

Supporting Information

TiCl₄-promoted Cyclization Reactions of Aminoacetals and Ethenetricarboxylates Leading to Nitrogen-containing Heterocycles

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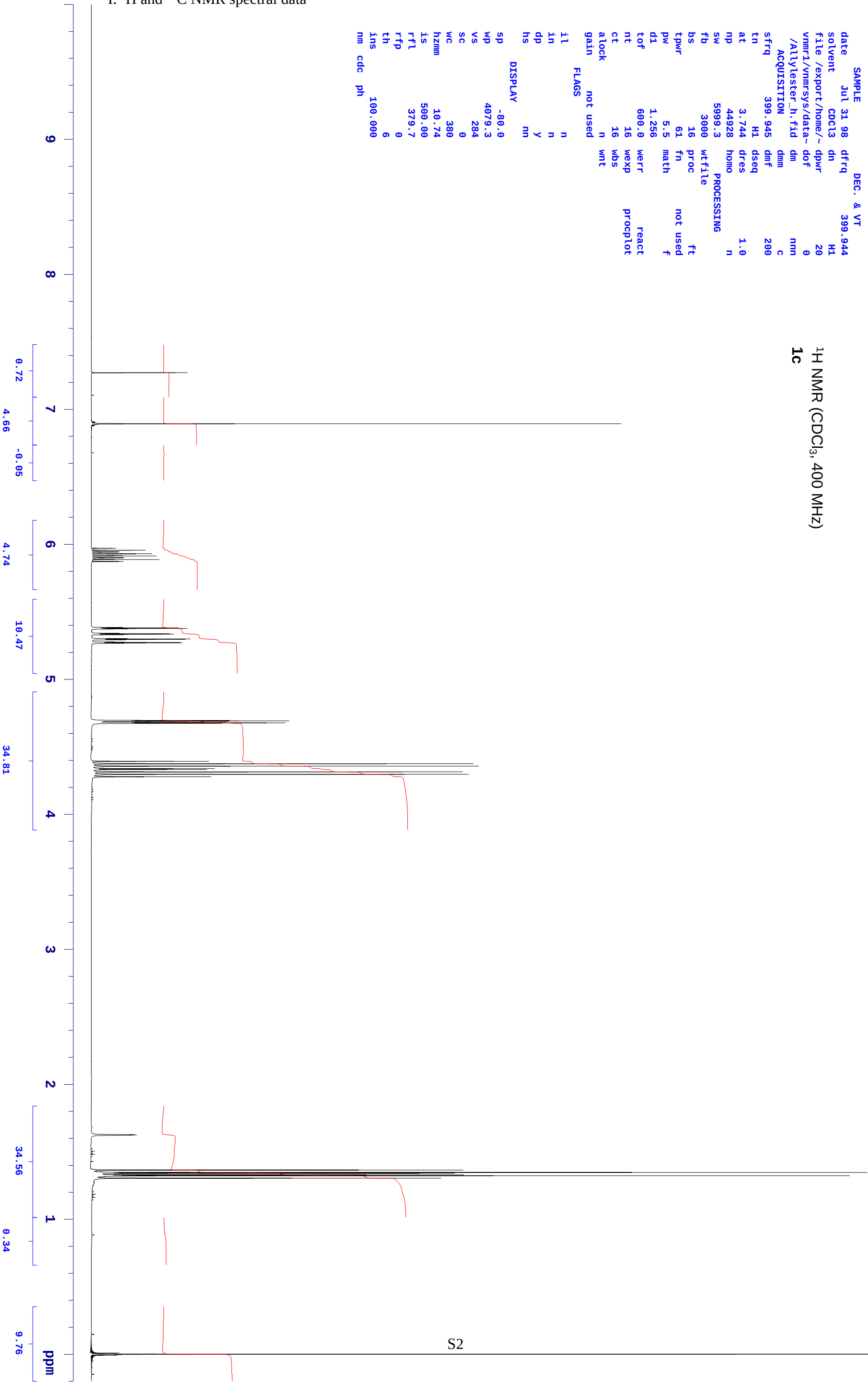
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Allylester_h

exp2 std1h

SAMPLE			DEC. & VT	
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tn	H1	dseq		
at	3.744	dres	1.0	
np	44928	homo	n	
sw	5999.3	PROCESSING		
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tpwr	61	fn	not used	
pw	5.5	math	f	
dl	1.256			
tof	600.0	werr	react	
nt	16	wexp	procp1ot	
ct	16	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nm			
DISPLAY				
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wp	4079.3			
vs	284			
sc	0			
wc	380			
hzmm	10.74			
is	500.00			
rfl	379.7			
rfp	0			
th	6			
ins	100.000			
nm	cdc	ph		

¹H NMR (CDCl₃, 400 MHz)
1c



I. ¹H and ¹³C NMR spectral data

Allylester_c

exp3 std13c

SAMPLE

DEC. & VT

date

Jul 31 98

dfrq

399.944

solvent

CDCl3

dn

H1

file

/export/home/~

dpwr

42

vmr1/vnmrsys/data-

dof

0

/Allylester_c.fid

dm

yyy

ACQUISITION

dm

w

sfrq

100.576

dmf

11056

tn

C13

dseq

garpl

at

1.199

dres

1.0

np

59968

homo

n

sw

25000.0

PROCESSING

fb

14000

lb

1.00

bs

16

wtfile

tpwr

50

proc

ft

pw

3.7

fn

not used

d1

0.801

math

f

tof

1000.0

nt

20000

werr

react

ct

20000

wexp

procplot

alock

n

wbs

gain

not used

wnt

FLAGS

il

n

in

n

dp

y

hs

nm

DISPLAY

sp

-1998.2

wp

24999.2

vs

322

sc

0

wc

380

hzmm

2.37

is

500.00

rfl

1999.0

rfp

0

th

17

ins

500.000

