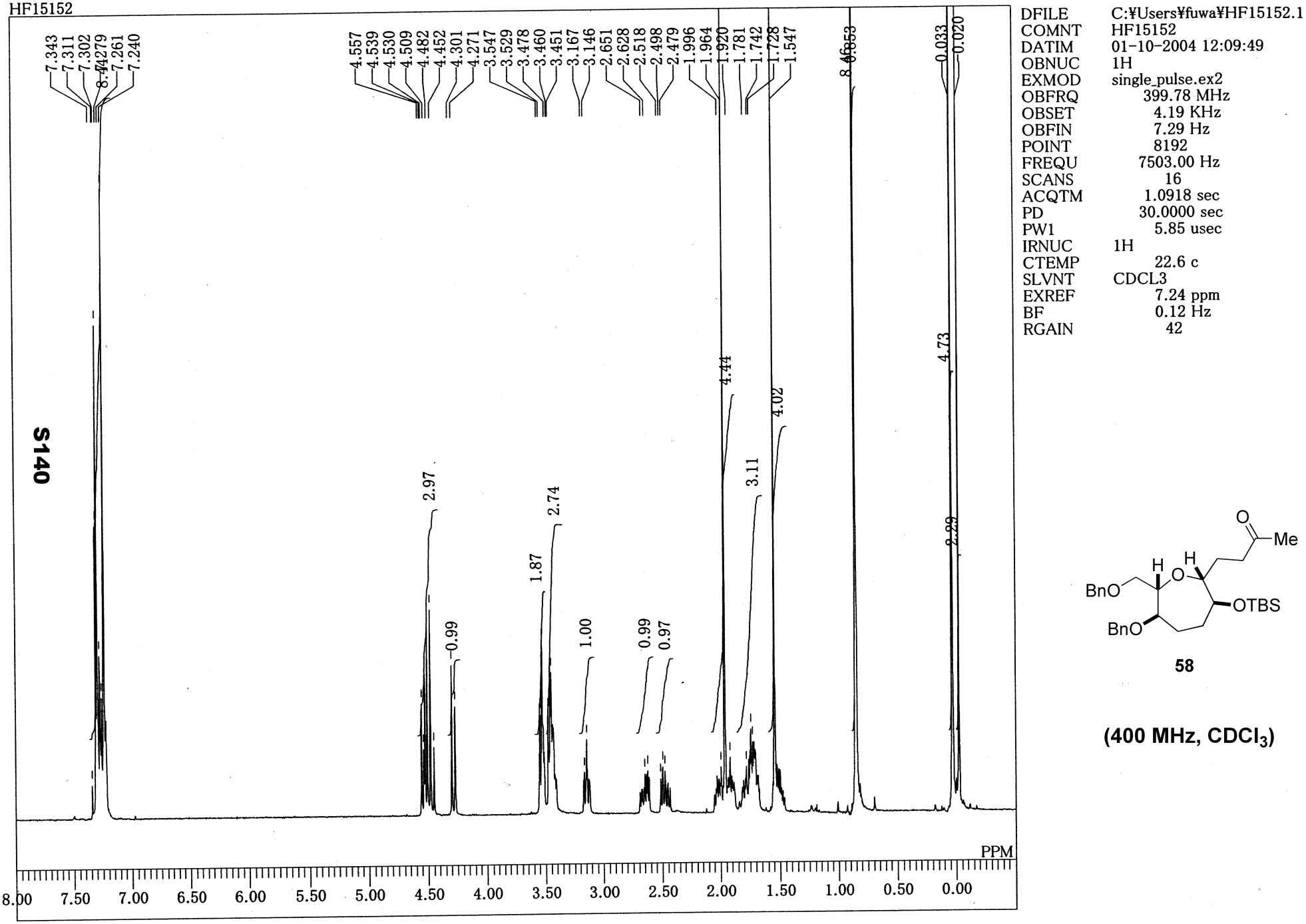
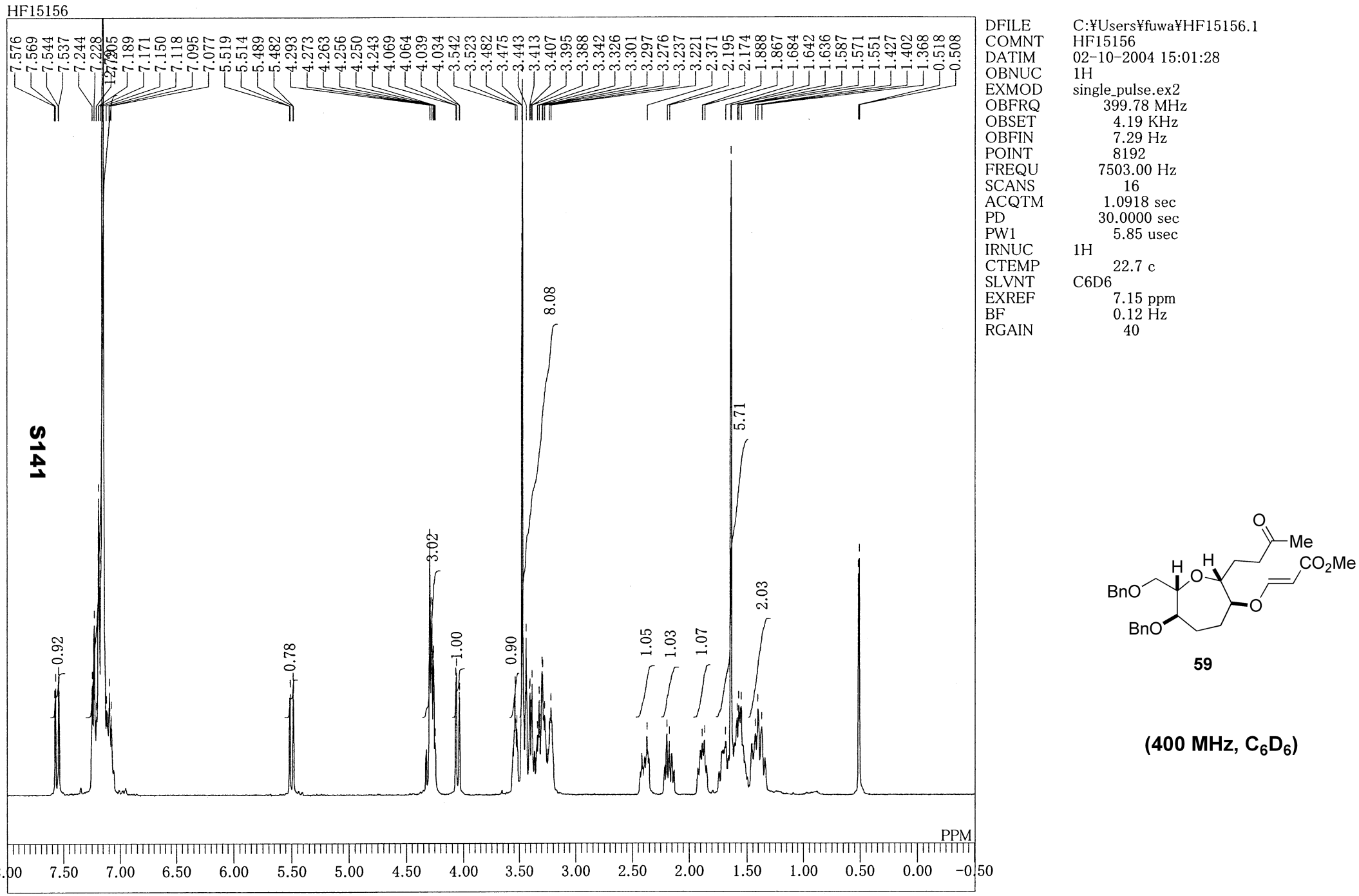


DFILE	C:¥Users¥fuwa¥HF15152.1
COMNT	HF15152
DATIM	01-10-2004 12:09:49
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.6 c
SLVNT	CDCL3
EXREF	7.24 ppm
BF	0.12 Hz
RGAIN	42

58

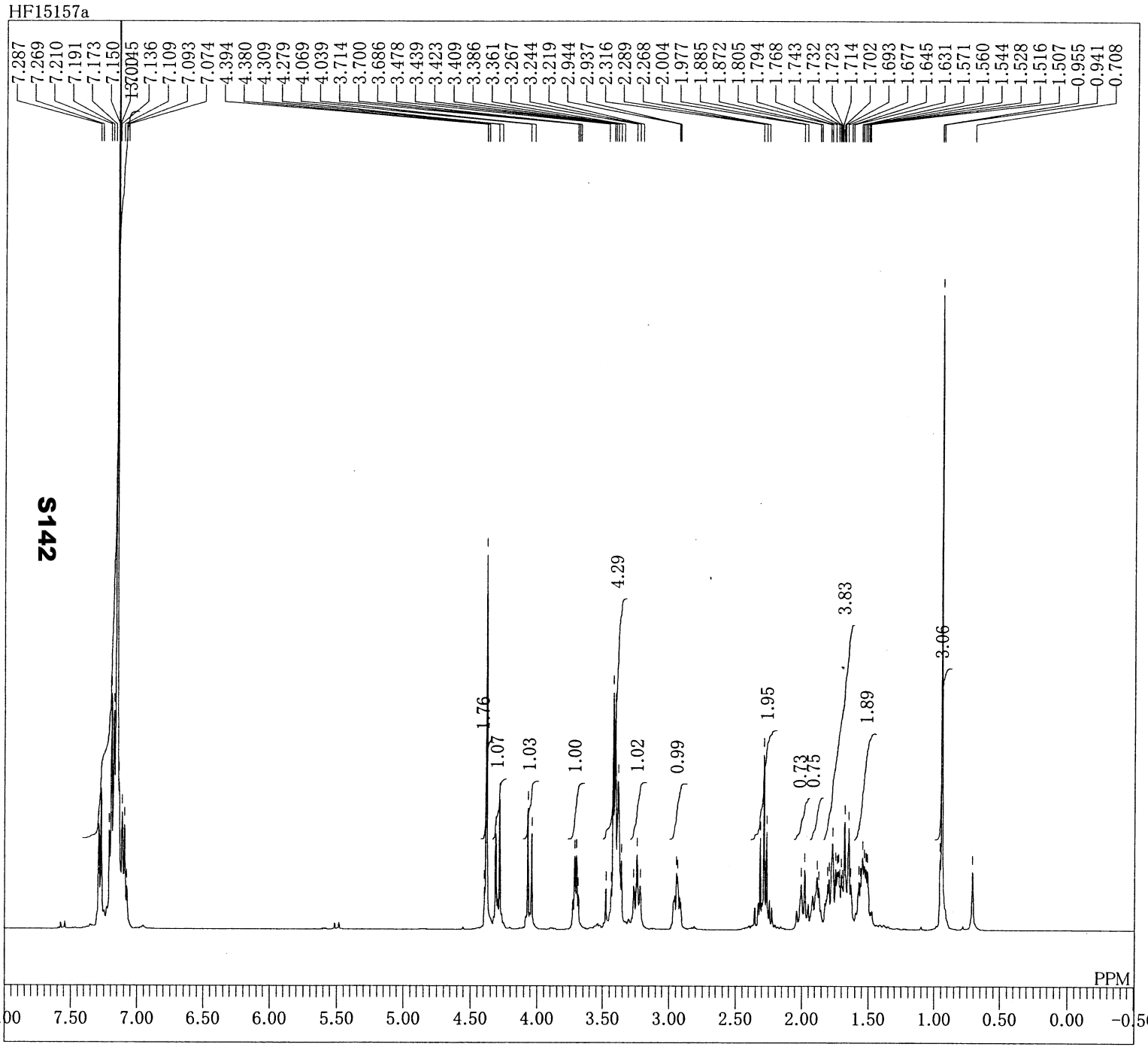
(400 MHz, $CDCl_3$)



DFILE	C:¥Users¥fuwa¥HF15156.1
COMNT	HF15156
DATIM	02-10-2004 15:01:28
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.7 c
SLVNT	C6D6
EXREF	7.15 ppm
BF	0.12 Hz
RGAIN	40

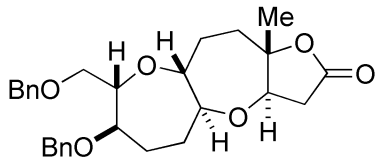
59

(400 MHz, C_6D_6)



S142

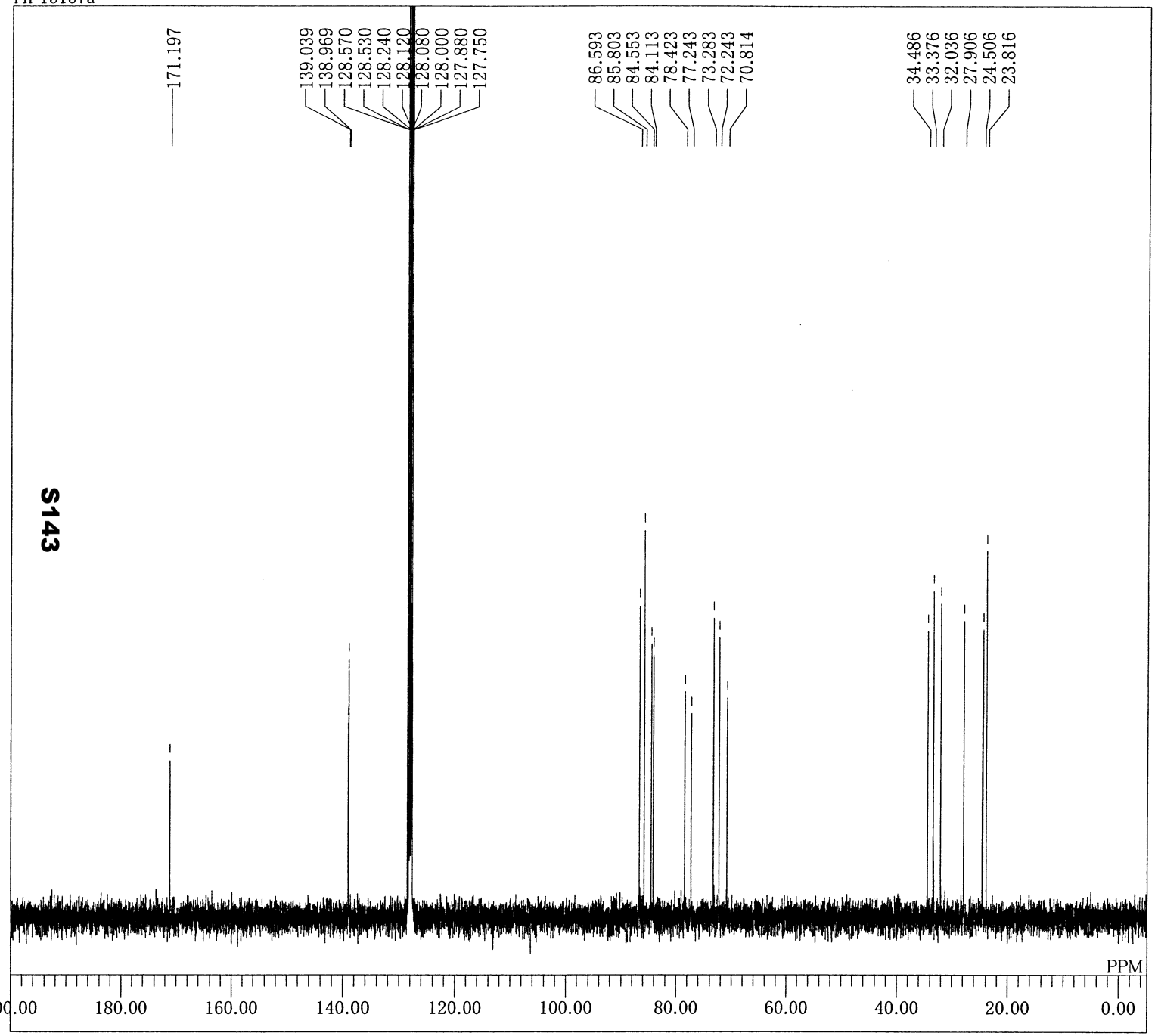
DFILE	C:¥Users¥fuwa¥HF15157a.1
COMNT	HF15157a
DATIM	02-10-2004 18:16:50
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.6 c
SLVNT	C6D6
EXREF	7.15 ppm
BF	0.12 Hz
RGAIN	36



60

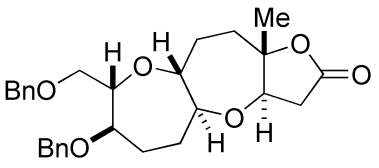
(400 MHz, C_6D_6)

HF15157a



S143

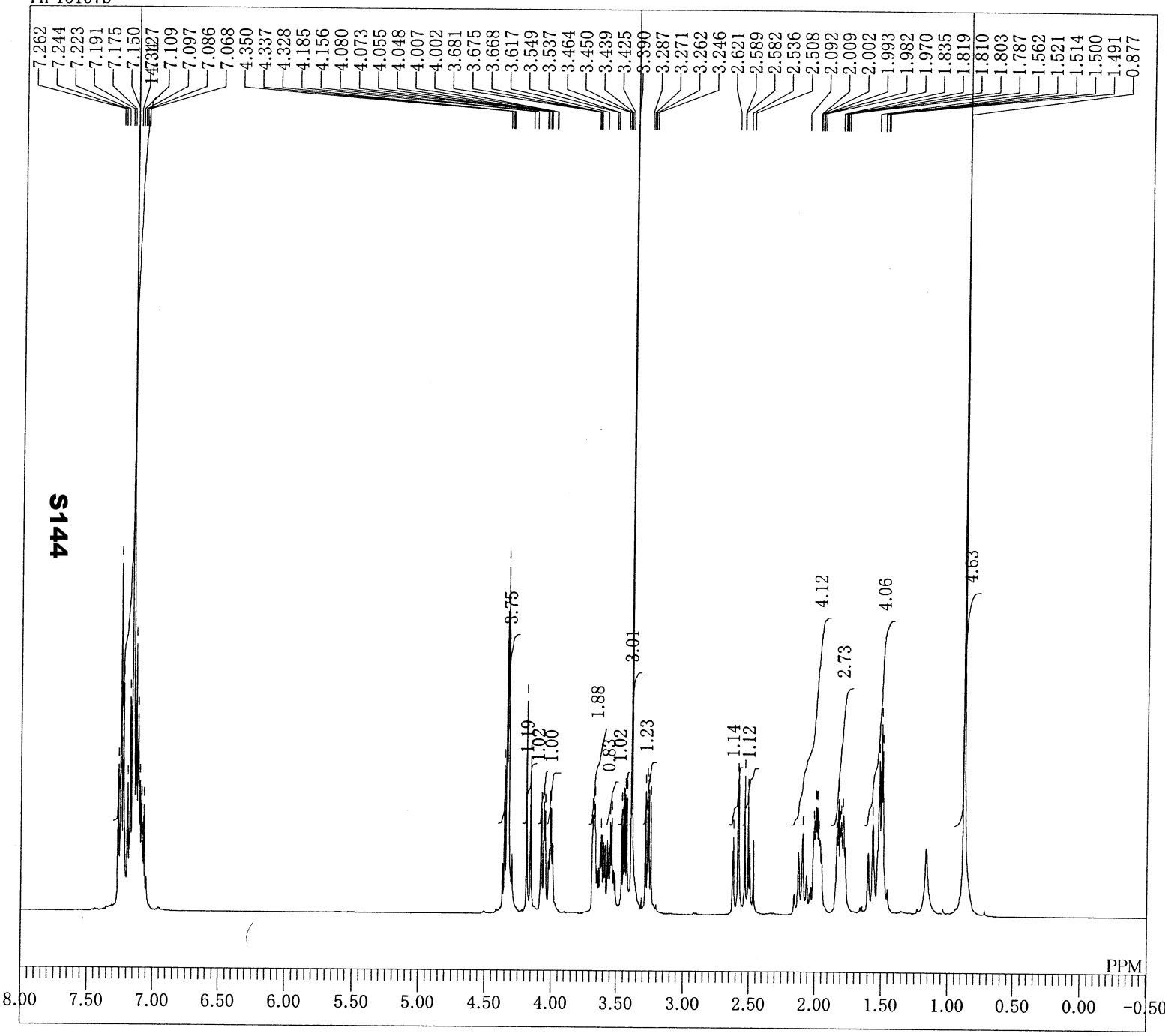
DFILE	C:¥Users¥fuwa¥HF15157a_bcm.1
COMNT	HF15157a
DATIM	02-10-2004 19:29:57
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	256
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.3 c
SLVNT	C6D6
EXREF	128.00 ppm
BF	0.12 Hz
RGAIN	60



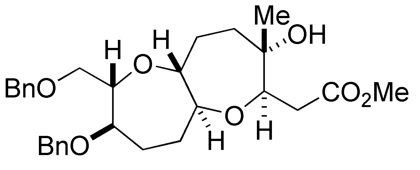
60

(100 MHz, C_6D_6)

HF15157b



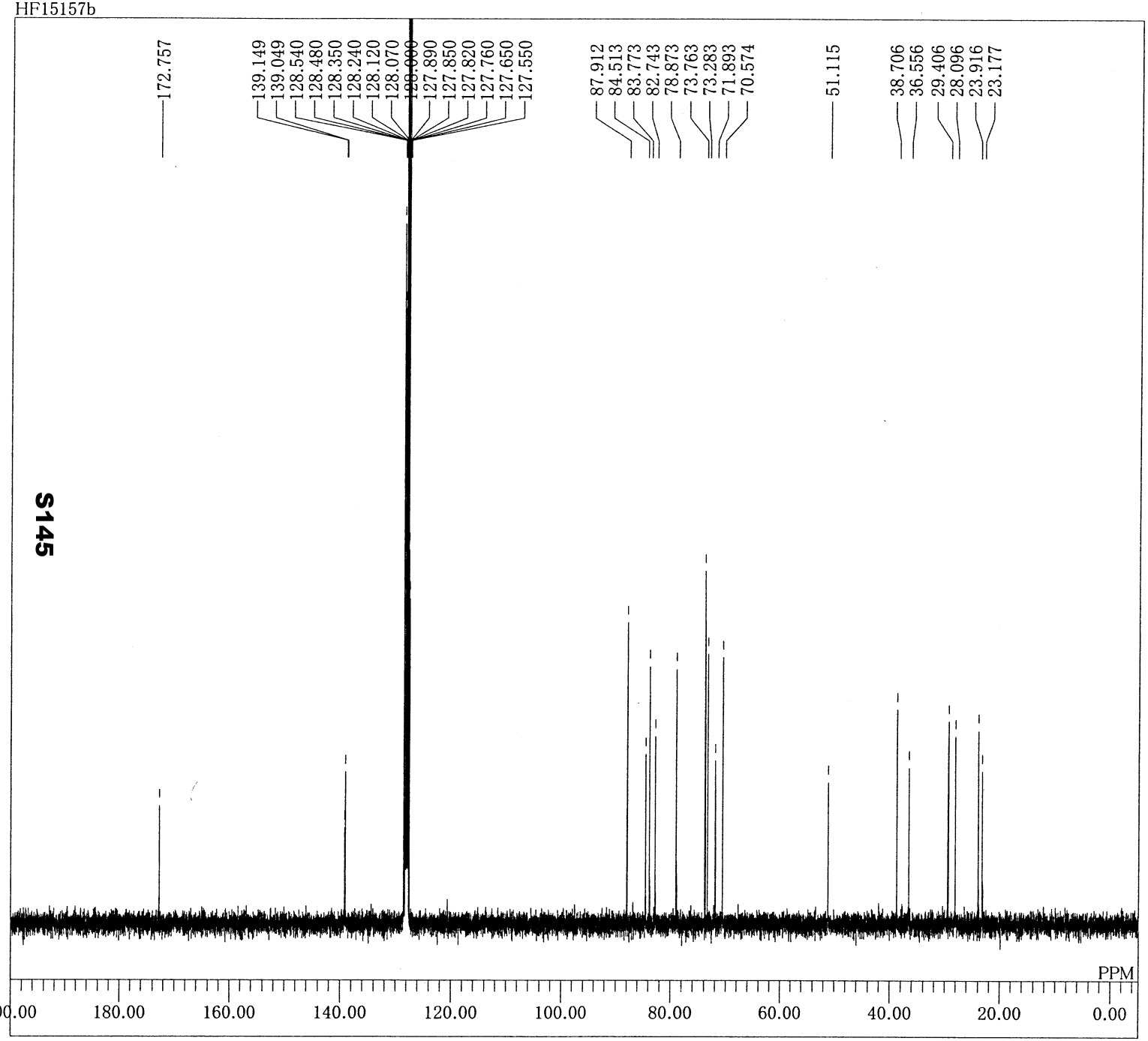
DFILE	C:¥Users¥fuwa¥HF15157b.1
COMNT	HF15157b
DATIM	02-10-2004 18:22:22
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.6 c
SLVNT	C6D6
EXREF	7.15 ppm
BF	0.12 Hz
RGAIN	36



61

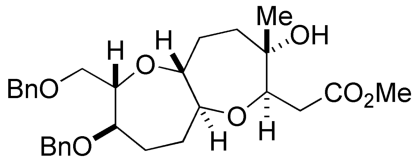
(400 MHz, C_6D_6)

HF15157b



S145

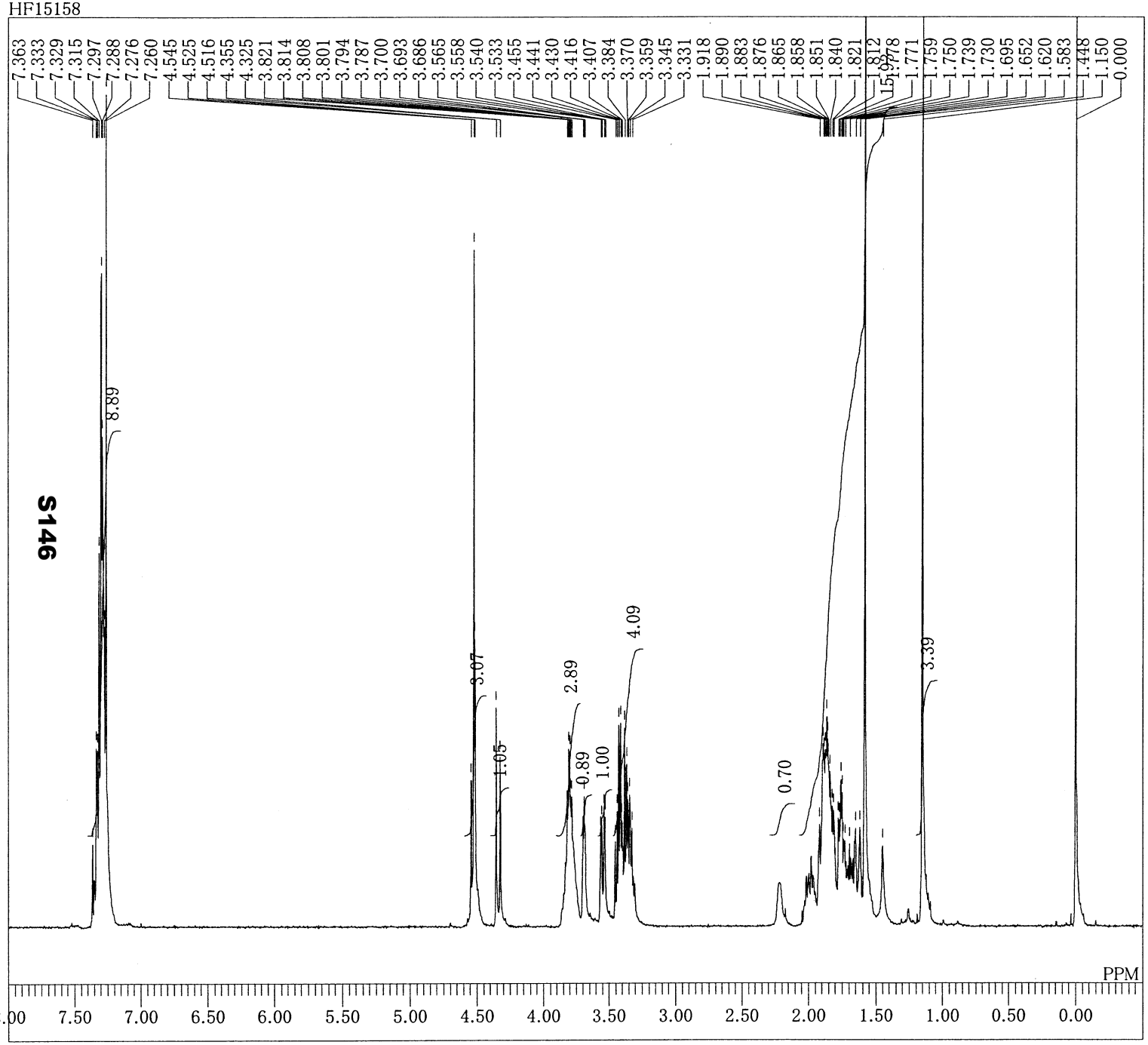
DFILE	C:¥Users¥fuwa¥HF15157b_bcm.1
COMNT	HF15157b
DATIM	02-10-2004 19:48:30
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	256
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.3 c
SLVNT	C6D6
EXREF	128.00 ppm
BF	0.12 Hz
RGAIN	60



61

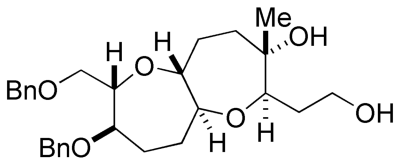
(100 MHz, C_6D_6)

HF15158



S146

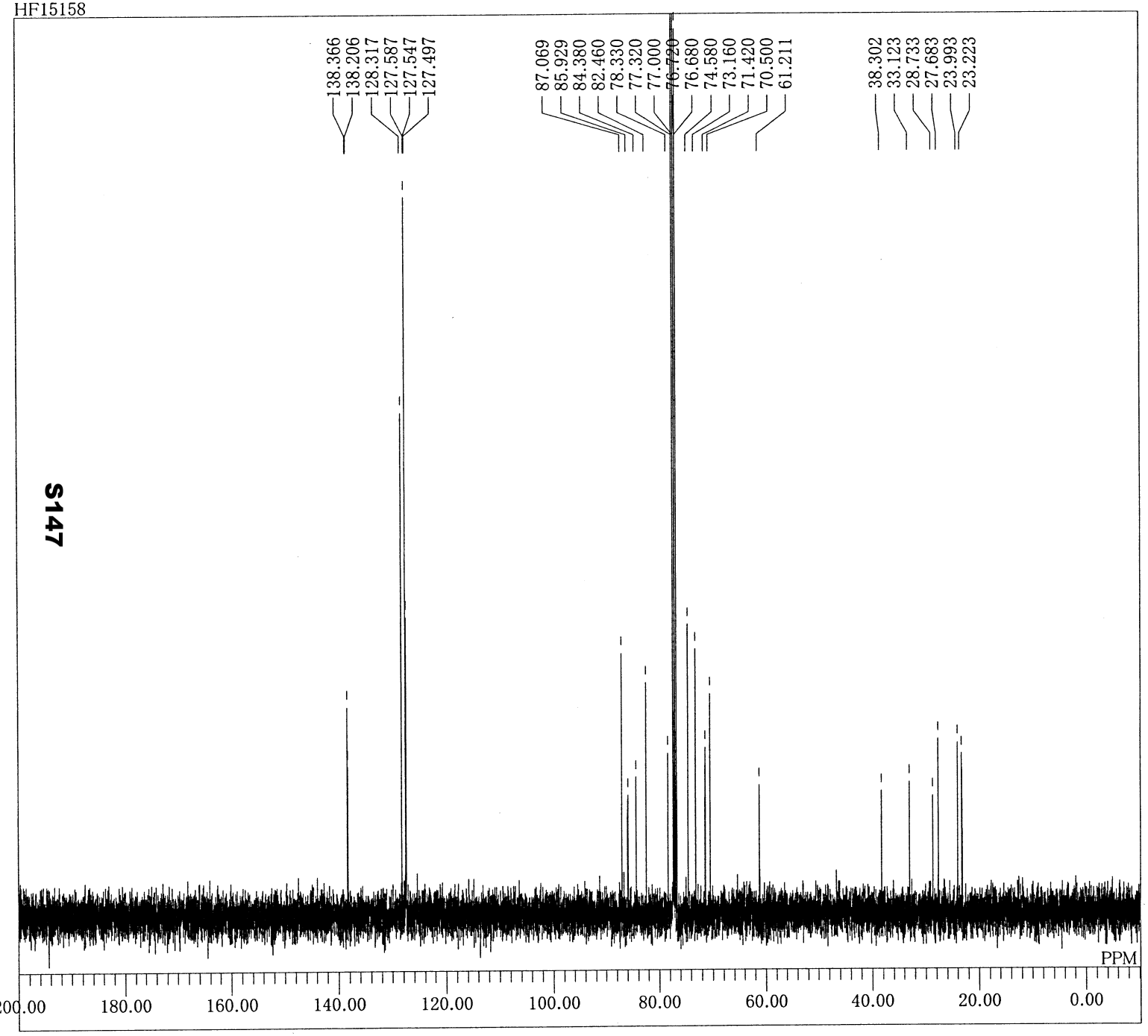
DFILE	C:¥Users¥fuwa¥HF15158CDCl3.1
COMNT	HF15158
DATIM	15-10-2004 14:44:50
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	42



62

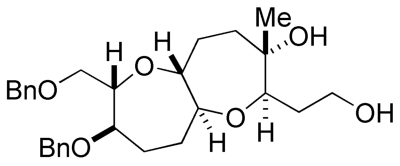
(400 MHz, $CDCl_3$)

HF15158



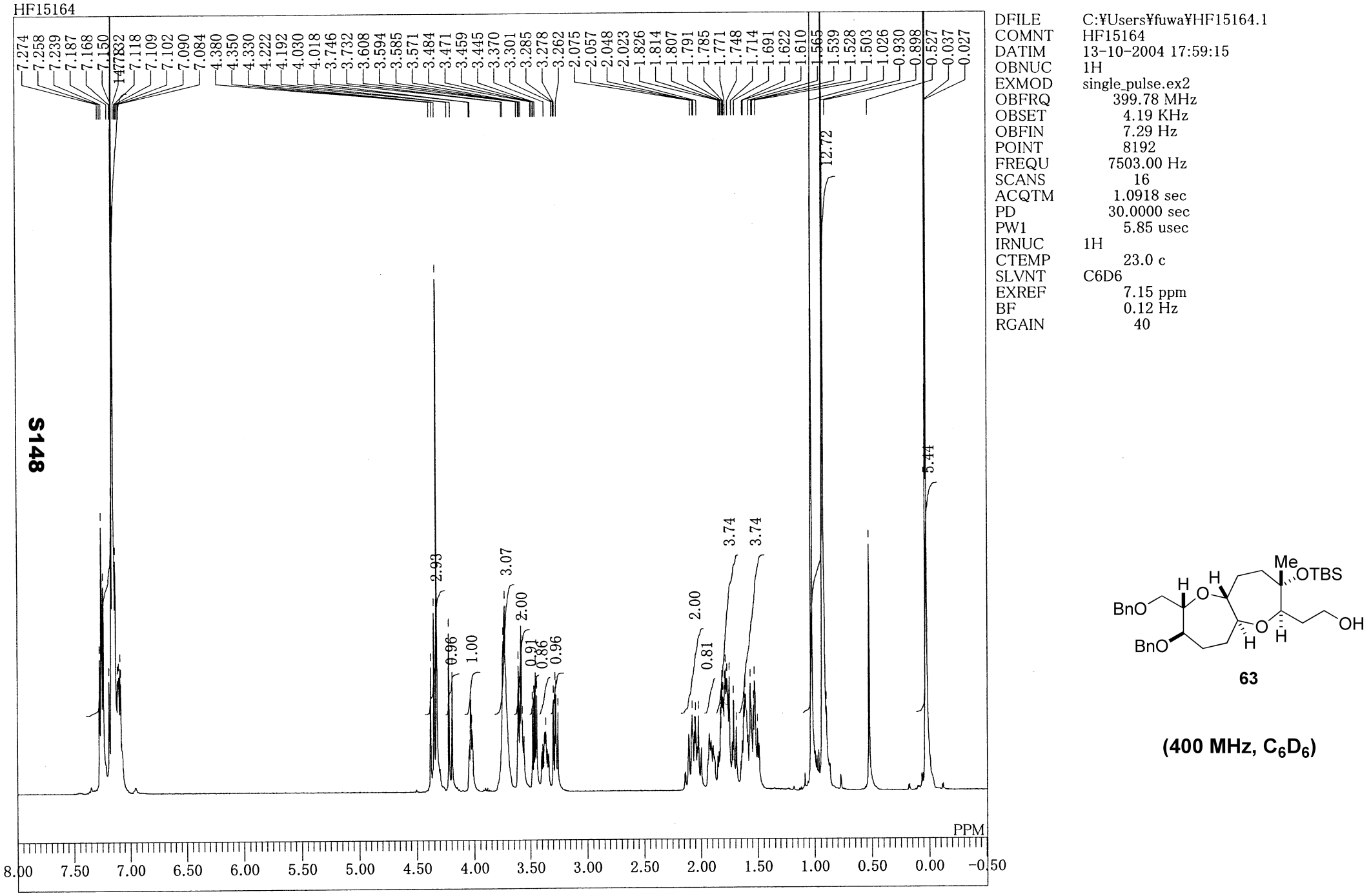
S147

DFILE	C:¥Users¥fuwa¥HF15158bcm.1
COMNT	HF15158
DATIM	15-10-2004 18:49:18
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	128
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	60



62

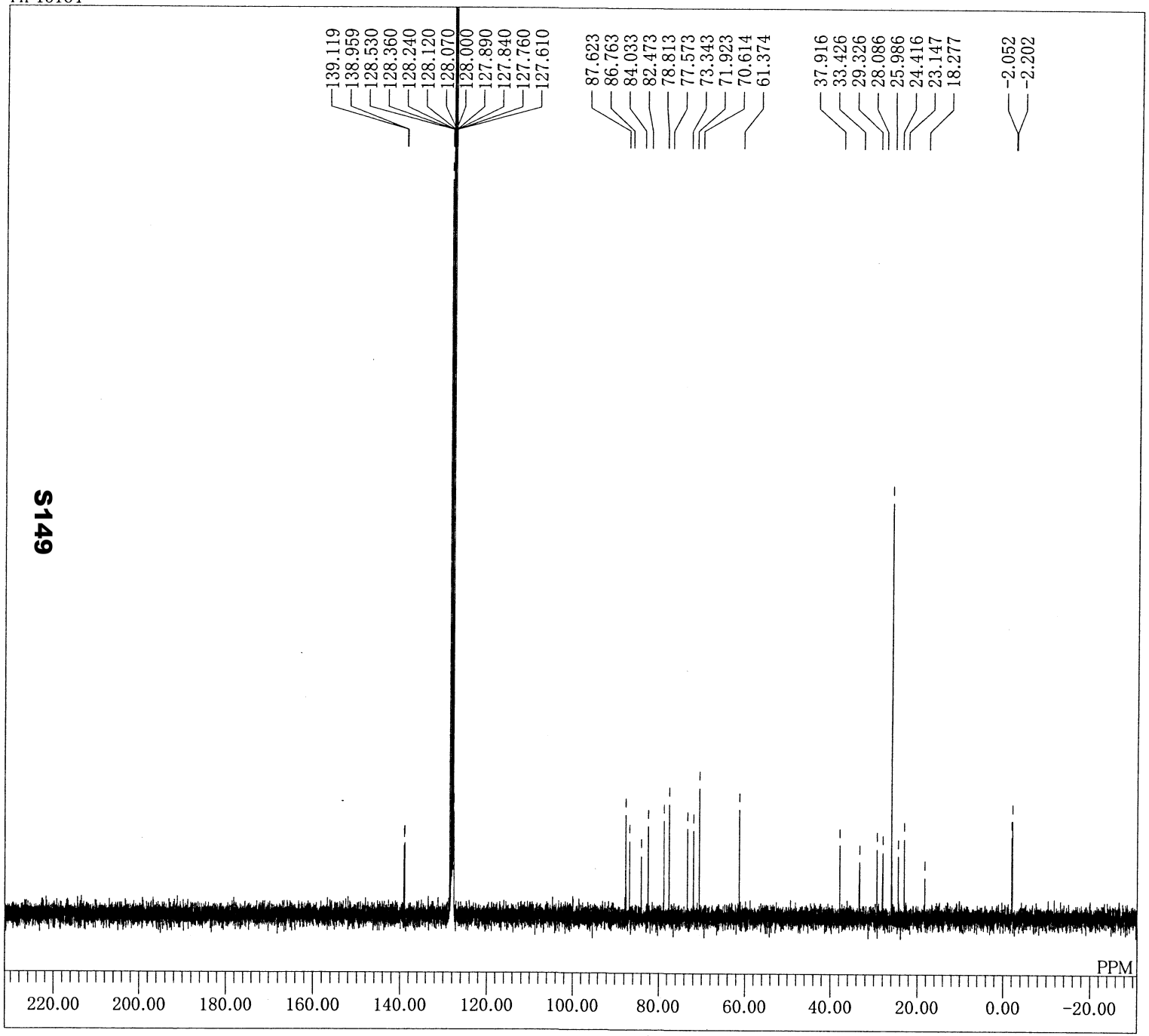
(100 MHz, $CDCl_3$)



63

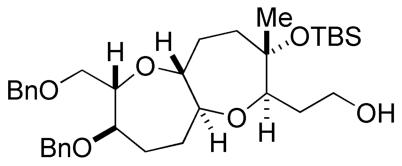
(400 MHz, C_6D_6)

HF15164



S149

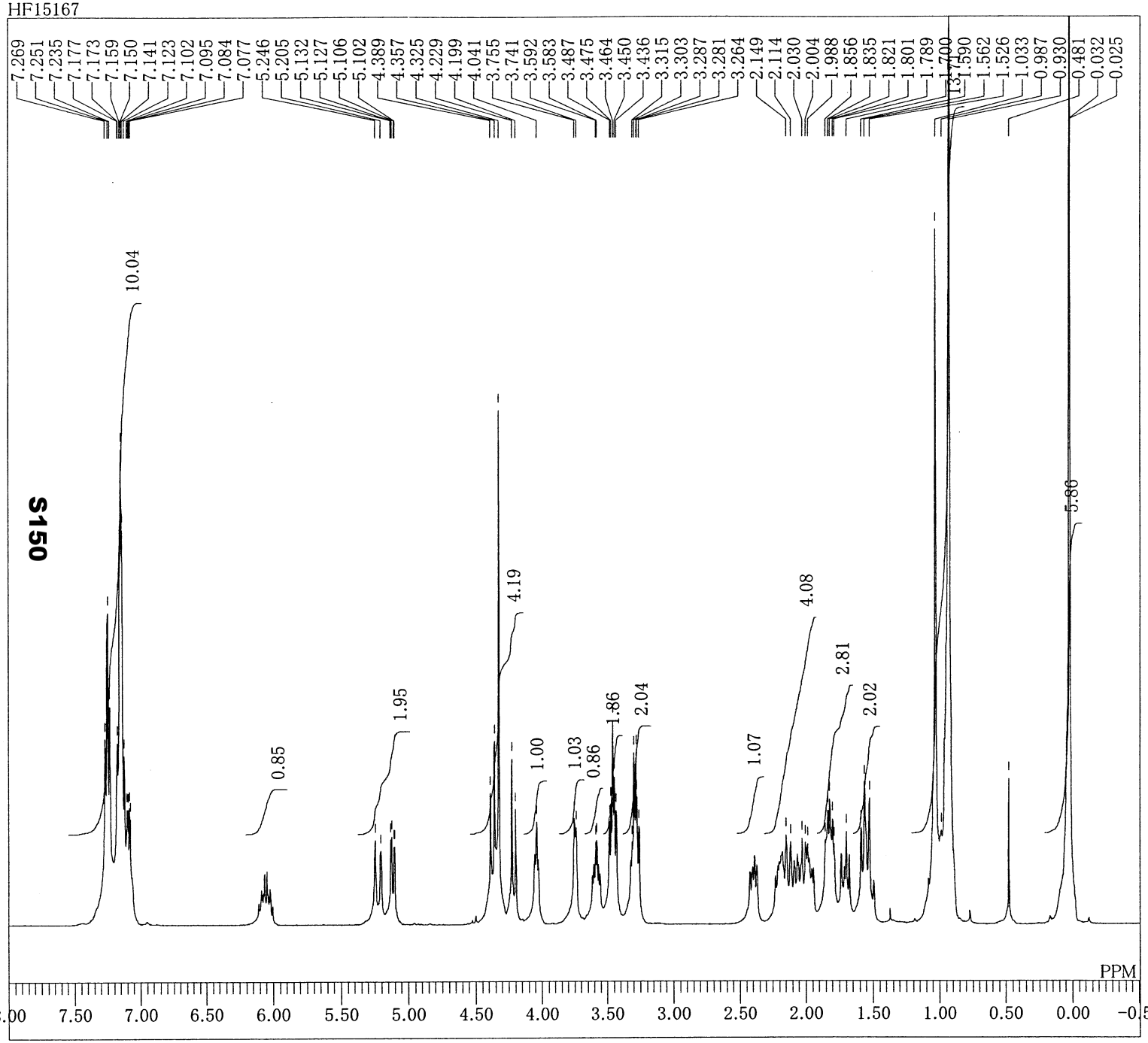
DFILE	C:¥Users¥fuwa¥HF15164bcm.1
COMNT	HF15164
DATIM	13-10-2004 18:18:13
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	384
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.5 c
SLVNT	C6D6
EXREF	128.00 ppm
BF	0.12 Hz
RGAIN	60



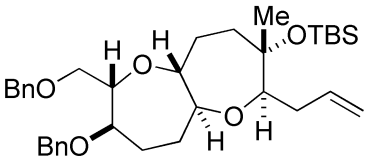
63

(100 MHz, C_6D_6)

HF15167



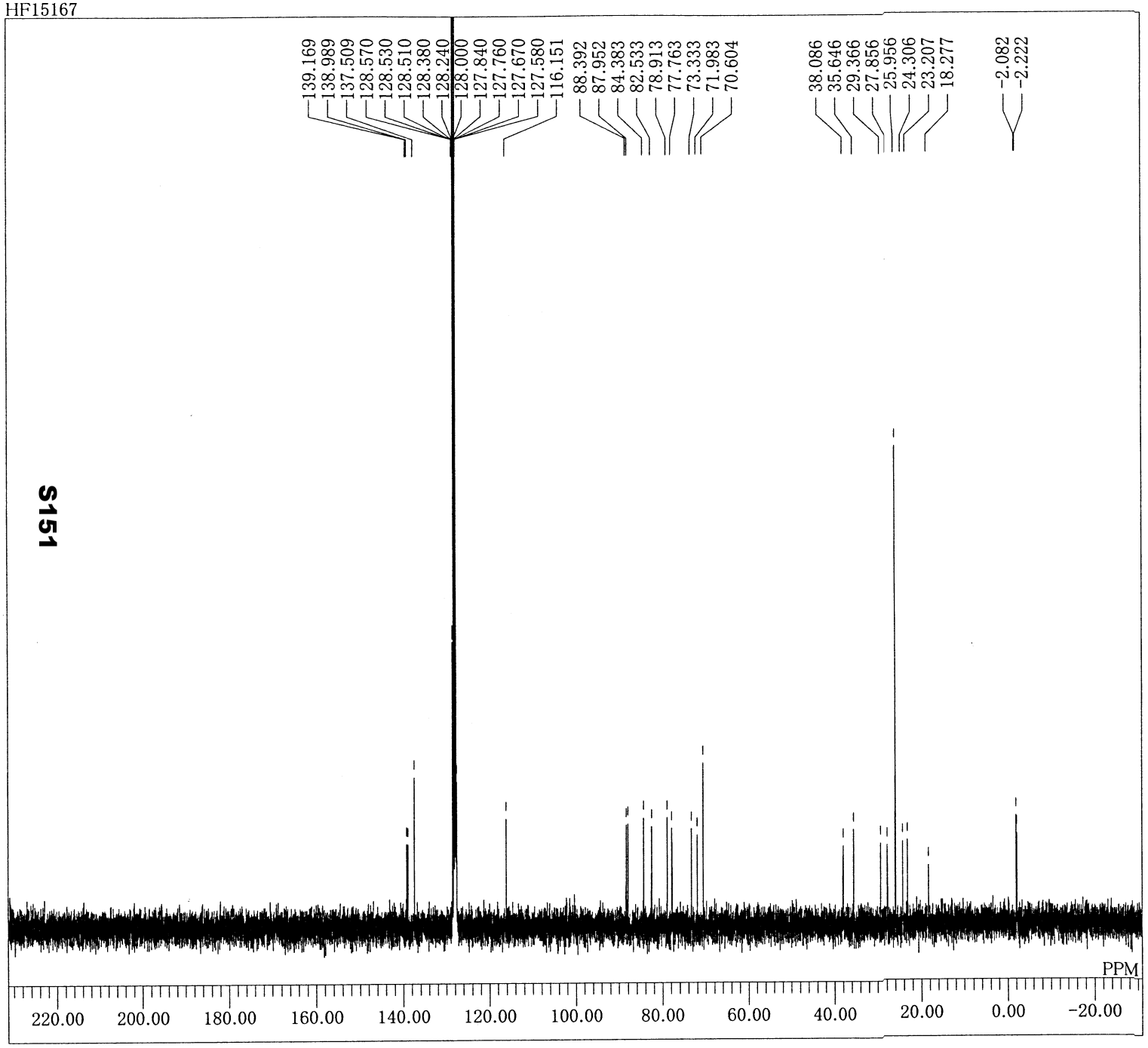
DFILE	C:¥Users¥fuwa¥HF15167.1
COMNT	HF15167
DATIM	18-10-2004 14:46:34
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.9 c
SLVNT	C6D6
EXREF	7.15 ppm
BF	0.12 Hz
RGAIN	36



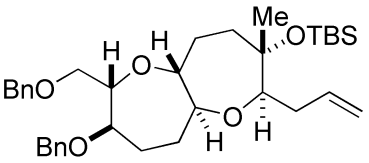
64

(400 MHz, C_6D_6)

HF15167

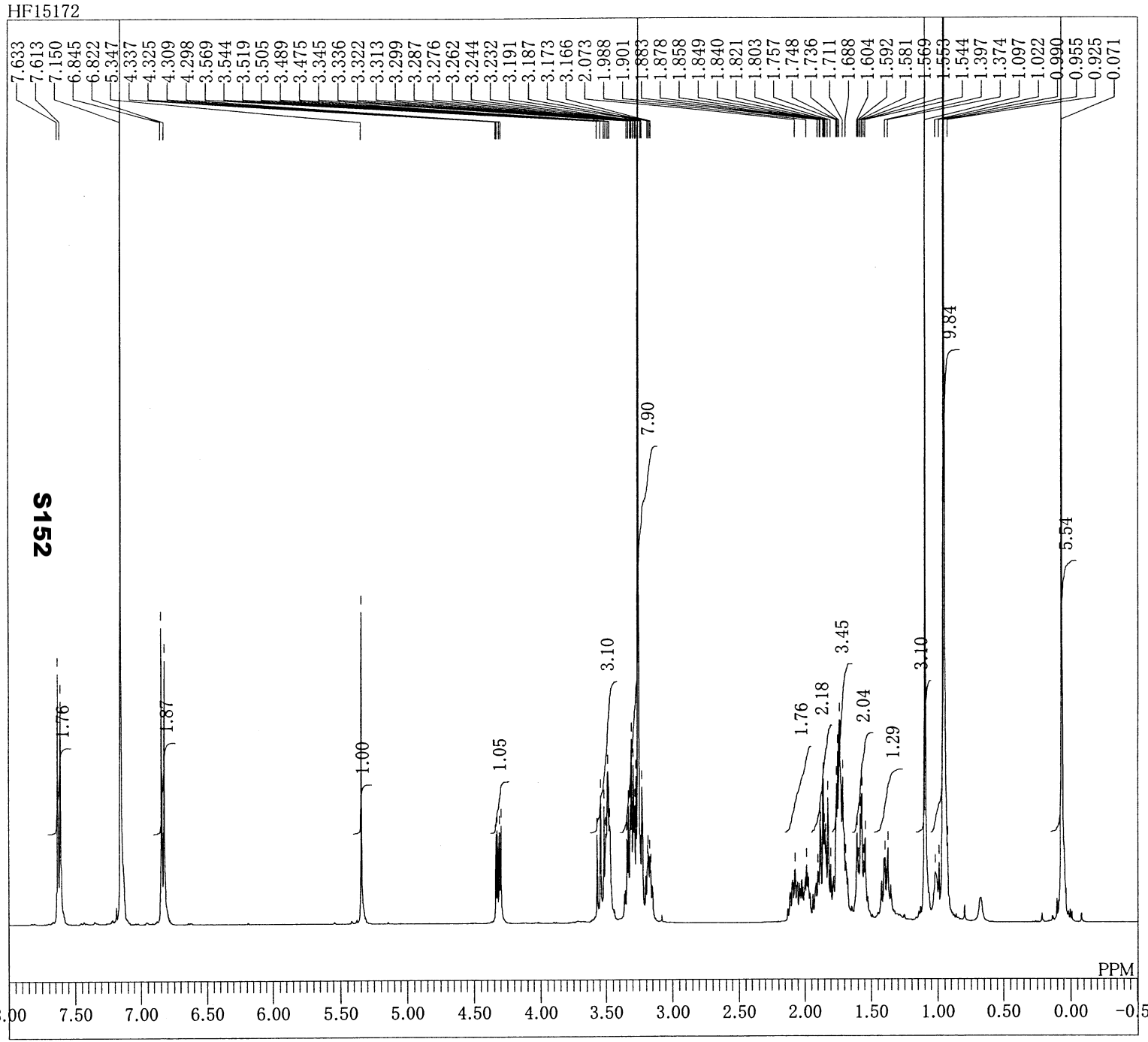


DFILE	C:¥Users¥fuwa¥HF15167bcm.1
COMNT	HF15167
DATIM	18-10-2004 14:57:52
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	192
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.4 c
SLVNT	C6D6
EXREF	128.00 ppm
BF	0.12 Hz
RGAIN	60

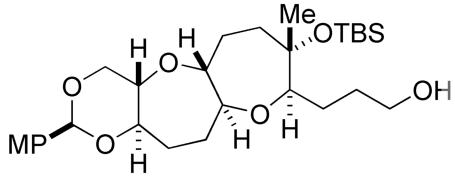


64

(100 MHz, C_6D_6)



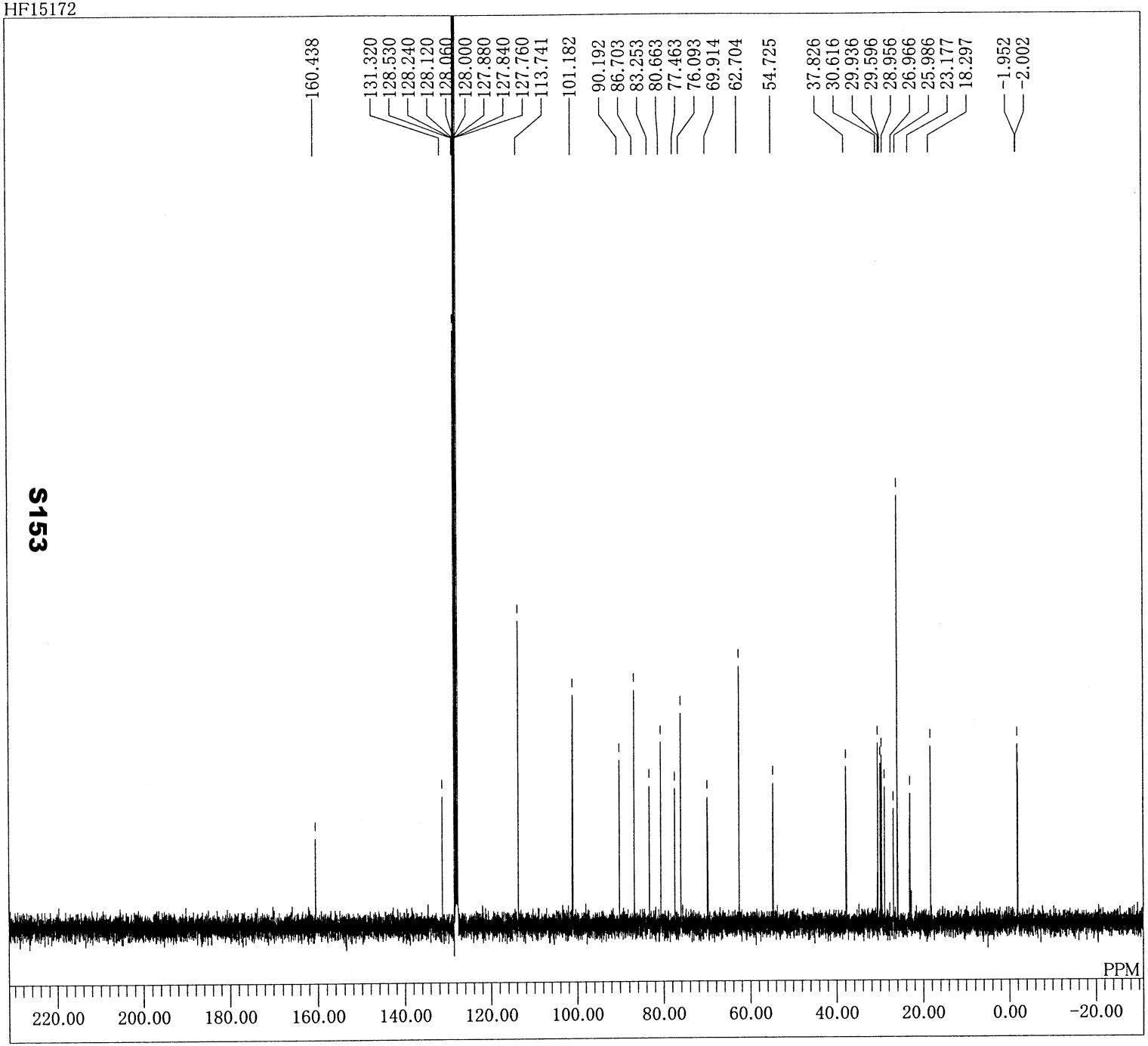
DFILE	C:¥Users¥fuwa¥HF15172.1
COMNT	HF15172
DATIM	19-10-2004 18:13:58
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.8 c
SLVNT	C6D6
EXREF	7.15 ppm
BF	0.12 Hz
RGAIN	36



65

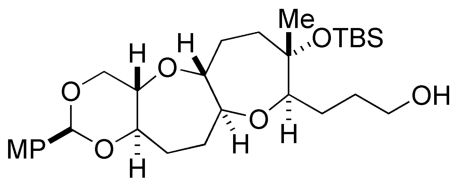
(400 MHz, C_6D_6)

HF15172



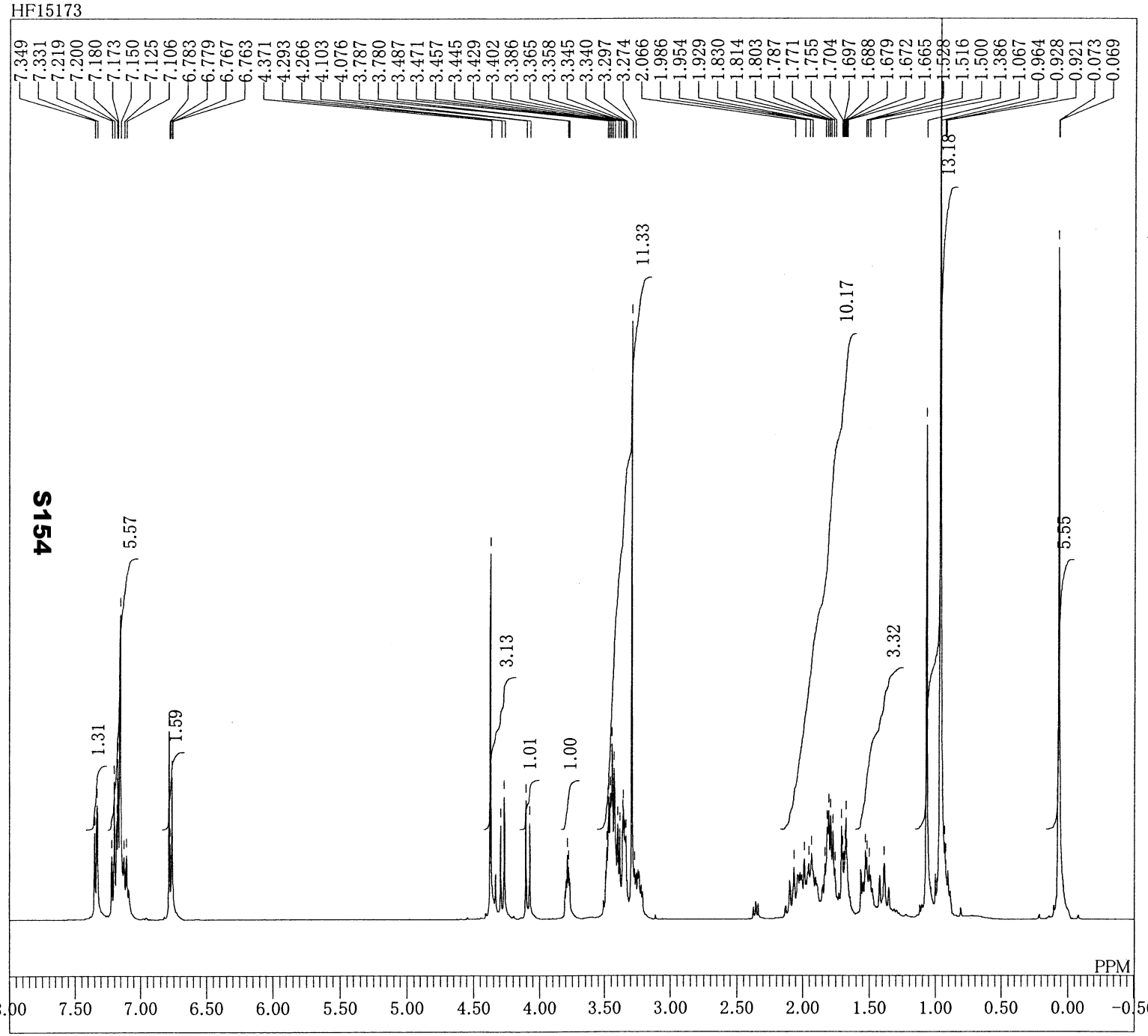
S153

DFILE	C:¥Users¥fuwa¥HF15172bcm.1
COMNT	HF15172
DATIM	19-10-2004 18:24:53
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	192
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.6 c
SLVNT	C6D6
EXREF	128.00 ppm
BF	0.12 Hz
RGAIN	60

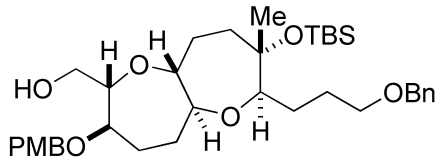


65

(100 MHz, C_6D_6)



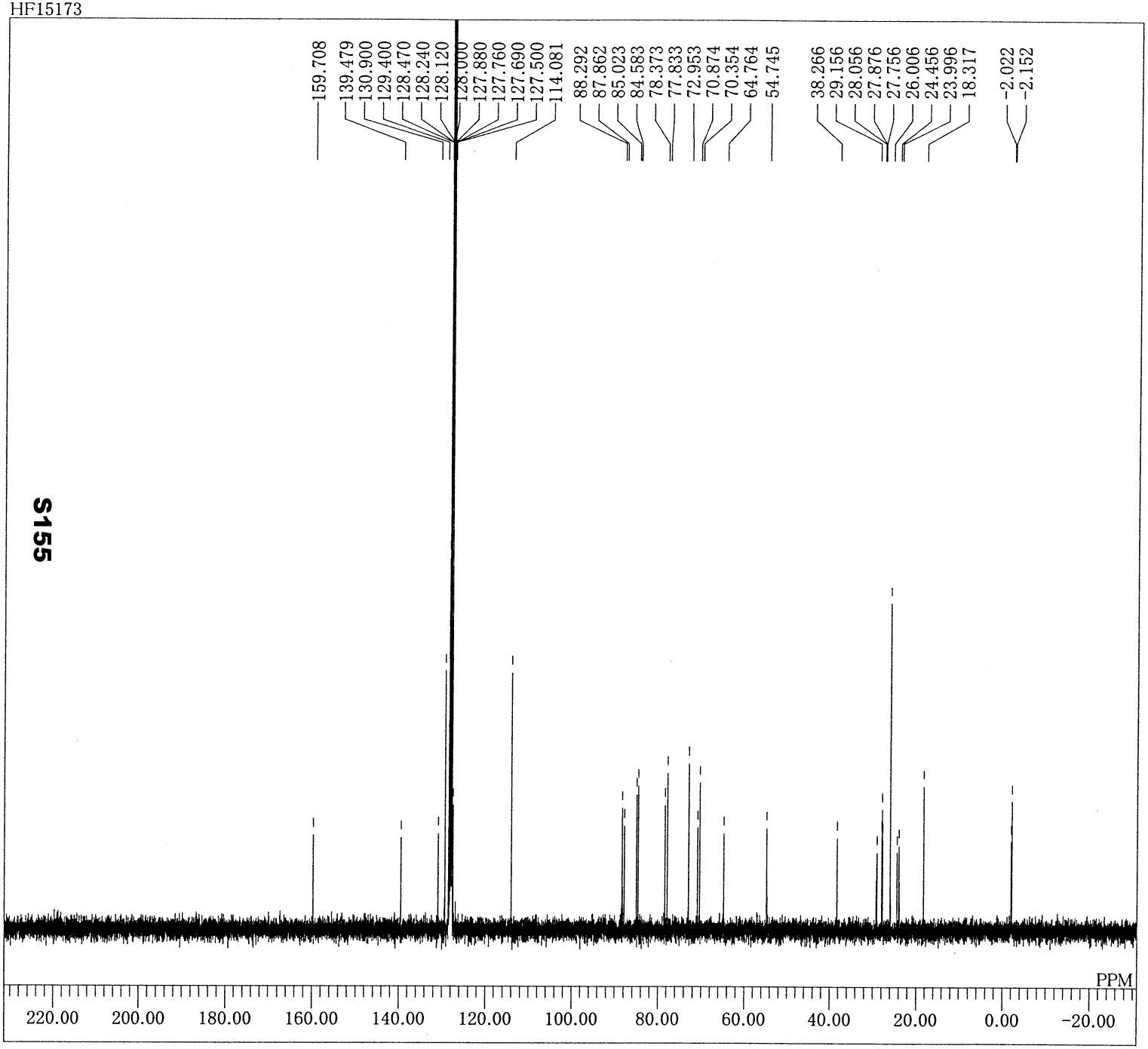
DFILE	C:¥Users¥fuwa¥HF15173.1
COMNT	HF15173
DATIM	20-10-2004 18:15:36
OBNUC	1H
EXMOD	single_pulse.ex2
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	8192
FREQU	7503.00 Hz
SCANS	16
ACQTM	1.0918 sec
PD	30.0000 sec
PW1	5.85 usec
IRNUC	1H
CTEMP	22.7 c
SLVNT	C6D6
EXREF	7.15 ppm
BF	0.12 Hz
RGAIN	36



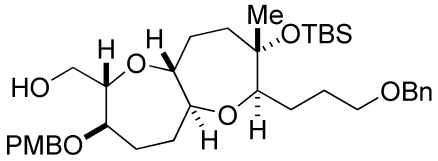
66

(400 MHz, C_6D_6)

HF15173



DFILE	C:¥Users¥fuwa¥HF15173bcm.1
COMNT	HF15173
DATIM	20-10-2004 18:26:27
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	32938.08 Hz
SCANS	192
ACQTM	0.9948 sec
PD	1.5000 sec
PW1	3.13 usec
IRNUC	1H
CTEMP	23.4 c
SLVNT	C6D6
EXREF	128.00 ppm
BF	0.12 Hz
RGAIN	60



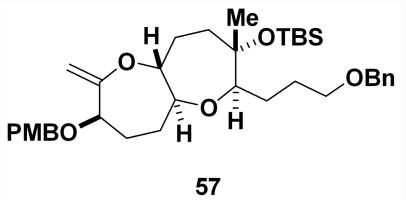
66

(100 MHz, C_6D_6)

Ebine III-30/C6D6

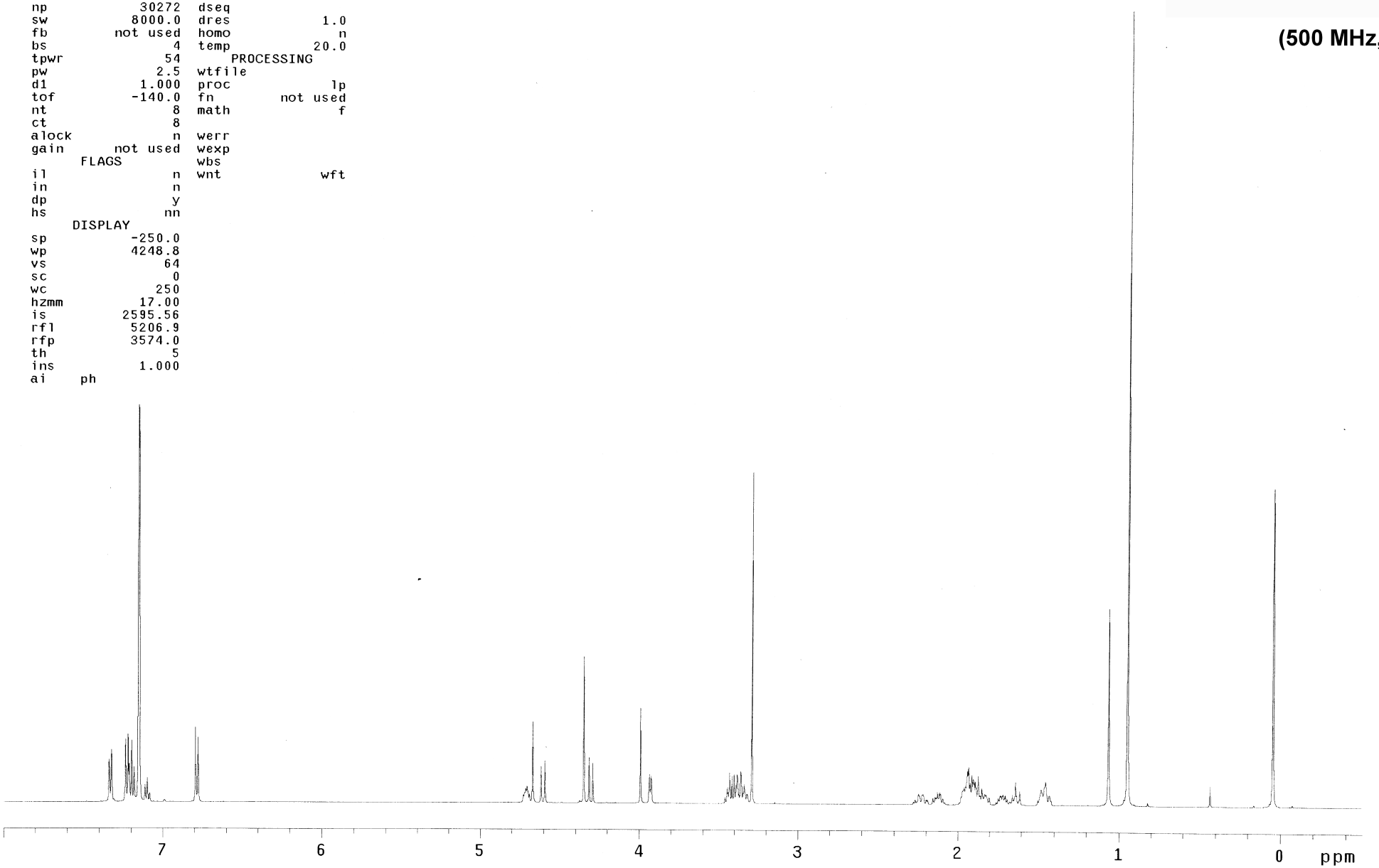
exp1 s2pul

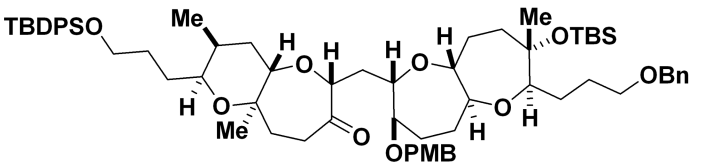
SAMPLE		DEC. & VT	
date	Jan 11 2005	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	8	math	f
ct	8		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	64		
sc	0		
wc	250		
hzmm	17.00		
is	2595.56		
rfl	5206.9		
rfp	3574.0		
th	5		
ins	1.000		
ai	ph		



57

(500 MHz, C_6D_6)





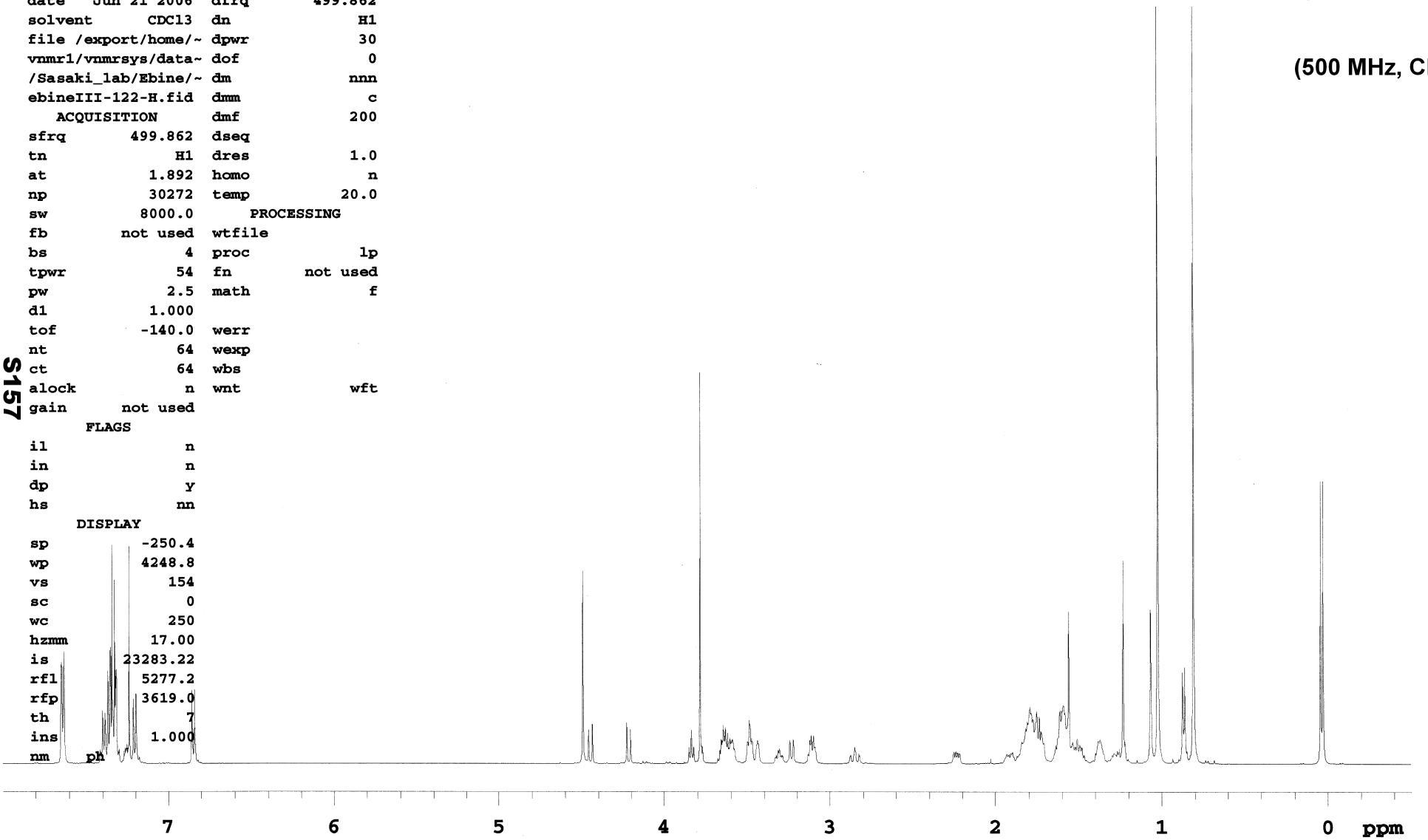
70

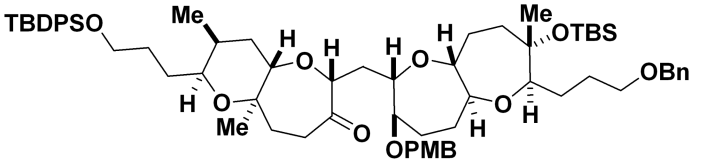
(500 MHz, $CDCl_3$)

STANDARD PROTON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Jun 21 2006	dfrq	499.862
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	30
vnmr1/vnmrsys/data~		dof	0
/Sasaki_lab/Ebine/~		dm	nnn
ebineIII-122-H.fid		dmm	c
ACQUISITION		dmf	200
sfrq	499.862	dseq	
tn	H1	dres	1.0
at	1.892	homo	n
np	30272	temp	20.0
sw	8000.0	PROCESSING	
fb	not used	wtfile	
bs	4	proc	lp
tpwr	54	fn	not used
pw	2.5	math	f
d1	1.000		
tof	-140.0	werr	
nt	64	wexp	
ct	64	wbs	
alock	n	wnt	wft
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.4		
wp	4248.8		
vs	154		
sc	0		
wc	250		
hzmm	17.00		
is	23283.22		
rfl	5277.2		
rfp	3619.0		
th	7		
ins	1.000		
nm	ph		





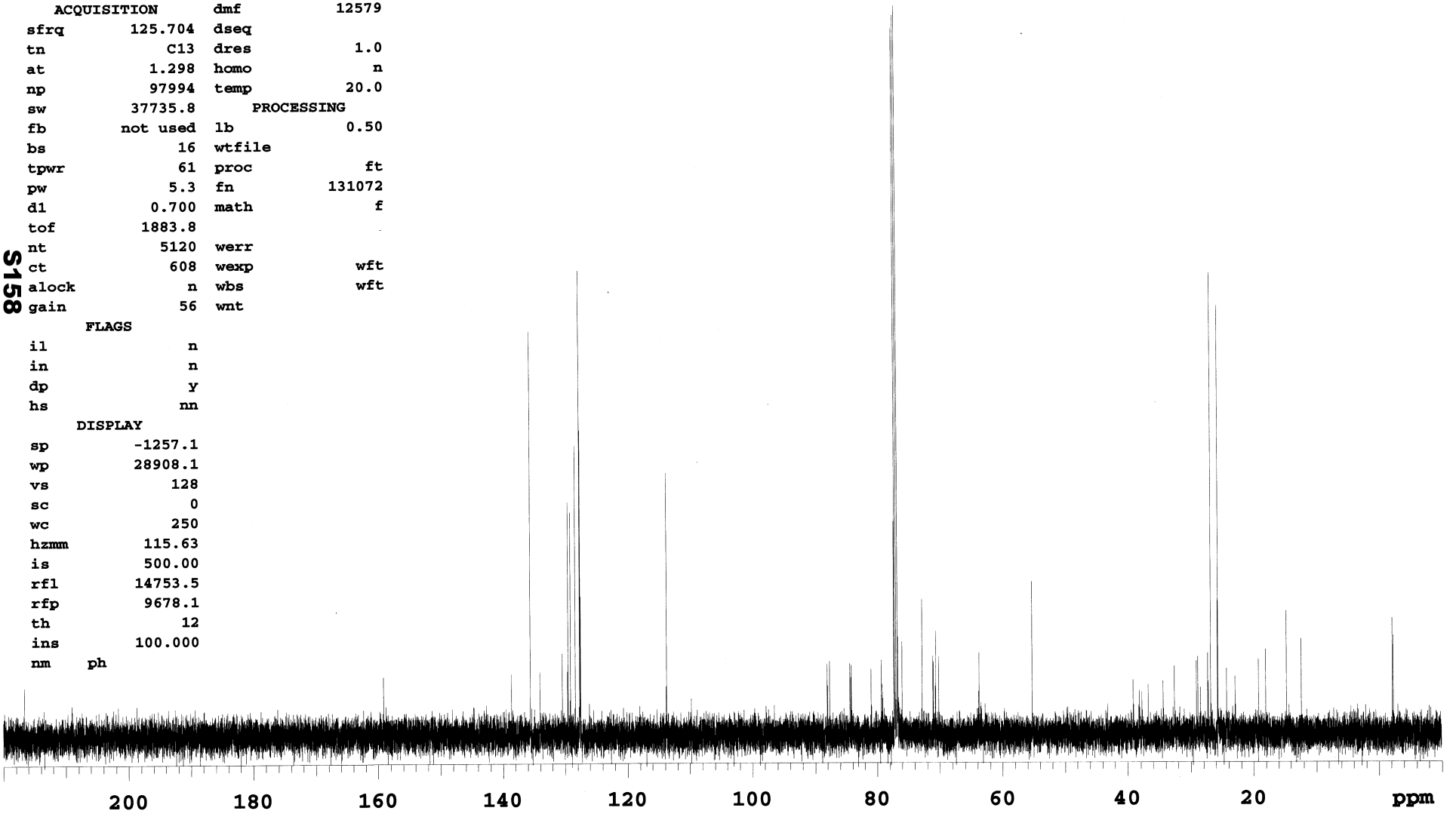
70

(125 MHz, $CDCl_3$)

STANDARD CARBON PARAMETERS

exp1 s2pul

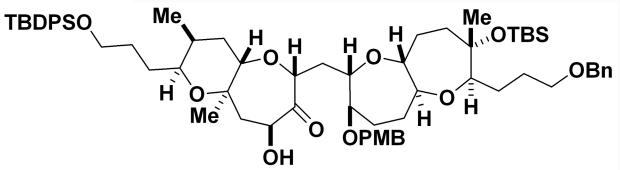
SAMPLE		DEC. & VT	
date	Jun 21 2006	dfrq	499.862
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	27
	vnmr1/vnmrsys/data~	dof	0
	/Sasaki_lab/Ebine/~	dm	YYY
	ebineIII-122-C.fid	dmm	w
ACQUISITION		dmf	12579
sfrq	125.704	dseq	
tn	C13	dres	1.0
at	1.298	homo	n
np	97994	temp	20.0
sw	37735.8	PROCESSING	
fb	not used	lb	0.50
bs	16	wtfile	
tpwr	61	proc	ft
pw	5.3	fn	131072
d1	0.700	math	f
tof	1883.8		
nt	5120	werr	
ct	608	wexp	wft
alock	n	wbs	wft
gain	56	wnt	
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1257.1		
wp	28908.1		
vs	128		
sc	0		
wc	250		
hzmm	115.63		
is	500.00		
rfl	14753.5		
rfp	9678.1		
th	12		
ins	100.000		
nm	ph		



STANDARD PROTON PARAMETERS

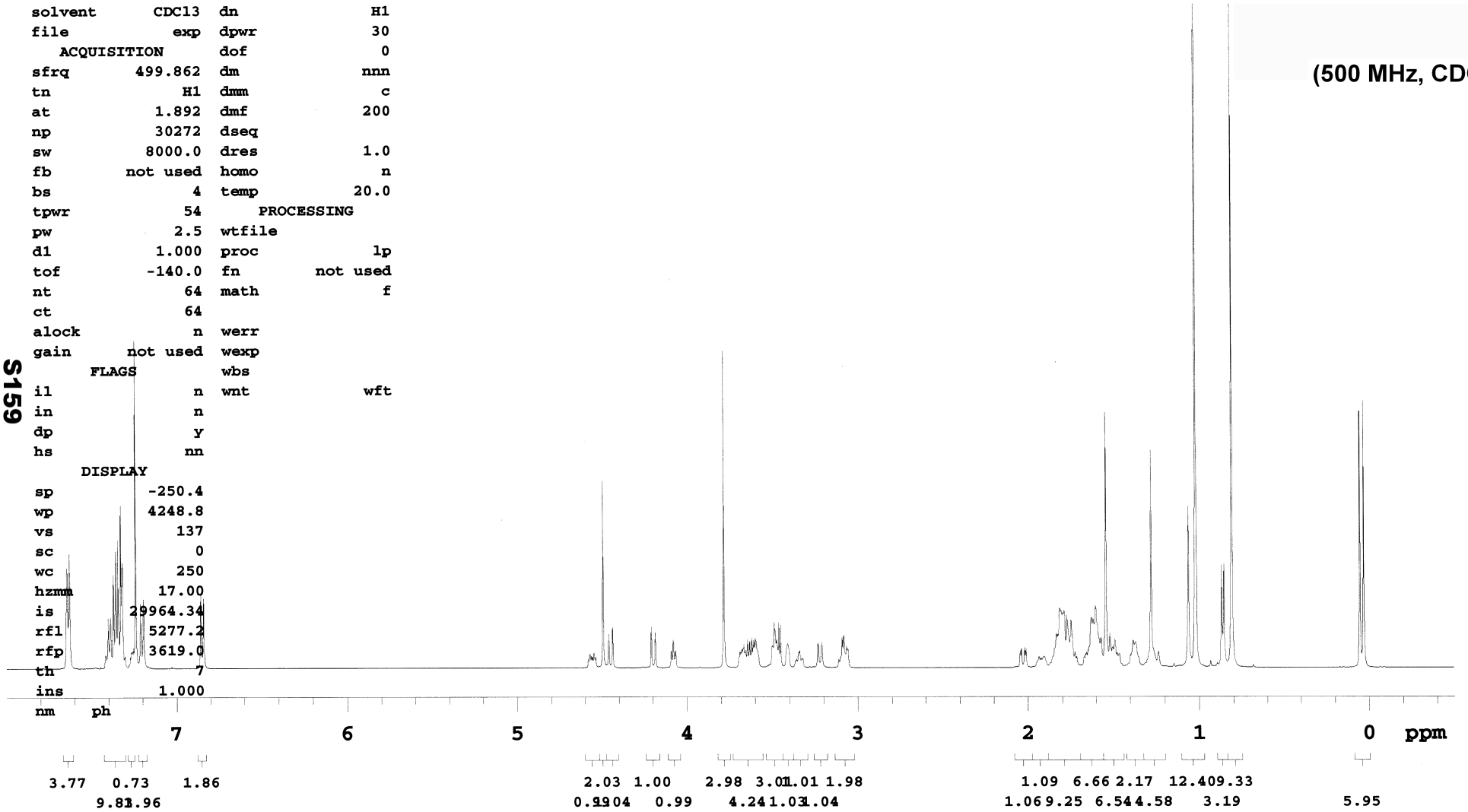
exp1 s2pul

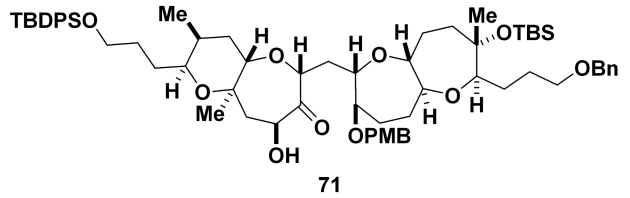
SAMPLE		DEC. & VT	
date	Jun 24 2006	dfrq	499.862
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.4		
wp	4248.8		
vs	137		
sc	0		
wc	250		
hzmm	17.00		
is	29964.34		
rfl	5277.2		
rfp	3619.0		
th	7		
ins	1.000		
nm	ph		



71

(500 MHz, $CDCl_3$)





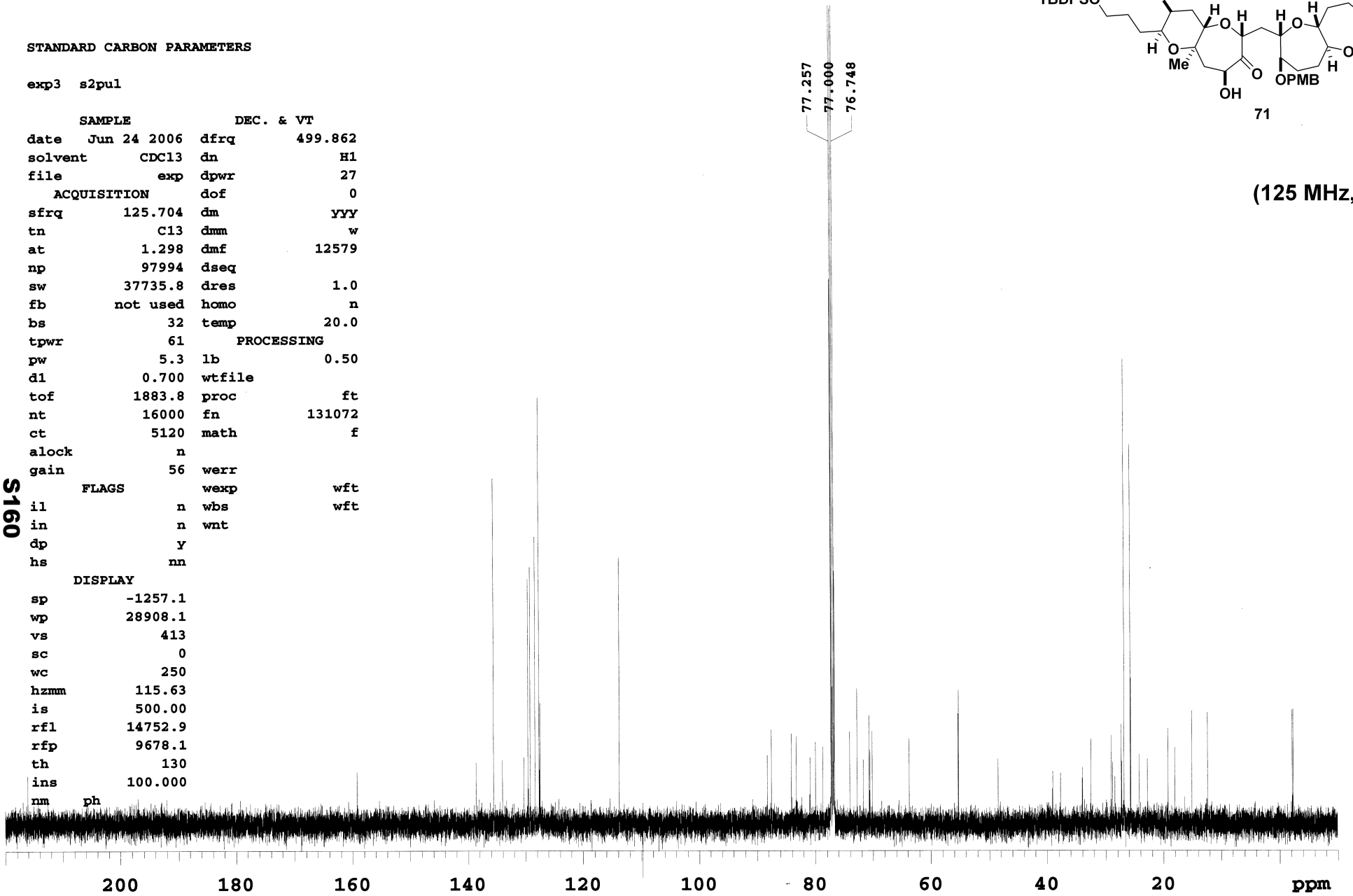
71

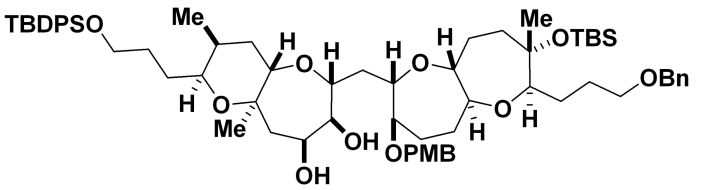
(125 MHz, $CDCl_3$)

STANDARD CARBON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Jun 24 2006	dfrq	499.862
solvent	CDCl3	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	32	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	16000	fn	131072
ct	5120	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1257.1		
wp	28908.1		
vs	413		
sc	0		
wc	250		
hzmm	115.63		
is	500.00		
rfl	14752.9		
rfp	9678.1		
th	130		
ins	100.000		
nm	ph		





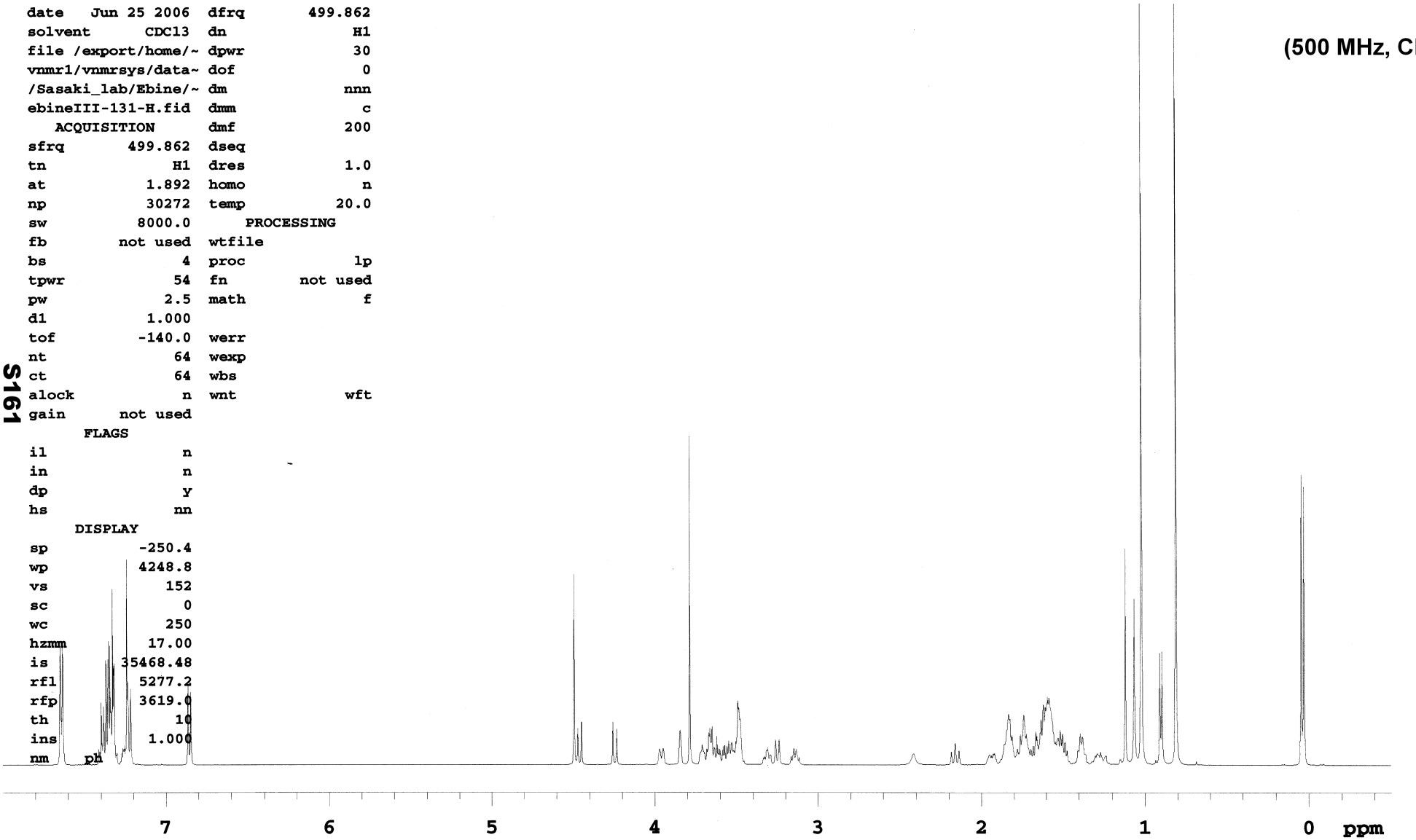
72

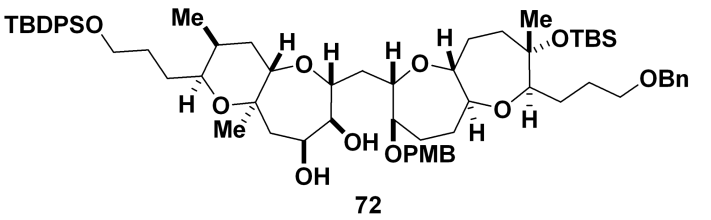
(500 MHz, $CDCl_3$)

STANDARD PROTON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Jun 25 2006	dfrq	499.862
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	30
	vnmr1/vnmrsys/data~	dof	0
	/Sasaki_lab/Ebine/~	dm	nnn
	ebineIII-131-H.fid	dmm	c
ACQUISITION		dmf	200
sfrq	499.862	dseq	
tn	H1	dres	1.0
at	1.892	homo	n
np	30272	temp	20.0
sw	8000.0	PROCESSING	
fb	not used	wtfile	
bs	4	proc	lp
tpwr	54	fn	not used
pw	2.5	math	f
d1	1.000		
tof	-140.0	werr	
nt	64	wexp	
ct	64	wbs	
alock	n	wnt	wft
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.4		
wp	4248.8		
vs	152		
sc	0		
wc	250		
hzmm	17.00		
is	35468.48		
rfl	5277.2		
rfp	3619.0		
th	10		
ins	1.000		
nm	ph		





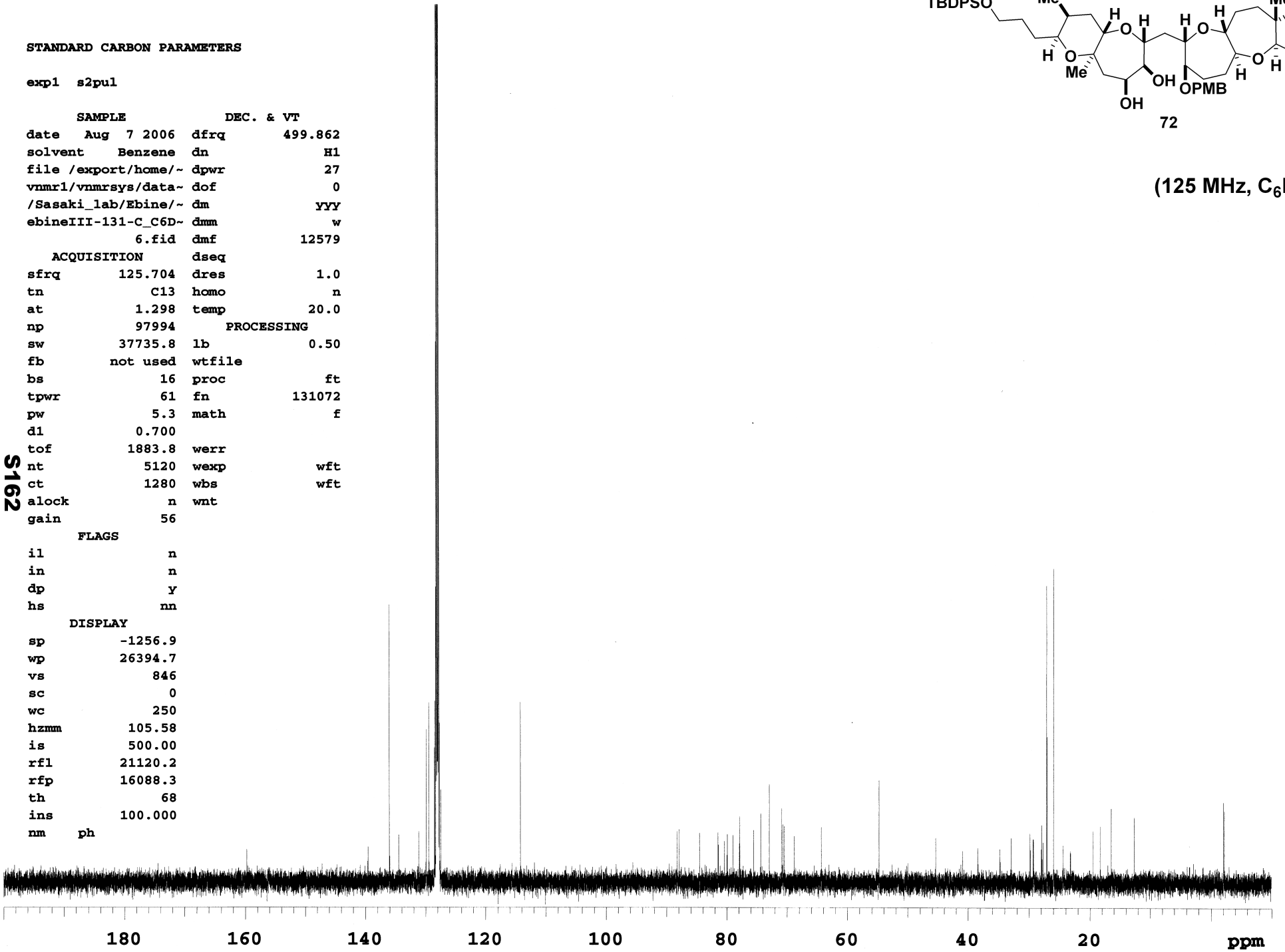
72

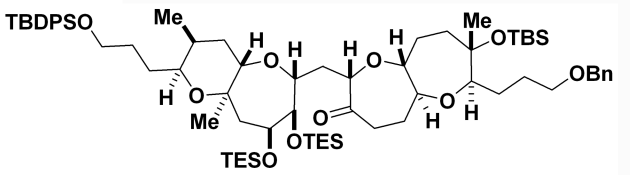
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Aug 7 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	/export/home/~	dpwr	27
	vnmr1/vnmrsys/data~	dof	0
	/Sasaki_lab/Ebine/~	dm	yyy
	ebineIII-131-C_C6D~	dmm	w
	6.fid	dmf	12579
ACQUISITION		dseq	
sfrq	125.704	dres	1.0
tn	C13	homo	n
at	1.298	temp	20.0
np	97994	PROCESSING	
sw	37735.8	lb	0.50
fb	not used	wtfile	
bs	16	proc	ft
tpwr	61	fn	131072
pw	5.3	math	f
d1	0.700		
tof	1883.8	werr	
nt	5120	wexp	wft
ct	1280	wbs	wft
alock	n	wnt	
gain	56		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	846		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21120.2		
rfp	16088.3		
th	68		
ins	100.000		
nm	ph		





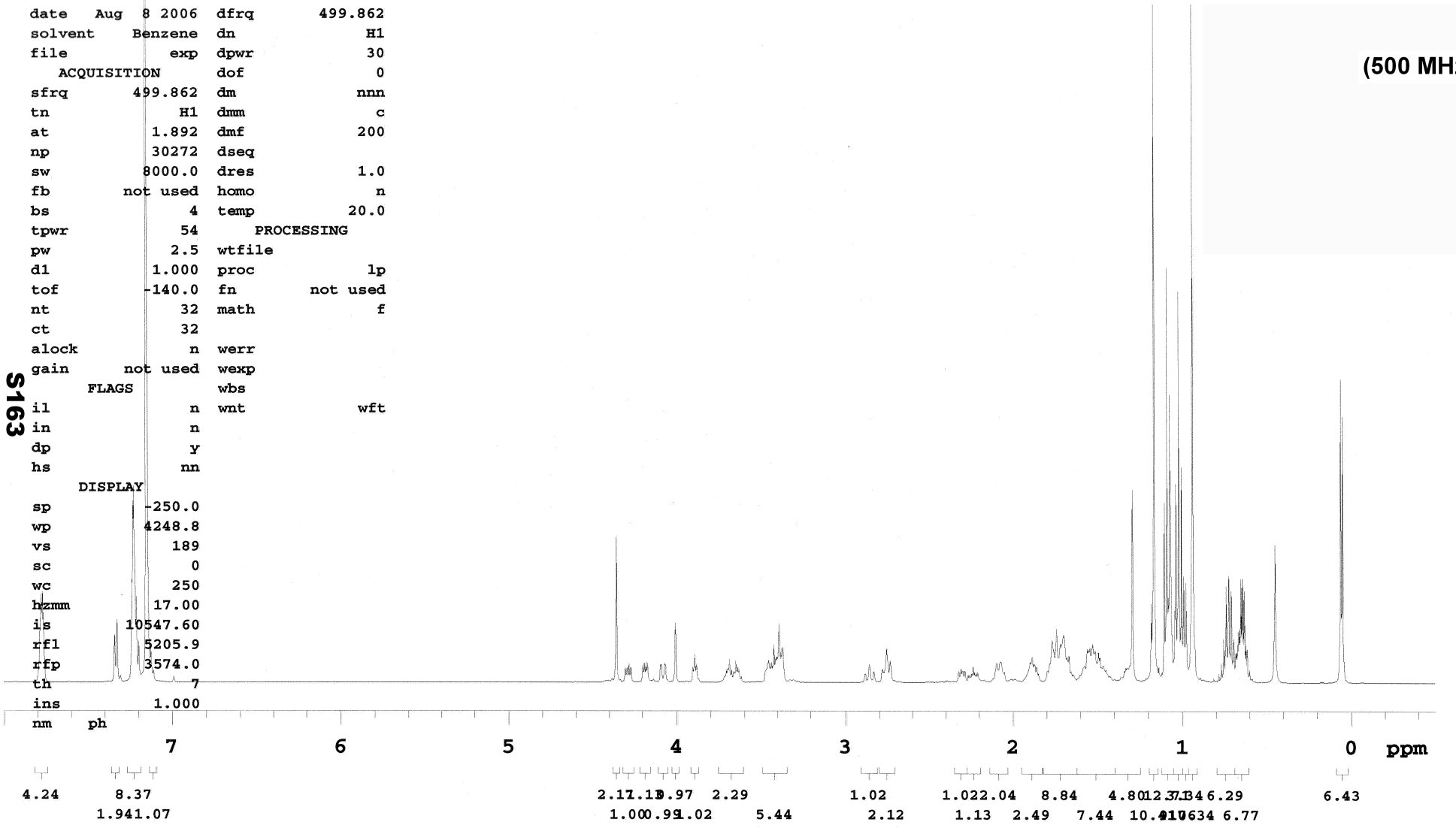
73

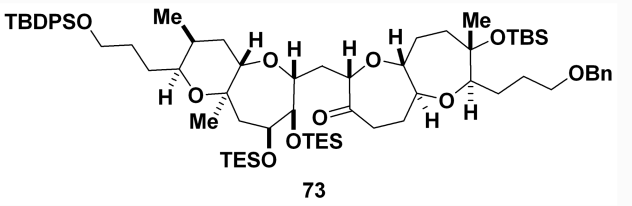
(500 MHz, C_6D_6)


```
STANDARD PROTON PARAMETERS

exp2  s2pul

      SAMPLE            DEC. & VT
date    Aug  8 2006  dfrq       499.862
solvent     Benzene  dn              H1
file            exp  dpwr            30
   ACQUISITION       dof              0
sfrq        499.862  dm             nnn
tn               H1  dmm              c
at            1.892  dmf            200
np            30272  dseq
sw           8000.0  dres           1.0
fb        not used   homo             n
bs                4  temp          20.0
tpwr             54      PROCESSING
pw              2.5  wtfile
d1            1.000  proc            lp
tof          -140.0  fn       not used
nt               32  math             f
ct               32
alock             n  werr
gain      not used   wexp
      FLAGS          wbs
il                n  wnt            wft
in                n
dp                y
hs               nn
     DISPLAY
sp           -250.0
wp           4248.8
vs              189
sc                0
wc              250
hzmm          17.00
is         10547.60
rfl          5205.9
rfp          3574.0
th                7
ins           1.000
nm    ph
```





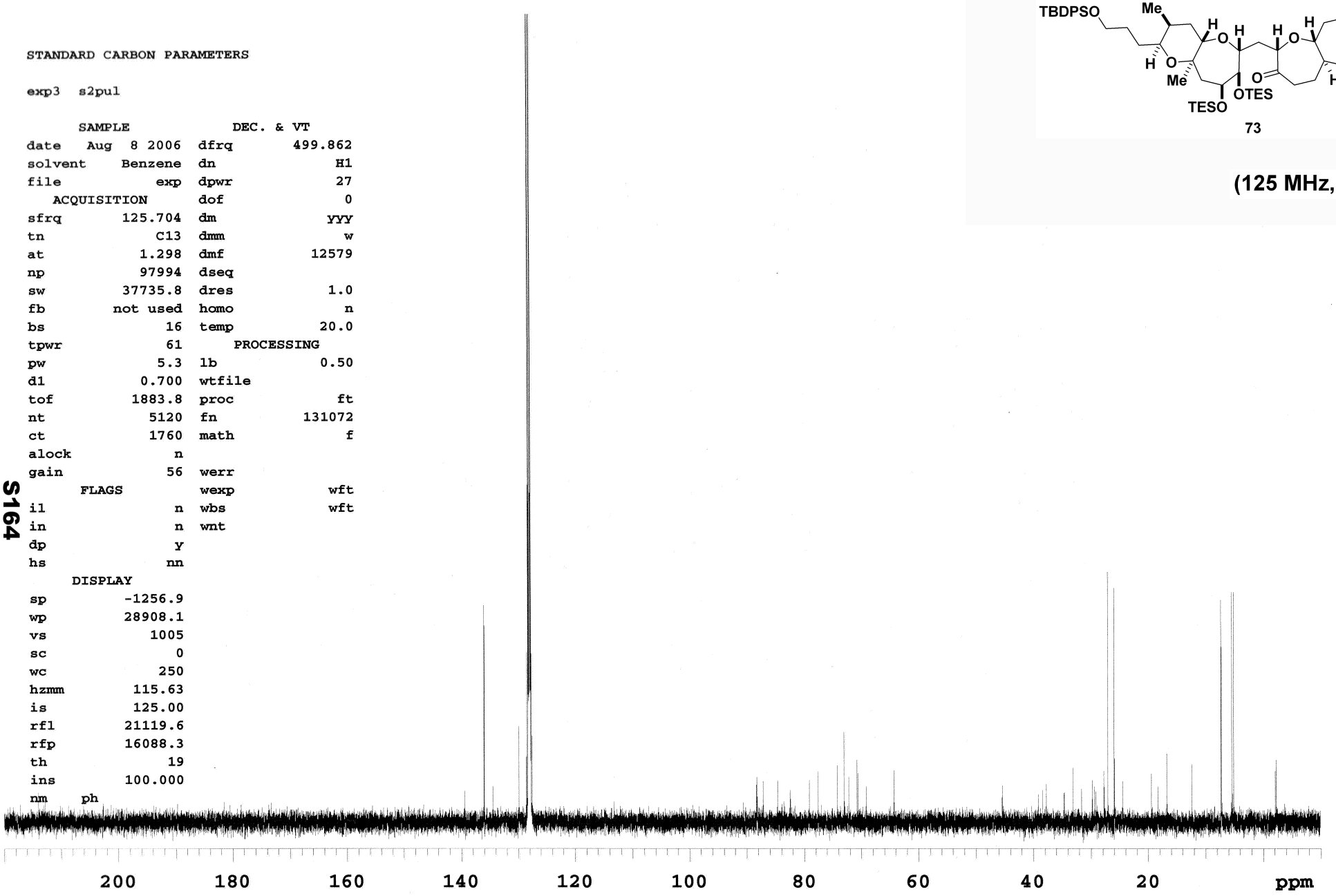
73

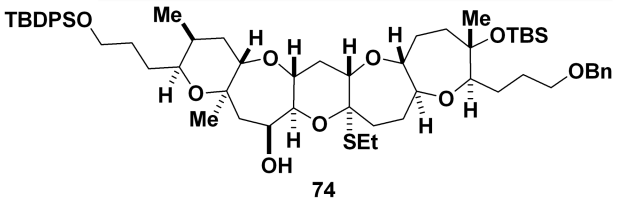
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Aug 8 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	YYY
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	1760	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	28908.1		
vs	1005		
sc	0		
wc	250		
hzmm	115.63		
is	125.00		
rfl	21119.6		
rfp	16088.3		
th	19		
ins	100.000		
nm	ph		





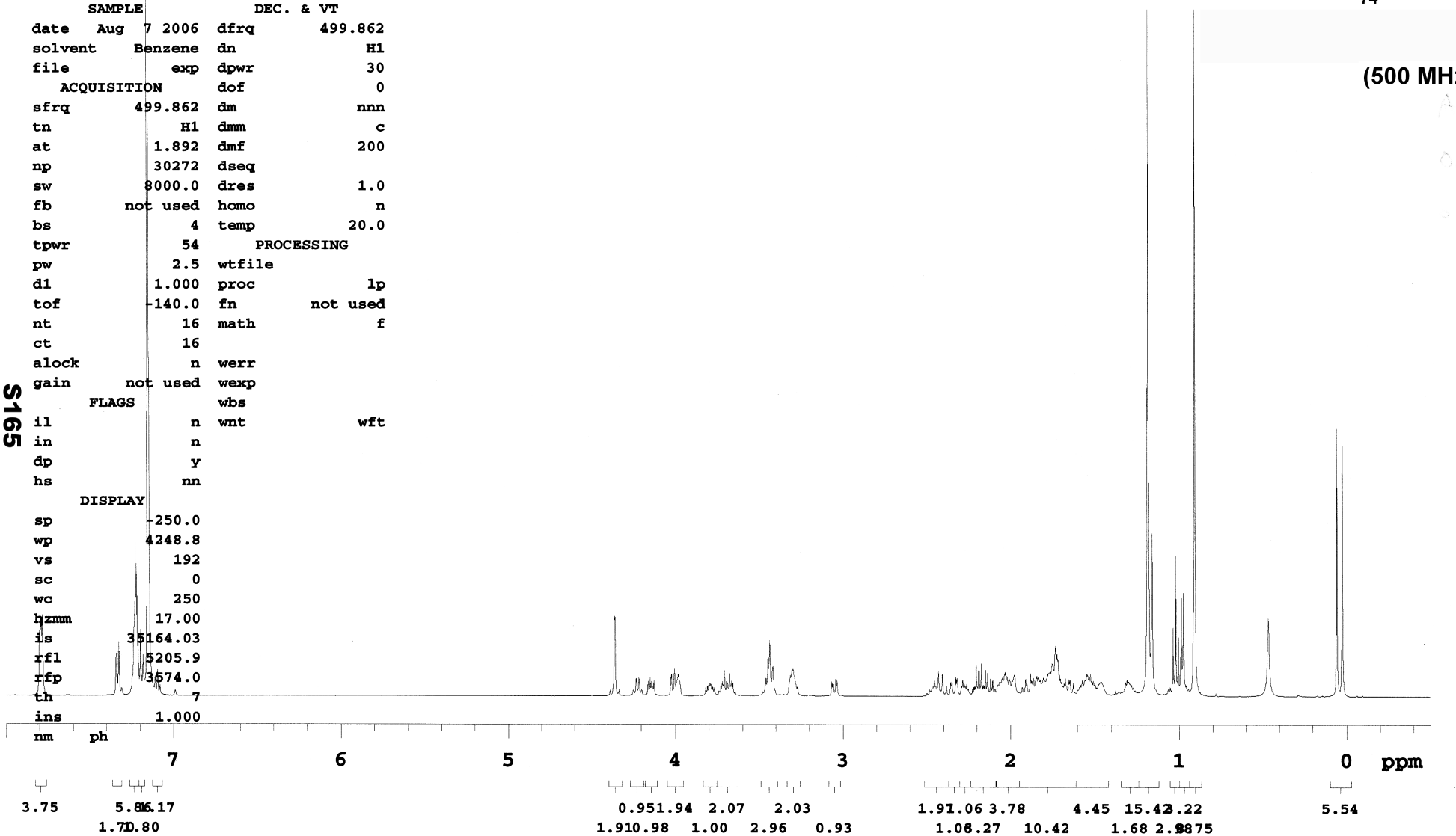
74

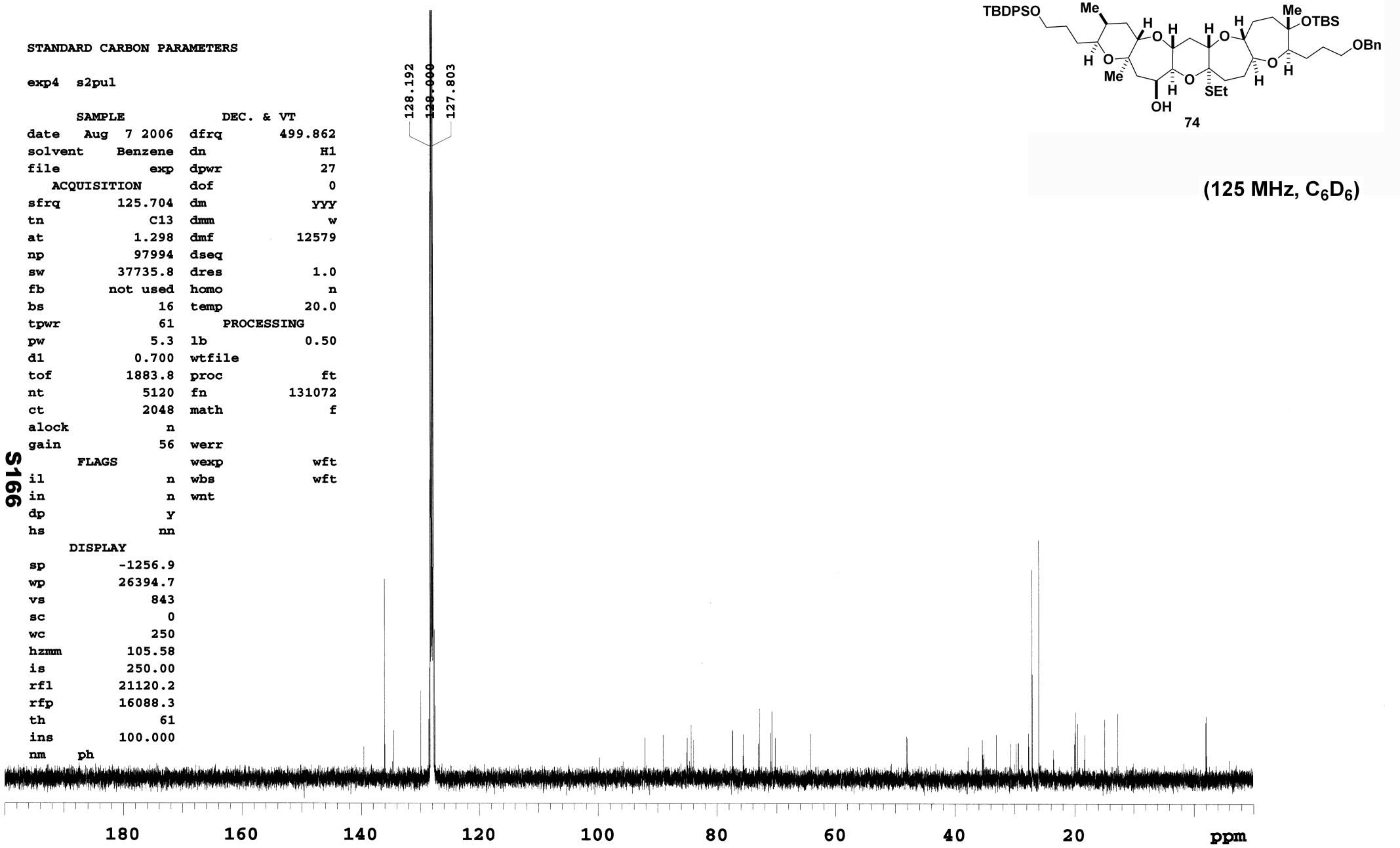
(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp3 s2pul

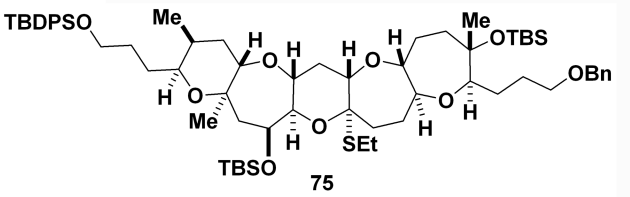
SAMPLE		DEC. & VT	
date	Aug 7 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	192		
sc	0		
wc	250		
hzmm	17.00		
is	35164.03		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		





74

(125 MHz, C_6D_6)



75

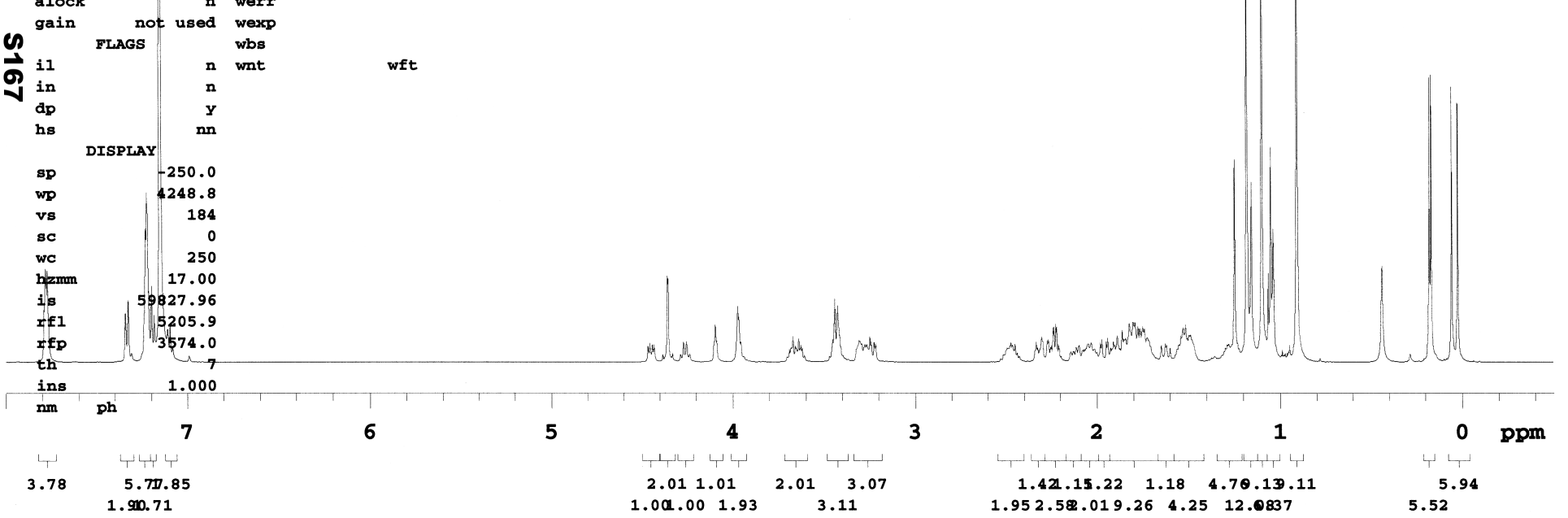
(500 MHz, C_6D_6)

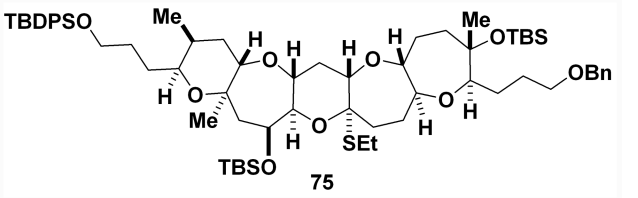
S167

STANDARD PROTON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Aug 7 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	32	math	f
ct	32		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	184		
sc	0		
wc	250		
hzmm	17.00		
is	59827.96		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		





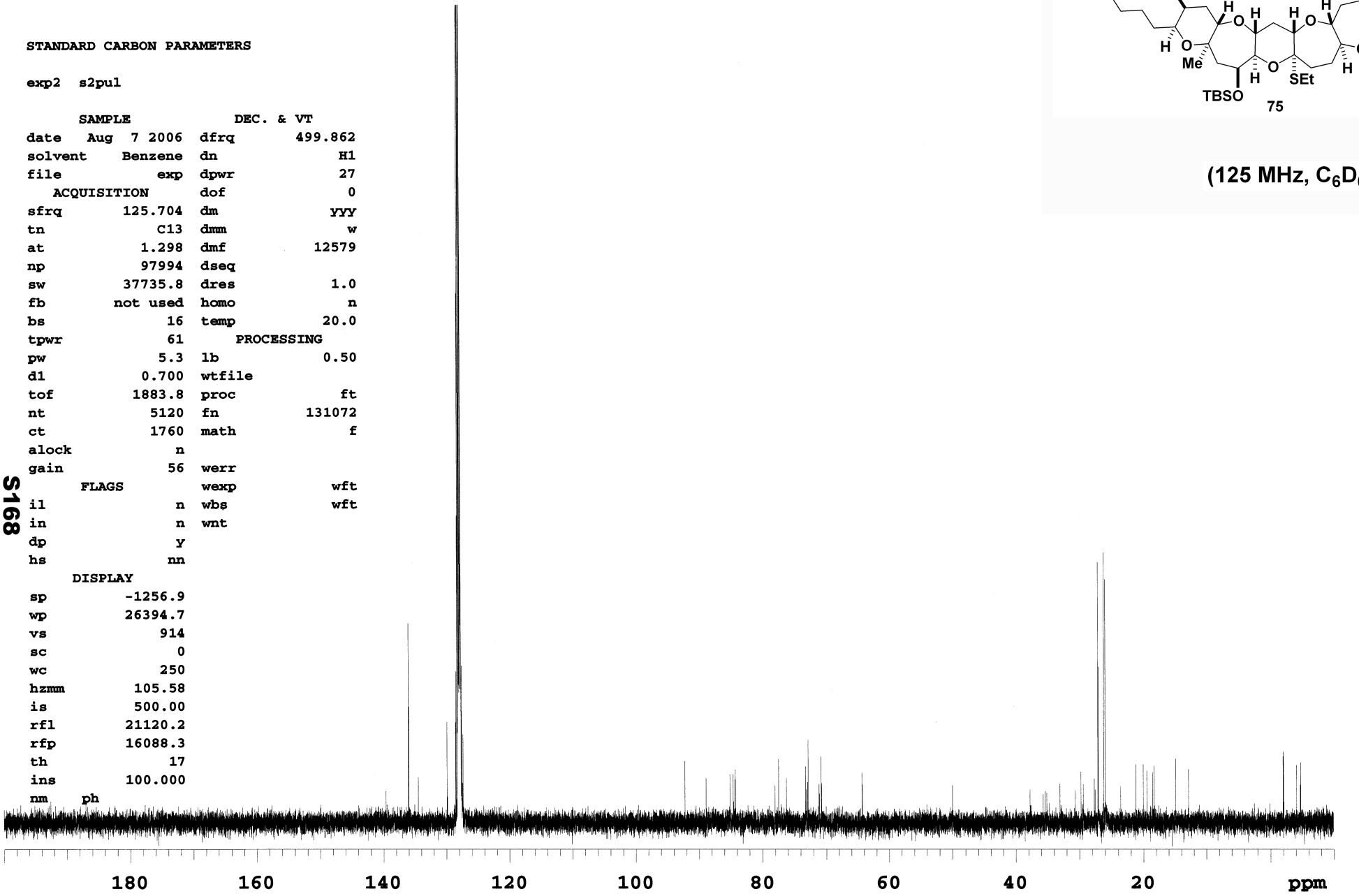
75

(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp2 s2pul

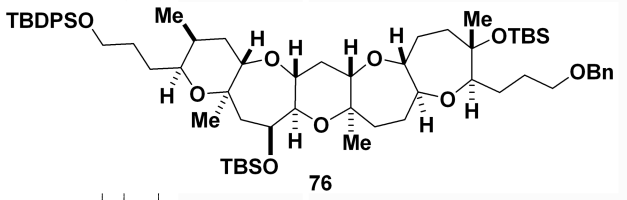
SAMPLE		DEC. & VT	
date	Aug 7 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	YYY
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	1760	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	914		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21120.2		
rfp	16088.3		
th	17		
ins	100.000		
nm	ph		



STANDARD PROTON PARAMETERS

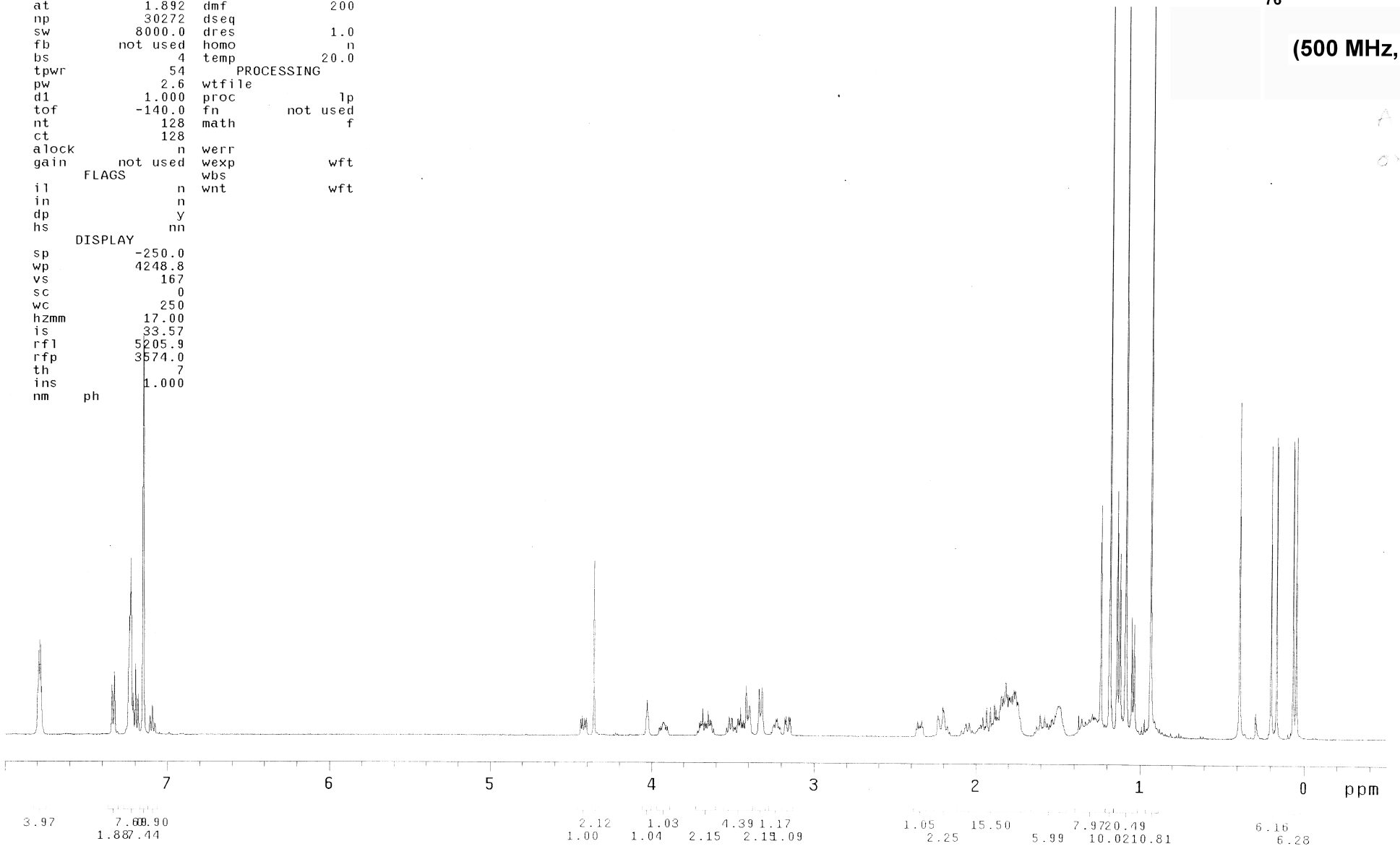
exp1 s2pul

SAMPLE		DEC. & VT	
date	Mar 19 2005	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.6	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	wft
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	167		
sc	0		
wc	250		
hzmm	17.00		
is	33.57		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		



76

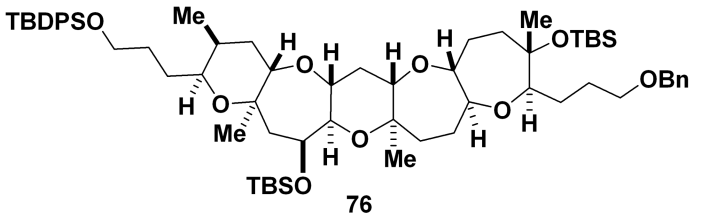
(500 MHz, C_6D_6)



III-106 ebine 9437 kouzou 05/3/19

Pulse Sequence: s2pul
 Solvent: Benzene
 Temp. 20.0 C / 293.1 K
User: 1-14-87
INOVA-600 "inova600"

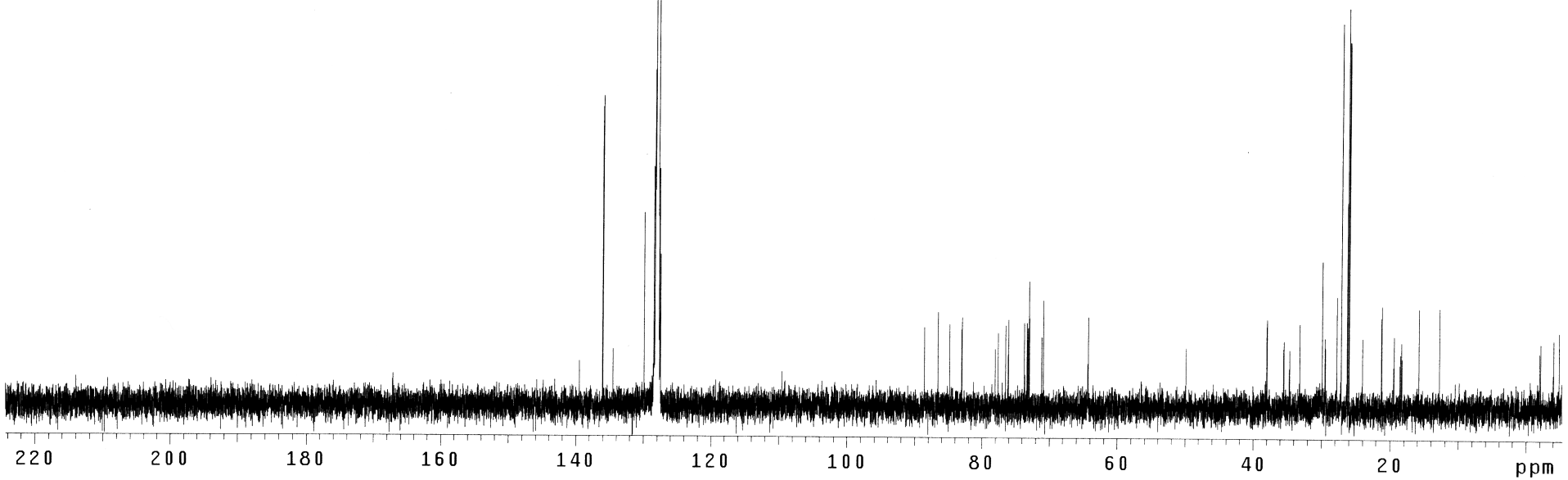
 Relax. delay 0.800 sec
 Pulse 45.0 degrees
 Acq. time 0.867 sec
 Width 34632.0 Hz
 36864 repetitions
OBSERVE C13, 150.8482663 MHz
DECOUPLE H1, 599.9153002 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 0.5 Hz
 Gauss apodization 0.388 sec
FT size 131072
Total time 23 hr, 16 min, 20 sec

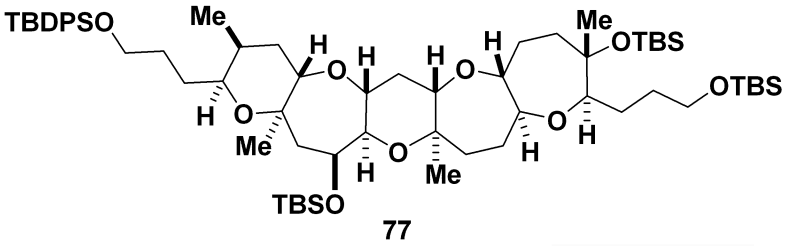


76

(125 MHz, C_6D_6)

S170





77

(500 MHz, C_6D_6)

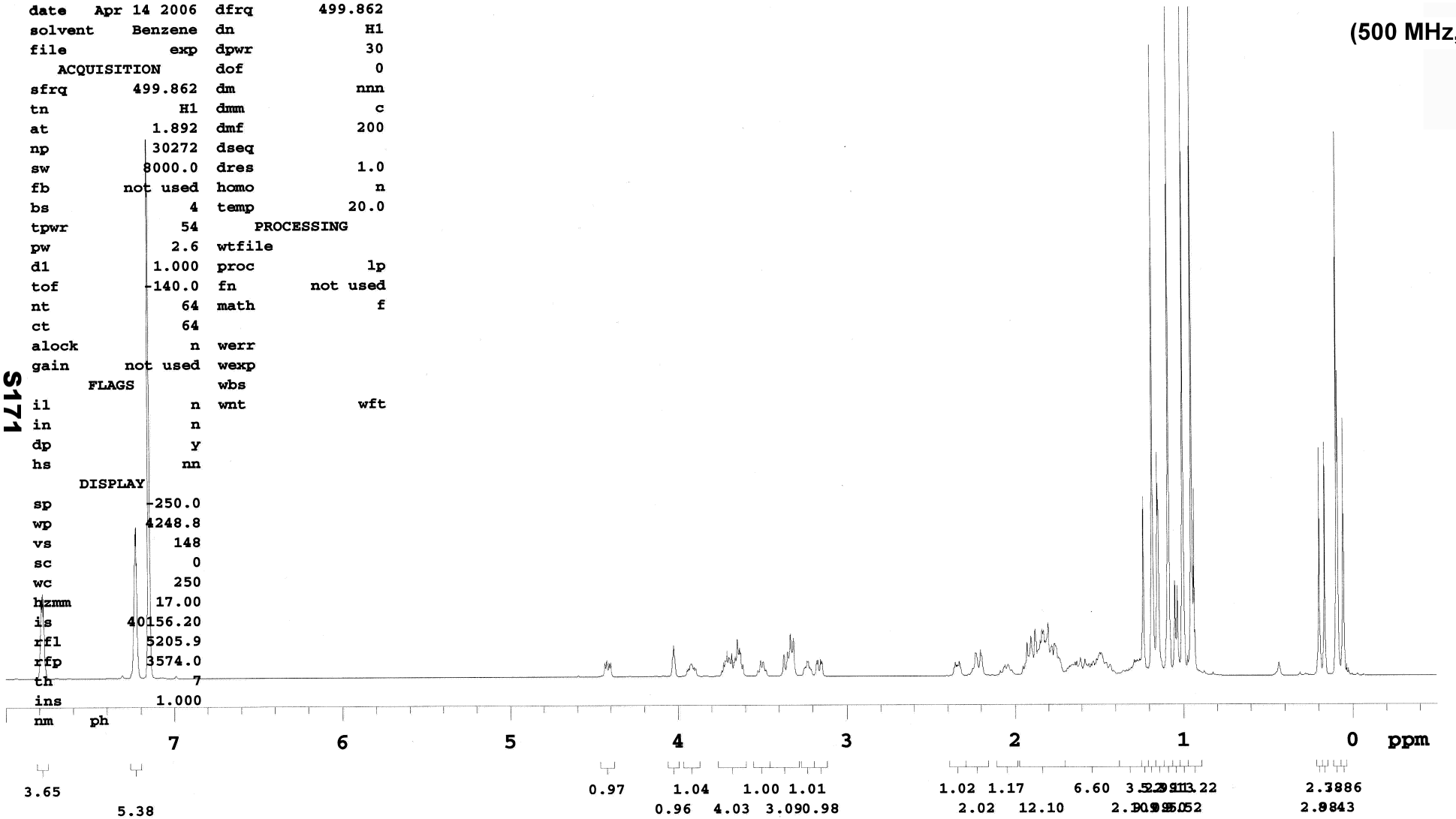
S171

```
STANDARD PROTON PARAMETERS

exp1  s2pul

      SAMPLE
date    Apr 14 2006
solvent     Benzene
file             exp
   ACQUISITION
sfrq         499.862
tn                H1
at             1.892
np             30272
sw            8000.0
fb         not used
bs                4
tpwr             54
pw              2.6
d1            1.000
tof          -140.0
nt               64
ct               64
alock             n
gain       not used
      FLAGS
il                n
in                n
dp                y
hs               nn
     DISPLAY
sp            -250.0
wp            4248.8
vs               148
sc                 0
wc               250
hzmm           17.00
is          40156.20
rfl          5205.9
rfp          3574.0
th                 7
ins            1.000
nm    ph

      DEC. & VT
dfrq         499.862
dn                H1
dpwr              30
dof                0
dm               nnn
dmm                c
dmf              200
dseq
dres             1.0
homo               n
temp            20.0
     PROCESSING
wtfile
proc              lp
fn         not used
math               f
werr
wexp
wbs
wnt              wft
```

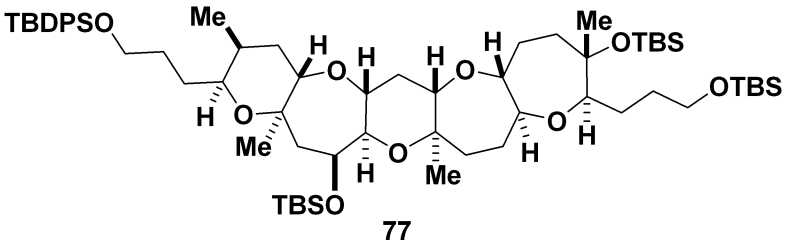


STANDARD CARBON PARAMETERS

Pulse Sequence: s2pul

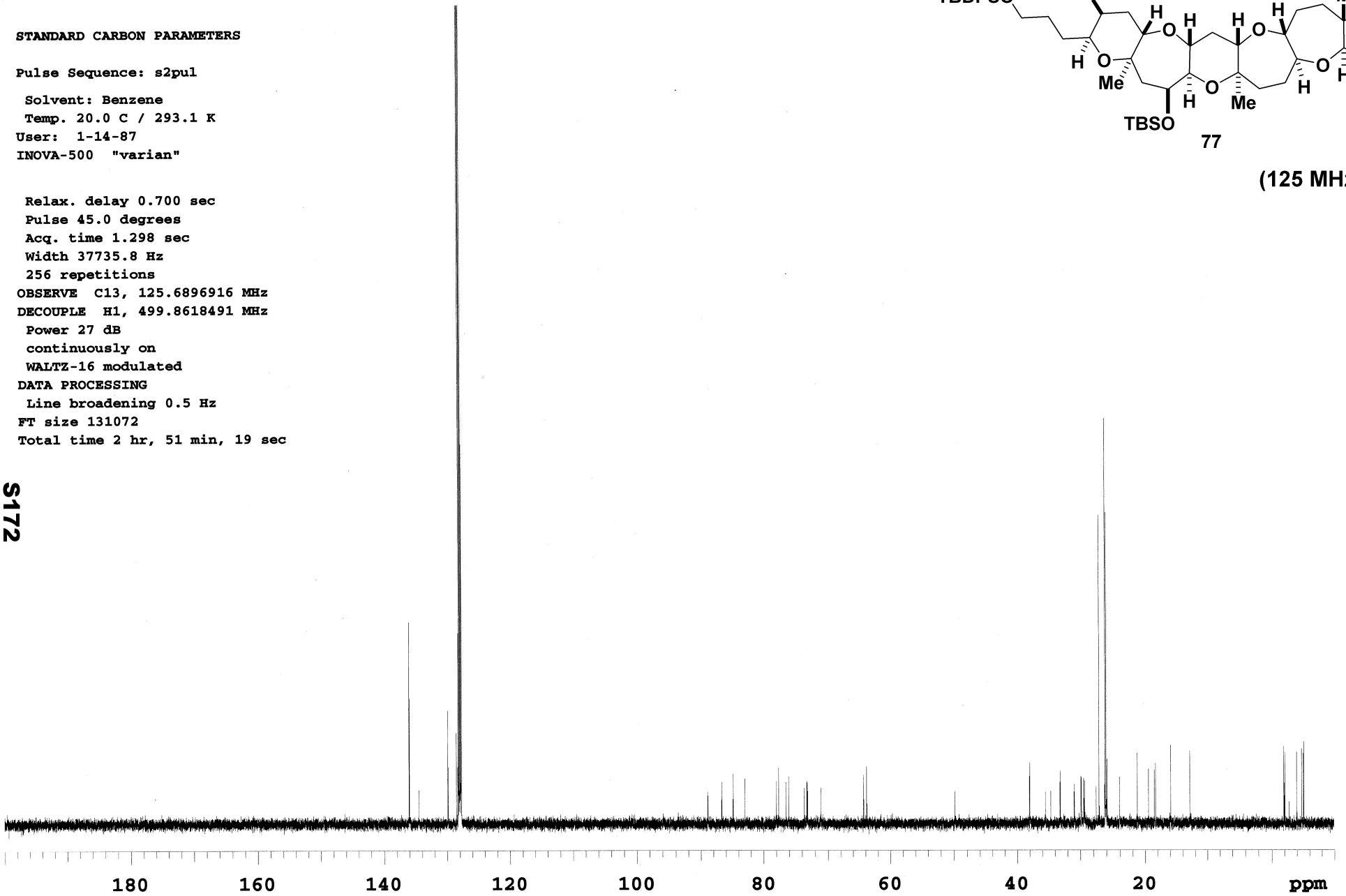
Solvent: Benzene
Temp. 20.0 C / 293.1 K
User: 1-14-87
INOVA-500 "varian"

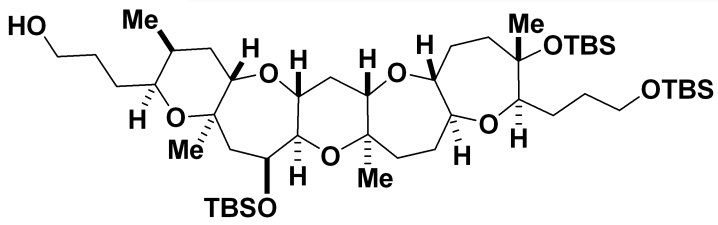
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.298 sec
Width 37735.8 Hz
256 repetitions
OBSERVE C13, 125.6896916 MHz
DECOUPLE H1, 499.8618491 MHz
Power 27 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 2 hr, 51 min, 19 sec



77

(125 MHz, C_6D_6)





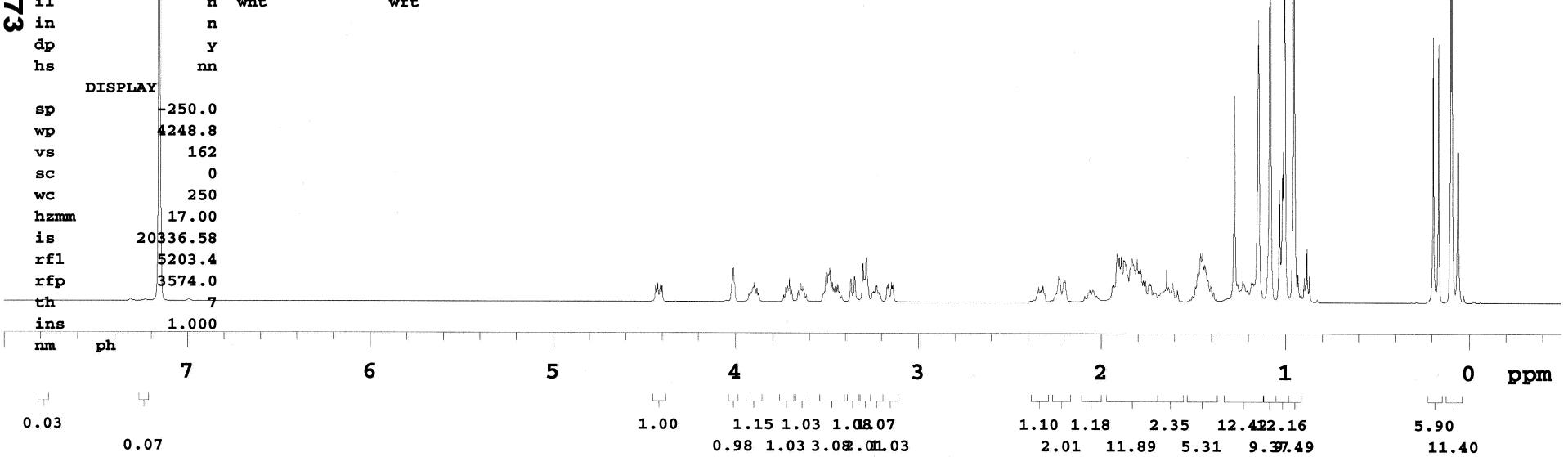
78

(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp1 s2pul

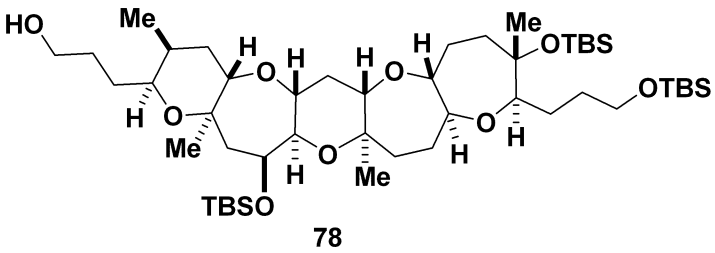
SAMPLE		DEC. & VT	
date	Apr 19 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	162		
sc	0		
wc	250		
hzmm	17.00		
is	20336.58		
rfl	5203.4		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		



STANDARD CARBON PARAMETERS

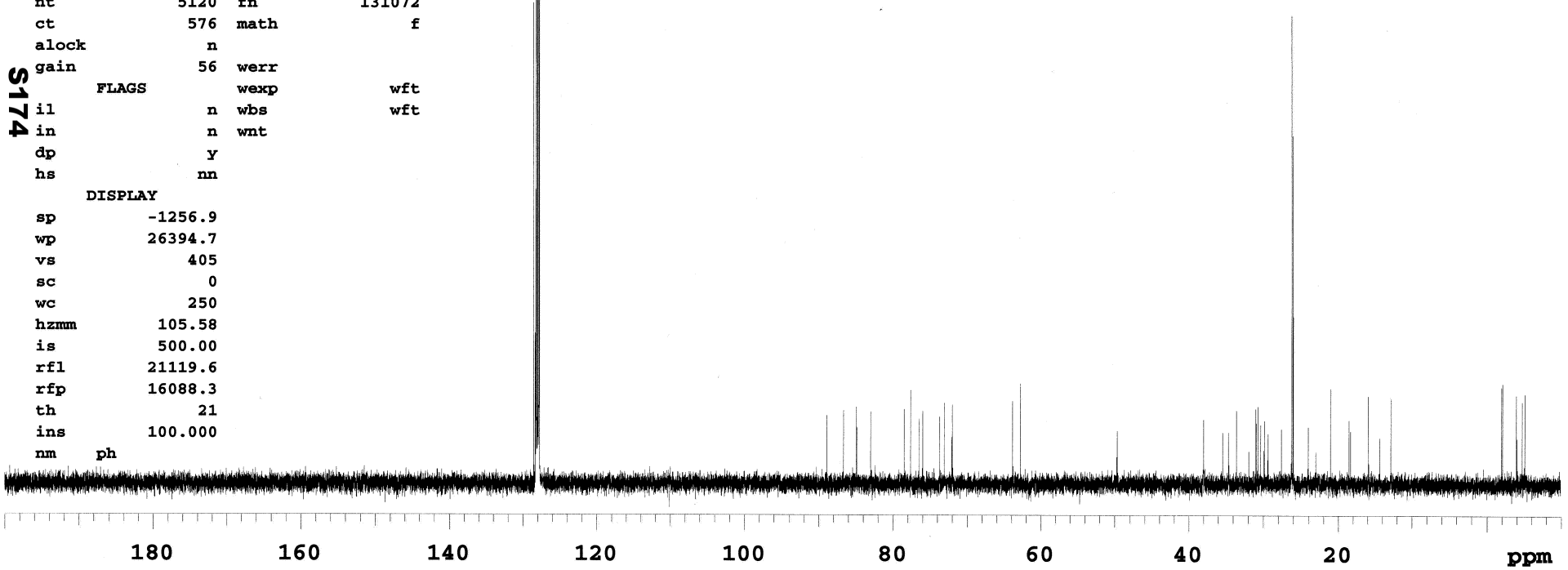
exp3 s2pul

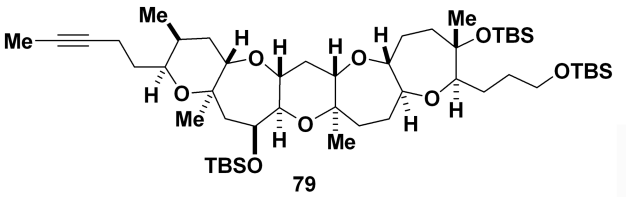
SAMPLE		DEC. & VT	
date	Apr 19 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	32	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	576	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	405		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21119.6		
rfp	16088.3		
th	21		
ins	100.000		
nm	ph		



78

(125 MHz, C_6D_6)





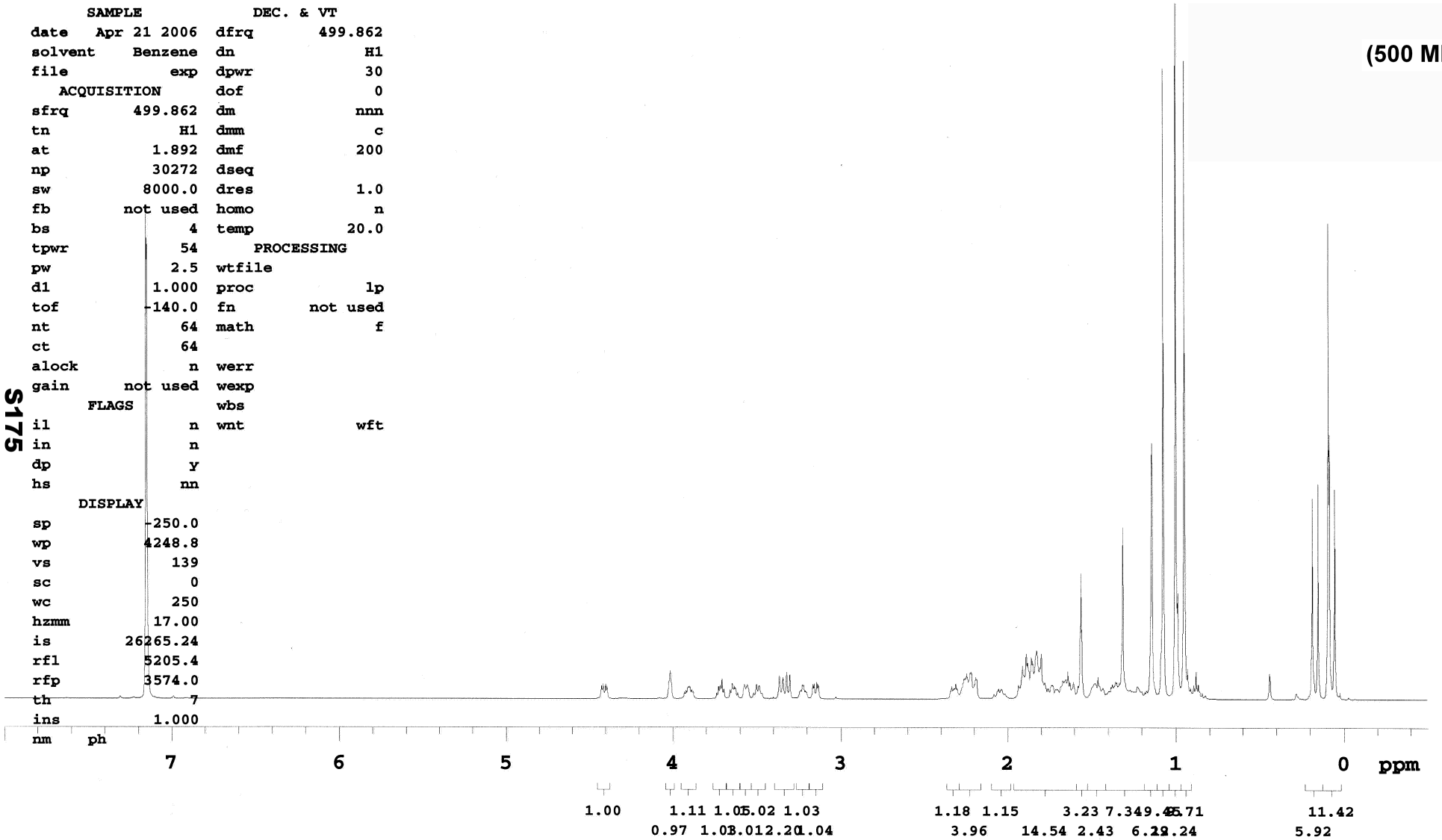
79

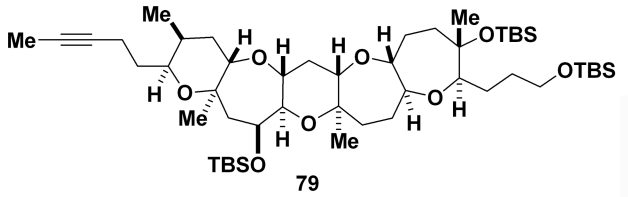
STANDARD PROTON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Apr 21 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	139		
sc	0		
wc	250		
hzmm	17.00		
is	26265.24		
rfl	5205.4		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		

(500 MHz, C_6D_6)





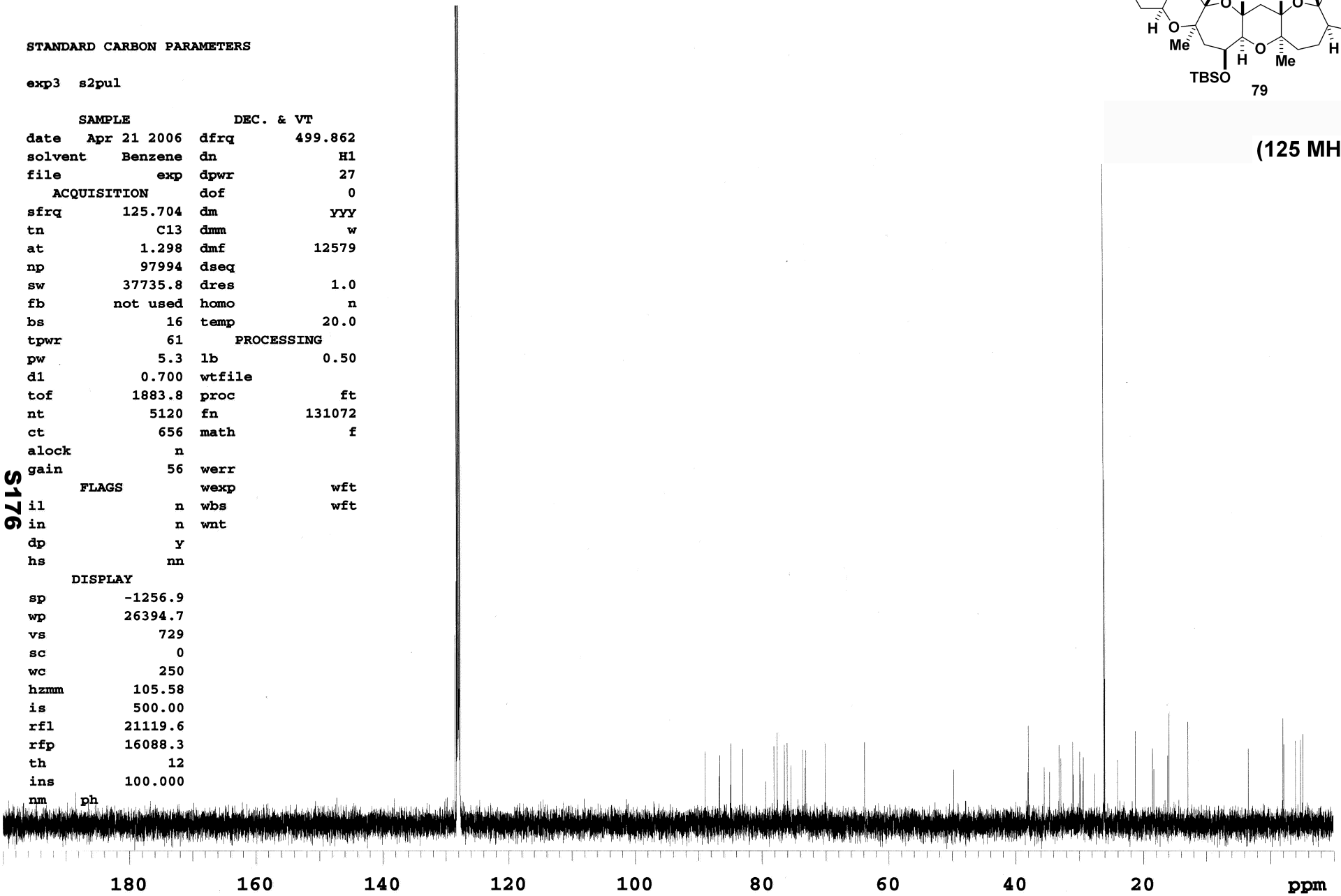
79

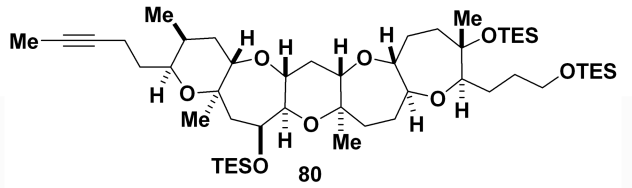
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Apr 21 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	656	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	729		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21119.6		
rfp	16088.3		
th	12		
ins	100.000		
nm	ph		





80

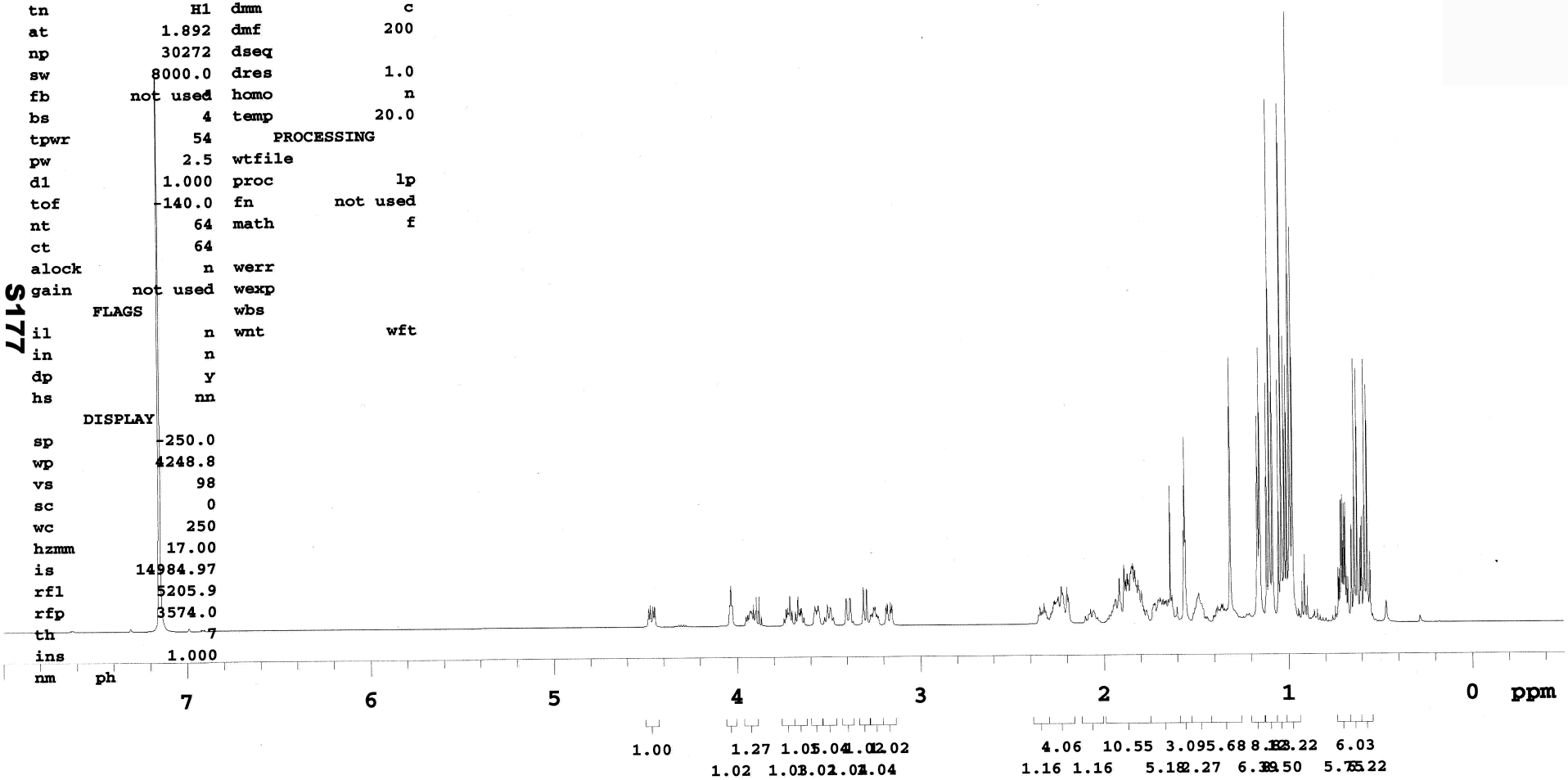
(500 MHz, C_6D_6)

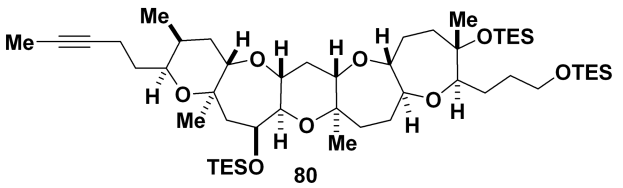
STANDARD PROTON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Apr 25 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	98		
sc	0		
wc	250		
hzmm	17.00		
is	14984.97		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		

S177





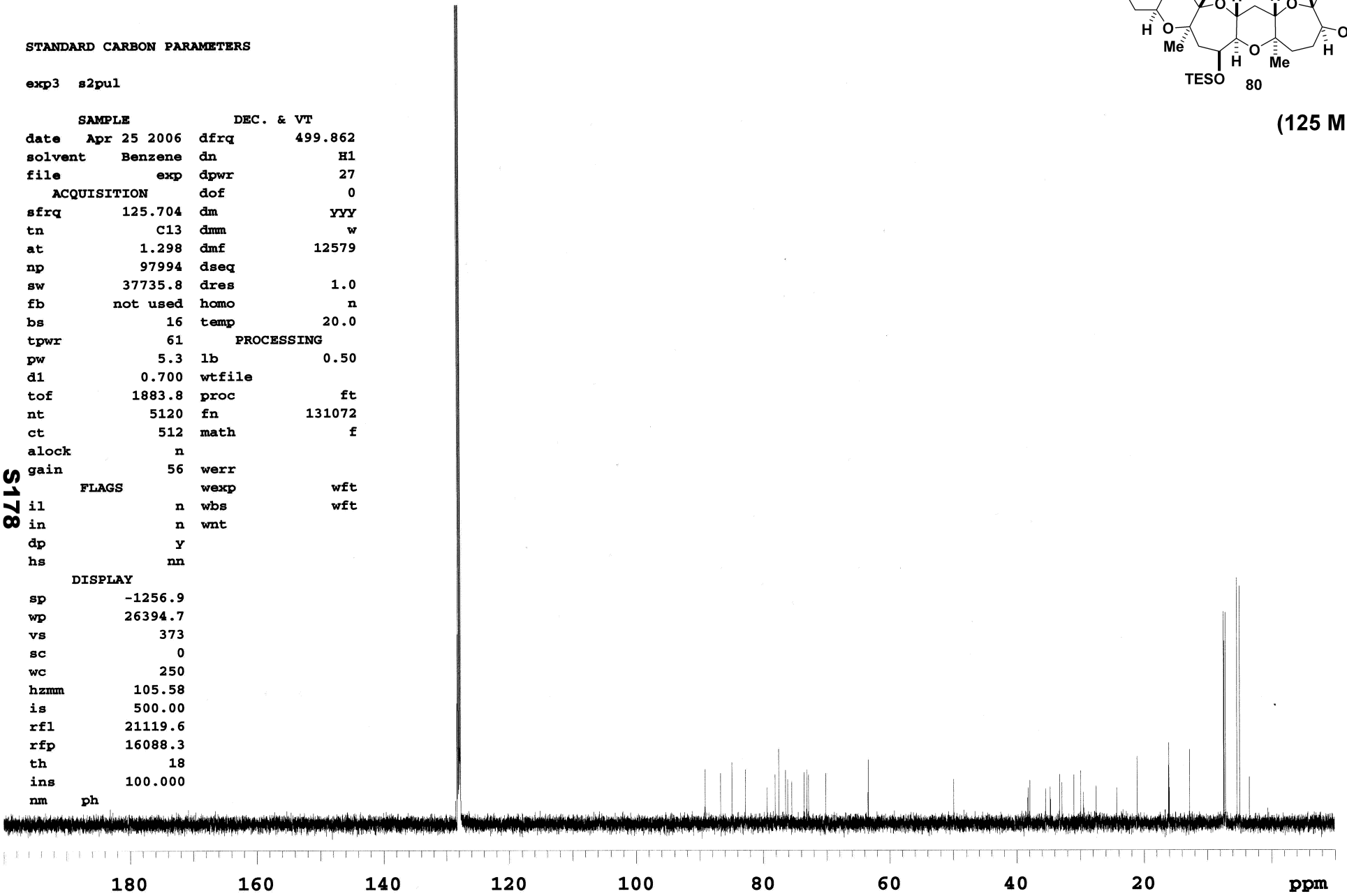
80

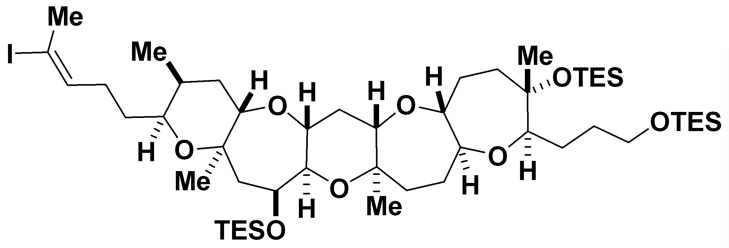
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Apr 25 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	YYY
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	512	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	373		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21119.6		
rfp	16088.3		
th	18		
ins	100.000		
nm	ph		





81

(500 MHz, C_6D_6)

S179

STANDARD PROTON PARAMETERS

exp3 s2pul

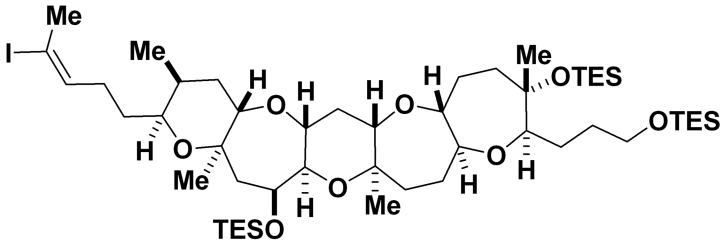
SAMPLE		DEC. & VT	
date	Apr 28 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.3		
wp	4248.8		
vs	115		
sc	0		
wc	250		
hzmm	17.00		
is	7889.77		
rfl	1640.6		
rfp	0		
th	7		
ins	1.000		

nm ph

7 6 5 4 3 2 1 0 ppm

0.05 0.02 0.08 0.10 0.99 2.01 1.04 1.71 4.70 15.04 3.15 9.18 11.25

0.16 0.67 0.01 0.98 1.00 1.02 2.22 1.02 1.11 1.58 3.17 5.61



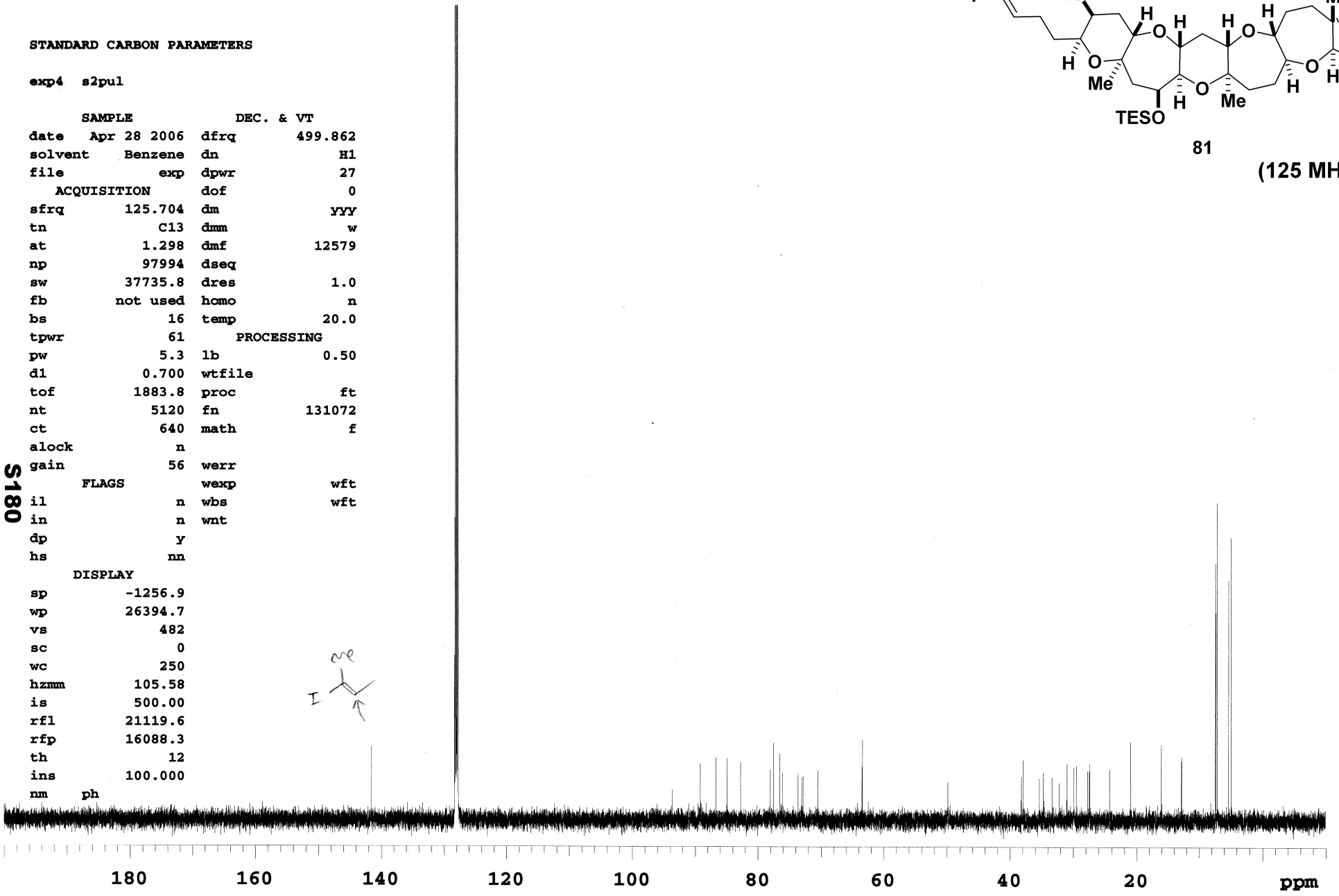
81

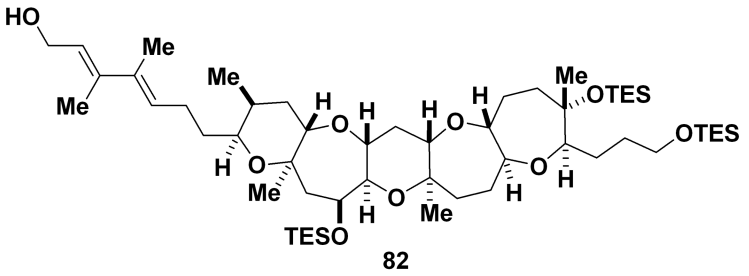
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp4 s2pul

SAMPLE		DEC. & VT	
date	Apr 28 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	640	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	482		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21119.6		
rfp	16088.3		
th	12		
ins	100.000		
nm	ph		





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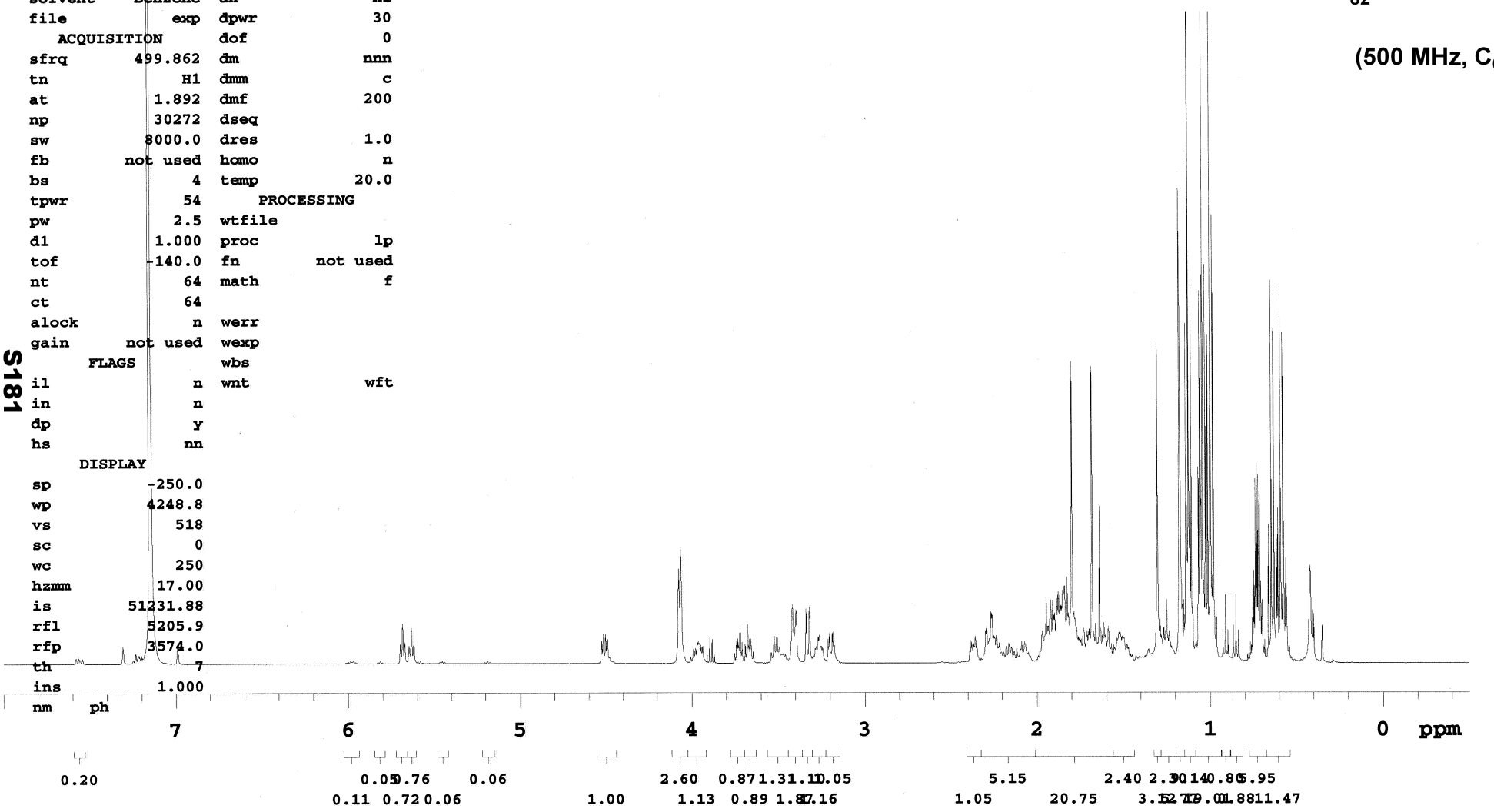
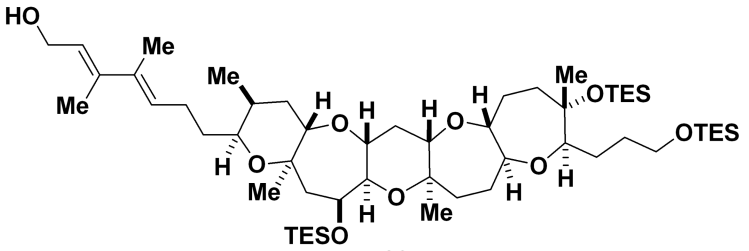
(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	May 2 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	518		
sc	0		
wc	250		
hzmm	17.00		
is	51231.88		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		





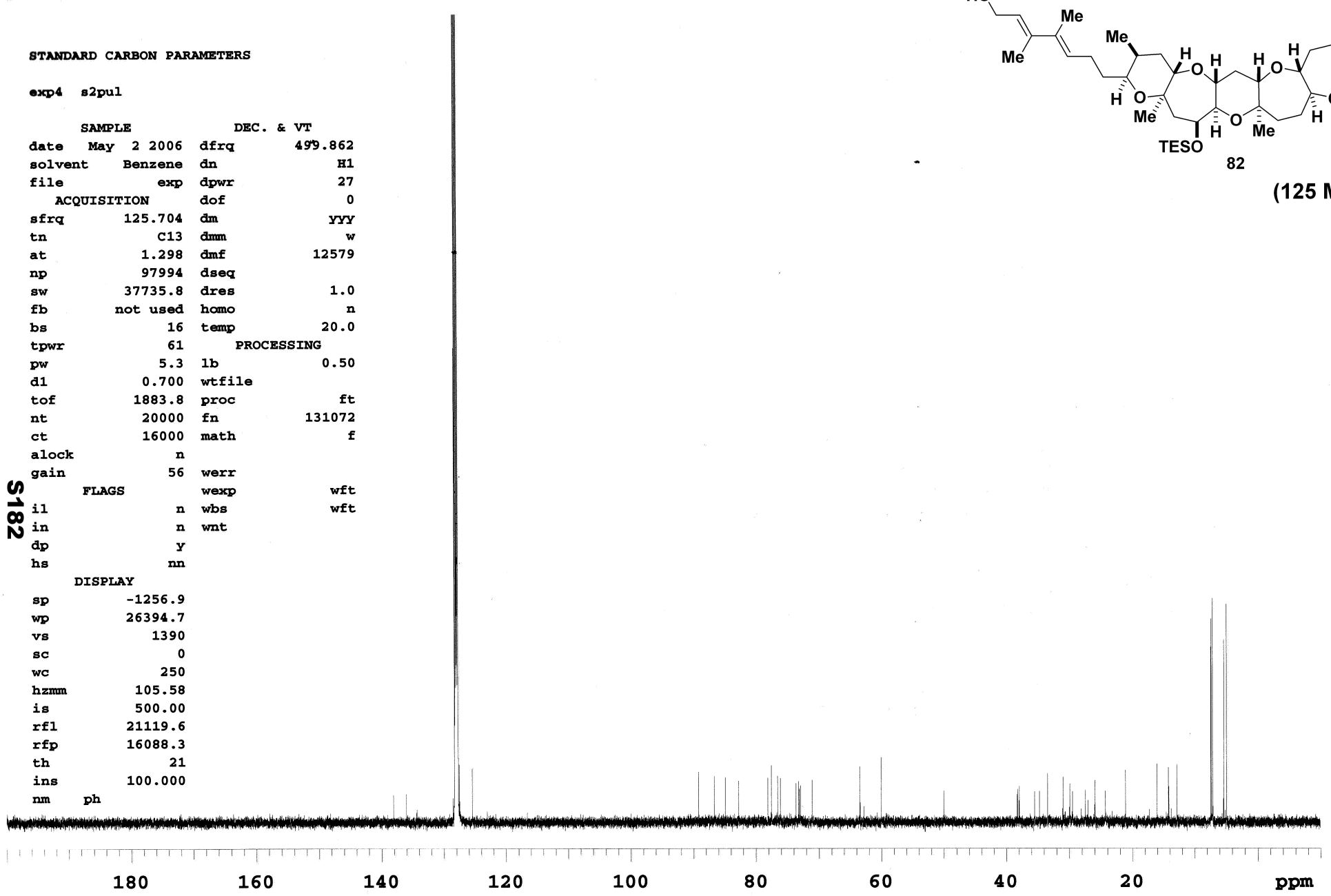
82

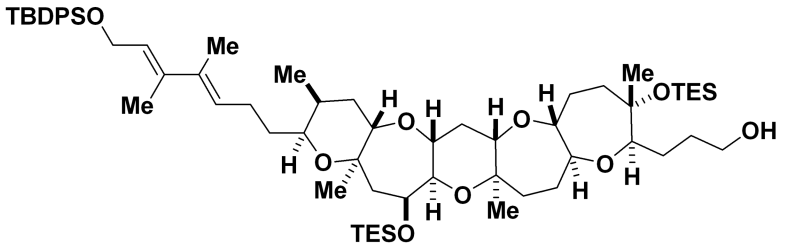
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp4 s2pul

SAMPLE		DEC. & VT	
date	May 2 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	20000	fn	131072
ct	16000	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	1390		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21119.6		
rfp	16088.3		
th	21		
ins	100.000		
nm	ph		





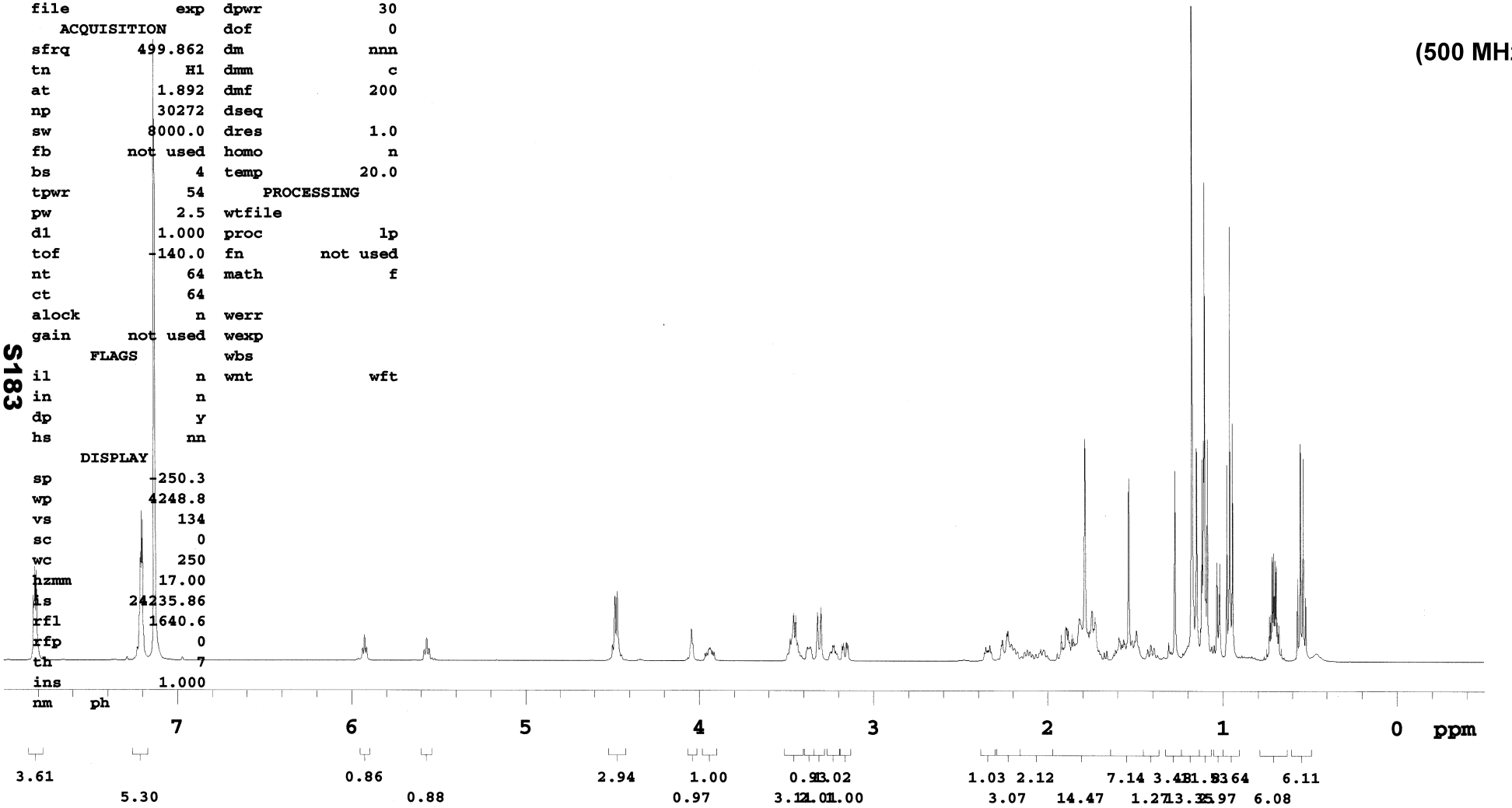
83

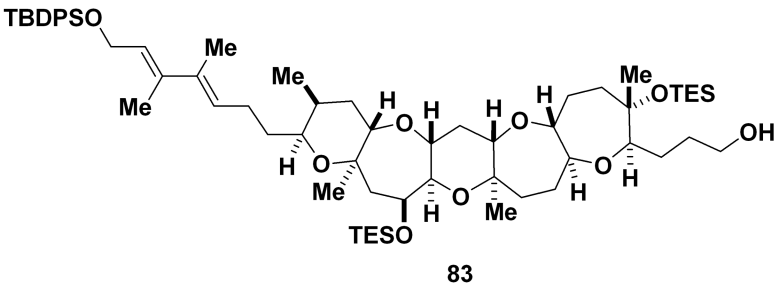
(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	May 30 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.3		
wp	4248.8		
vs	134		
sc	0		
wc	250		
hzmm	17.00		
is	24235.86		
rfl	1640.6		
rfp	0		
th	7		
ins	1.000		
nm	ph		





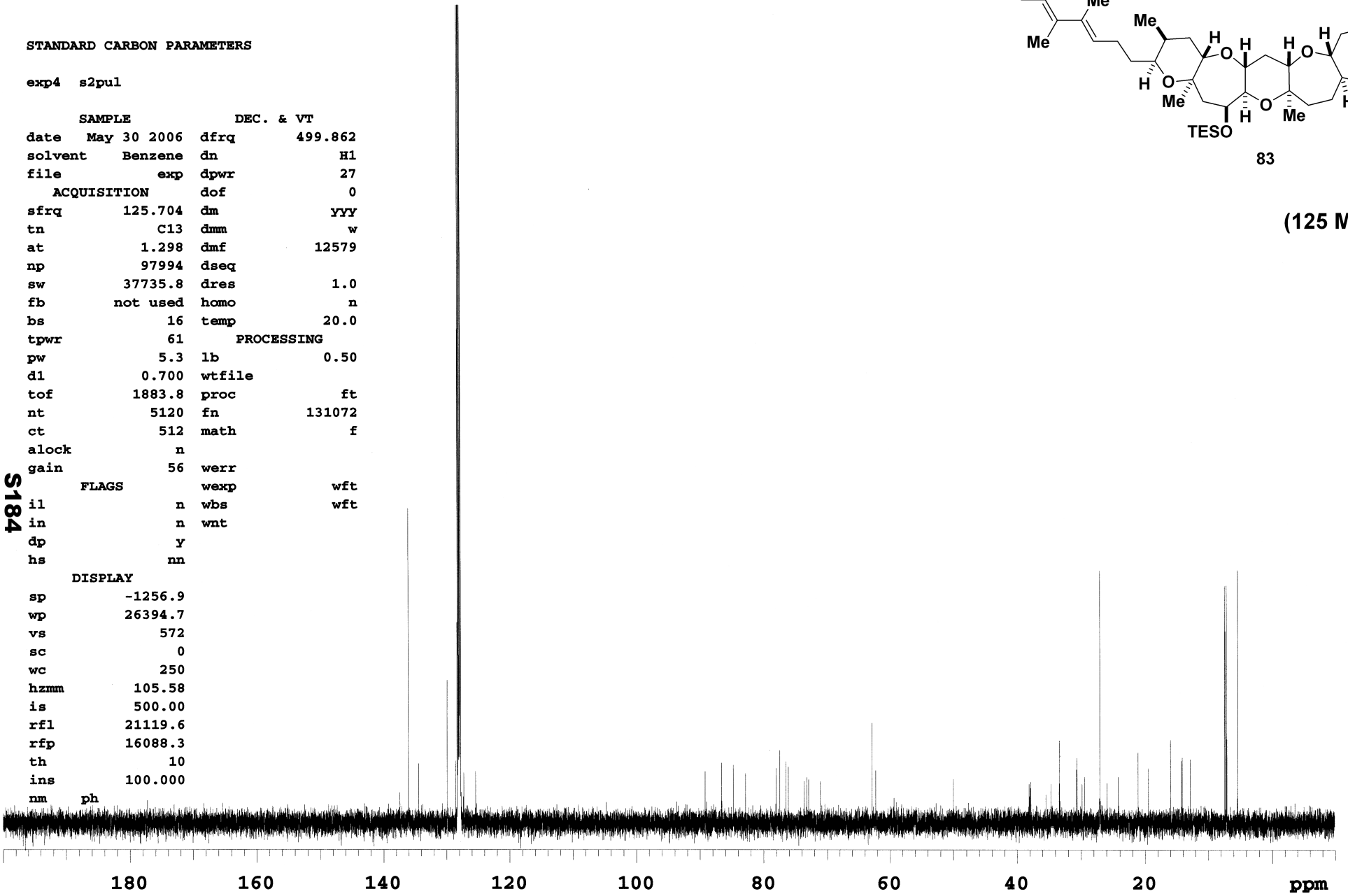
83

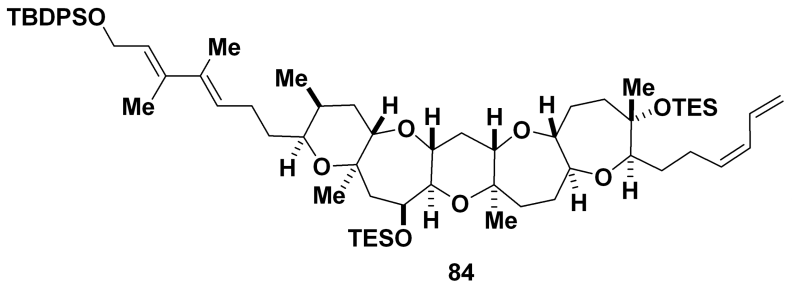
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp4 s2pul

SAMPLE		DEC. & VT	
date	May 30 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	YYY
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	512	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	572		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21119.6		
rfp	16088.3		
th	10		
ins	100.000		
nm	ph		





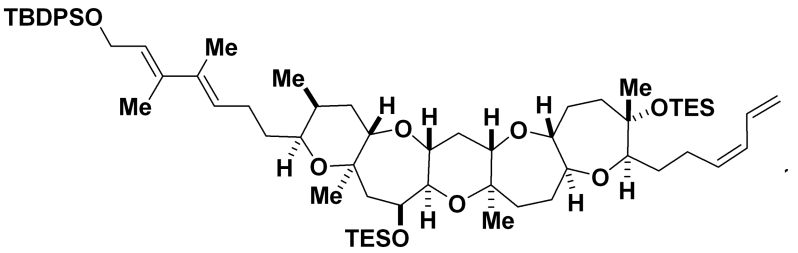
84

(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp1 s2pul

SAMPLE		DEC. & VT	
date	Jun 2 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	243		
sc	0		
wc	250		
hzmm	17.00		
is	36967.77		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		



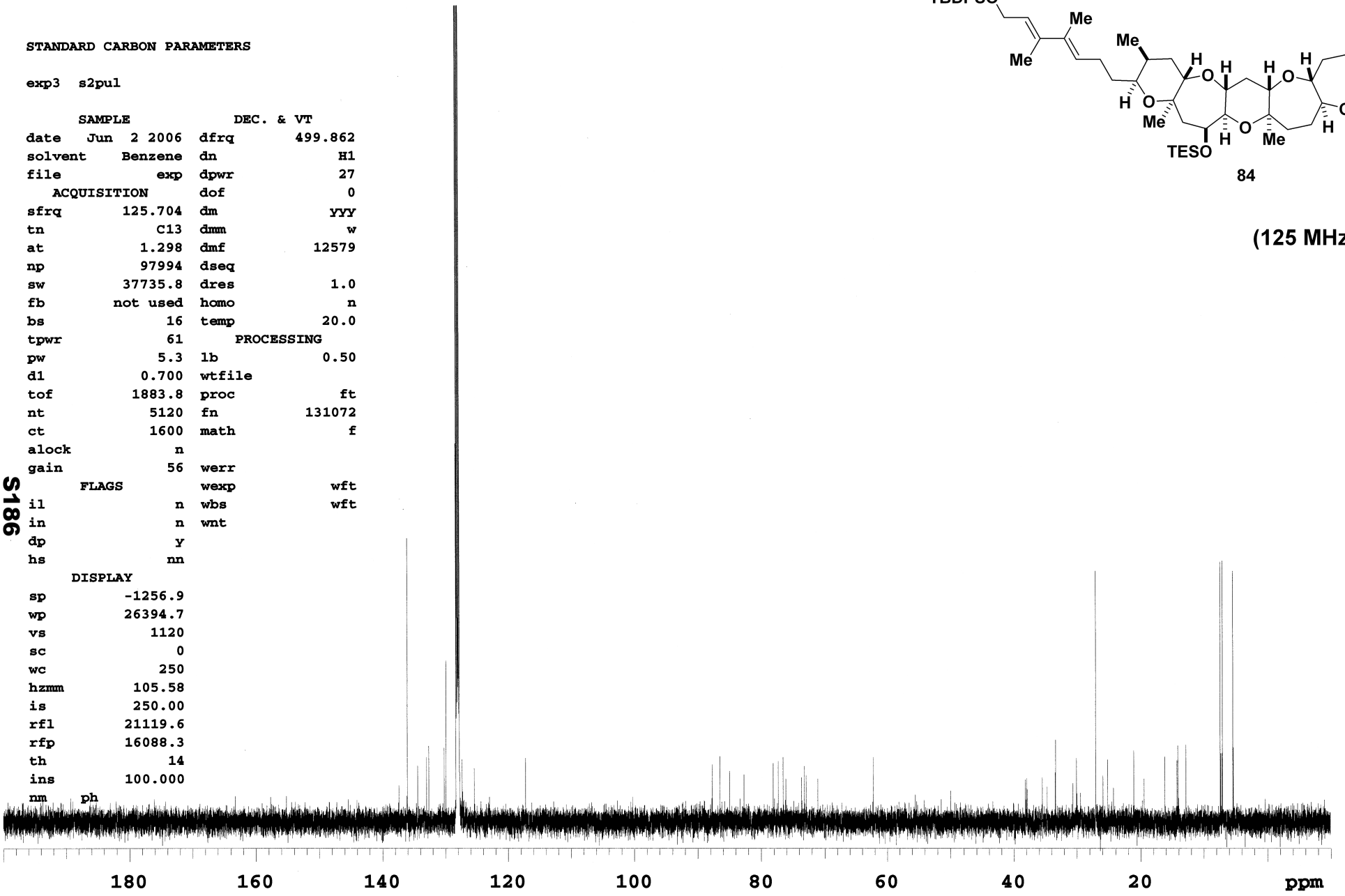
84

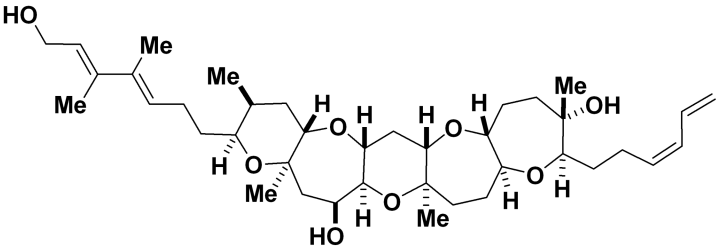
(125 MHz, C_6D_6)

STANDARD CARBON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Jun 2 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	1600	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	1120		
sc	0		
wc	250		
hzmm	105.58		
is	250.00		
rfl	21119.6		
rfp	16088.3		
th	14		
ins	100.000		
nm	ph		





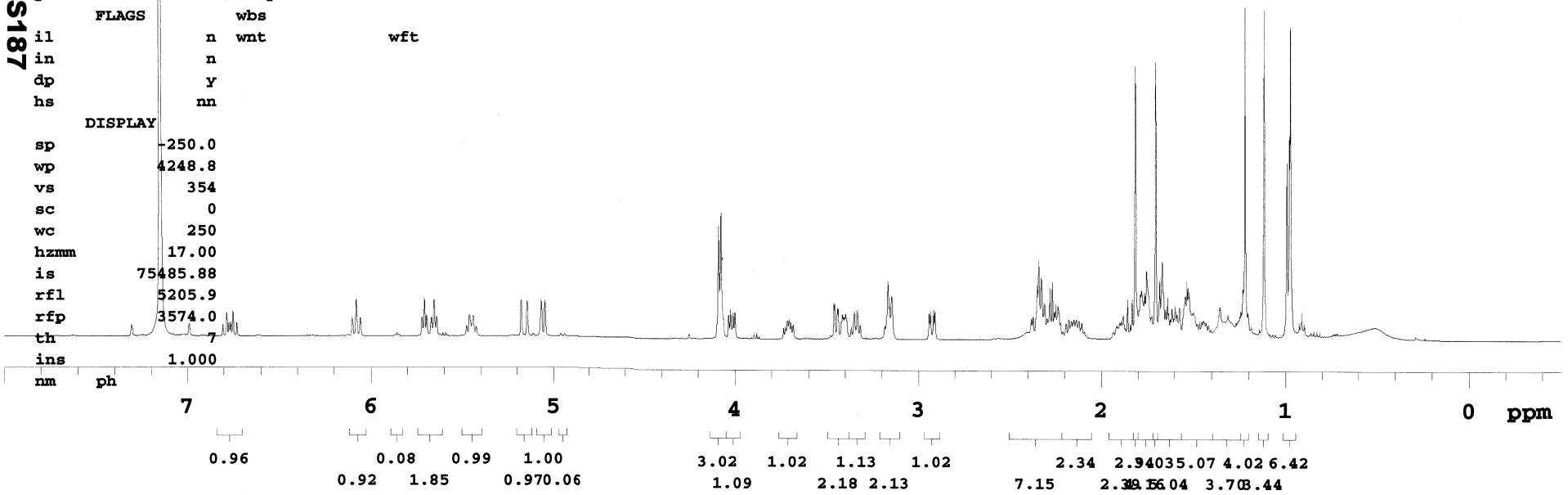
85

(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp1 s2pul

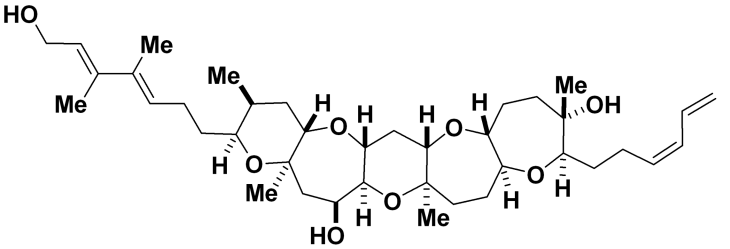
SAMPLE		DEC. & VT	
date	Jun 3 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	4248.8		
vs	354		
sc	0		
wc	250		
hzmm	17.00		
is	75485.88		
rfl	5205.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		



STANDARD CARBON PARAMETERS

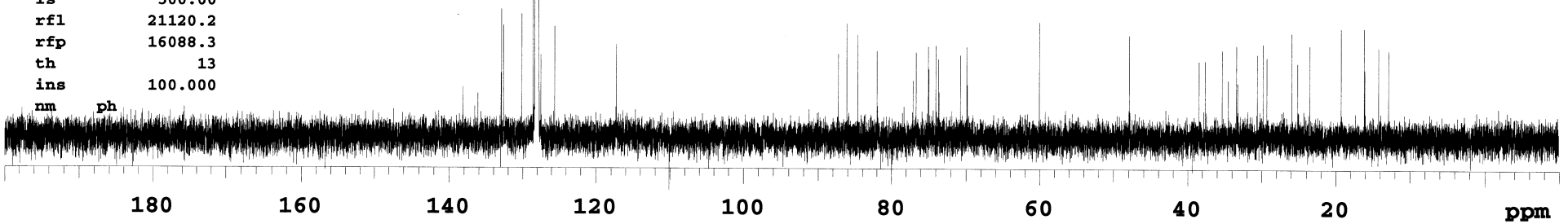
exp5 s2pul

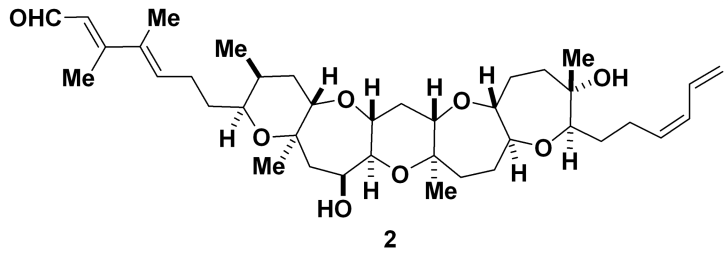
SAMPLE		DEC. & VT	
date	Jun 3 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	32	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	5120	fn	131072
ct	2432	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	1536		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21120.2		
rfp	16088.3		
th	13		
ins	100.000		
nm	ph		



85

(125 MHz, C_6D_6)





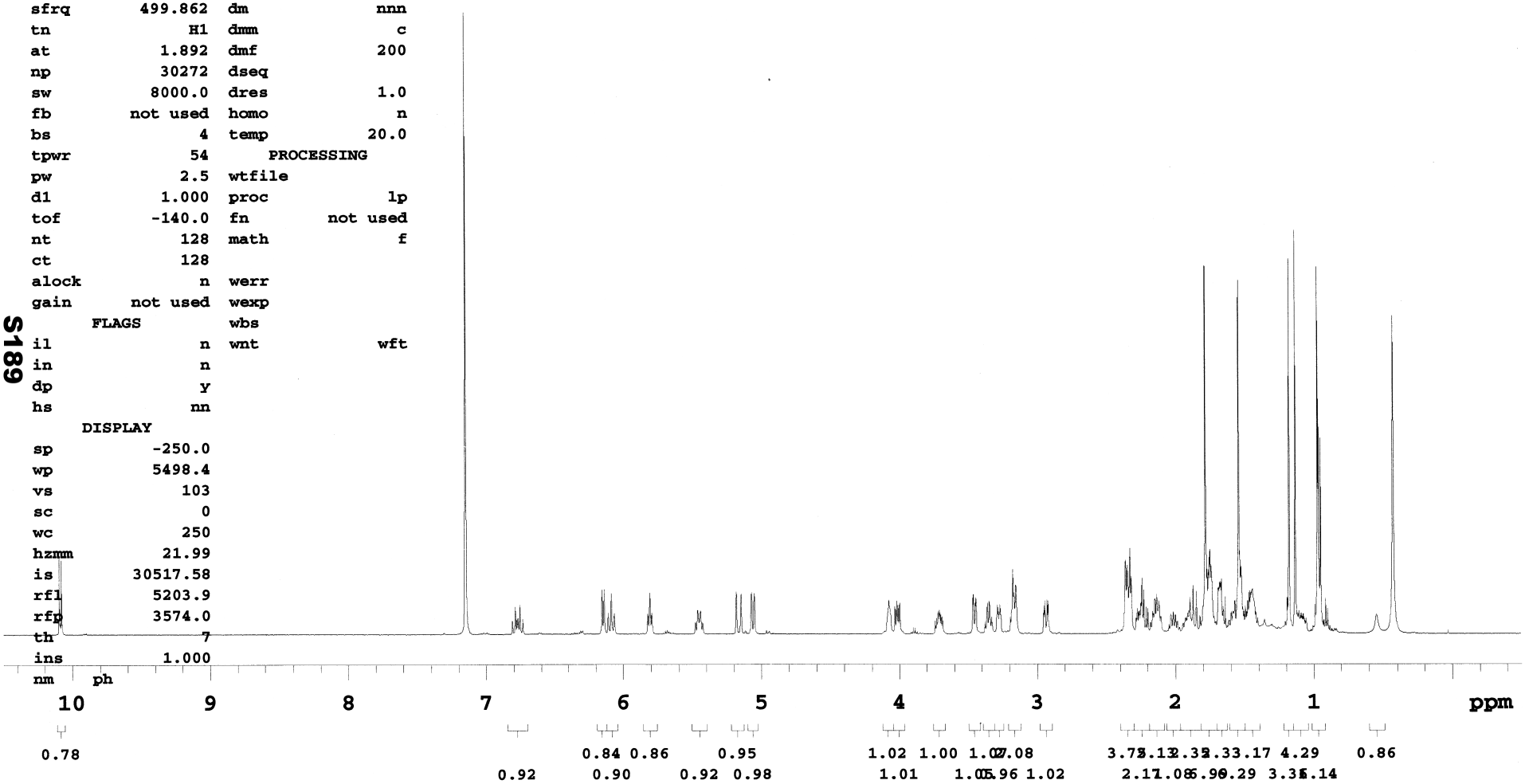
2

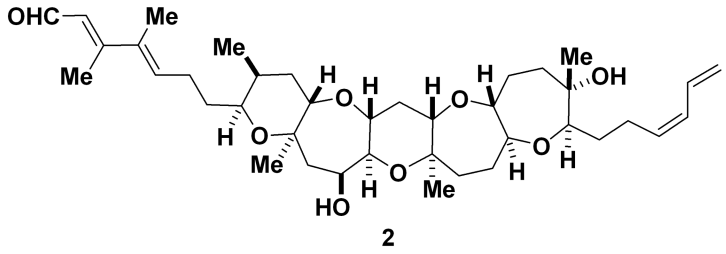
(500 MHz, C_6D_6)

STANDARD PROTON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Jun 19 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	499.862	dm	nnn
tn	H1	dmm	c
at	1.892	dmf	200
np	30272	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	4	temp	20.0
tpwr	54	PROCESSING	
pw	2.5	wtfile	
d1	1.000	proc	lp
tof	-140.0	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	wft
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-250.0		
wp	5498.4		
vs	103		
sc	0		
wc	250		
hzmm	21.99		
is	30517.58		
rfl	5203.9		
rfp	3574.0		
th	7		
ins	1.000		
nm	ph		

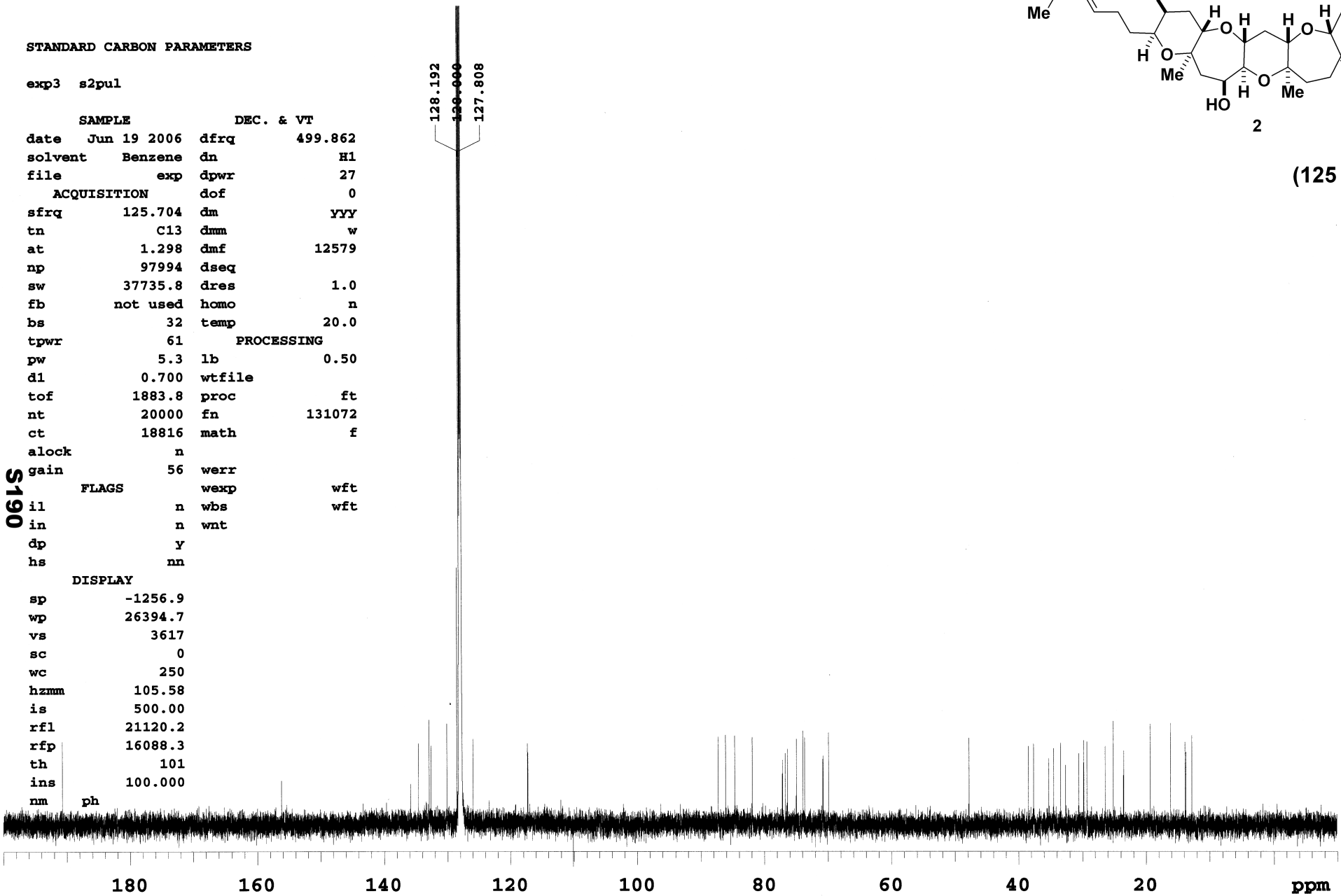




(125 MHz, C_6D_6)

S190

STANDARD CARBON PARAMETERS

exp3 s2pul

SAMPLE		DEC. & VT	
date	Jun 19 2006	dfrq	499.862
solvent	Benzene	dn	H1
file	exp	dpwr	27
ACQUISITION		dof	0
sfrq	125.704	dm	yyy
tn	C13	dmm	w
at	1.298	dmf	12579
np	97994	dseq	
sw	37735.8	dres	1.0
fb	not used	homo	n
bs	32	temp	20.0
tpwr	61	PROCESSING	
pw	5.3	lb	0.50
d1	0.700	wtfile	
tof	1883.8	proc	ft
nt	20000	fn	131072
ct	18816	math	f
alock	n		
gain	56	werr	
FLAGS		wexp	wft
il	n	wbs	wft
in	n	wnt	
dp	y		
hs	nn		
DISPLAY			
sp	-1256.9		
wp	26394.7		
vs	3617		
sc	0		
wc	250		
hzmm	105.58		
is	500.00		
rfl	21120.2		
rfp	16088.3		
th	101		
ins	100.000		
nm	ph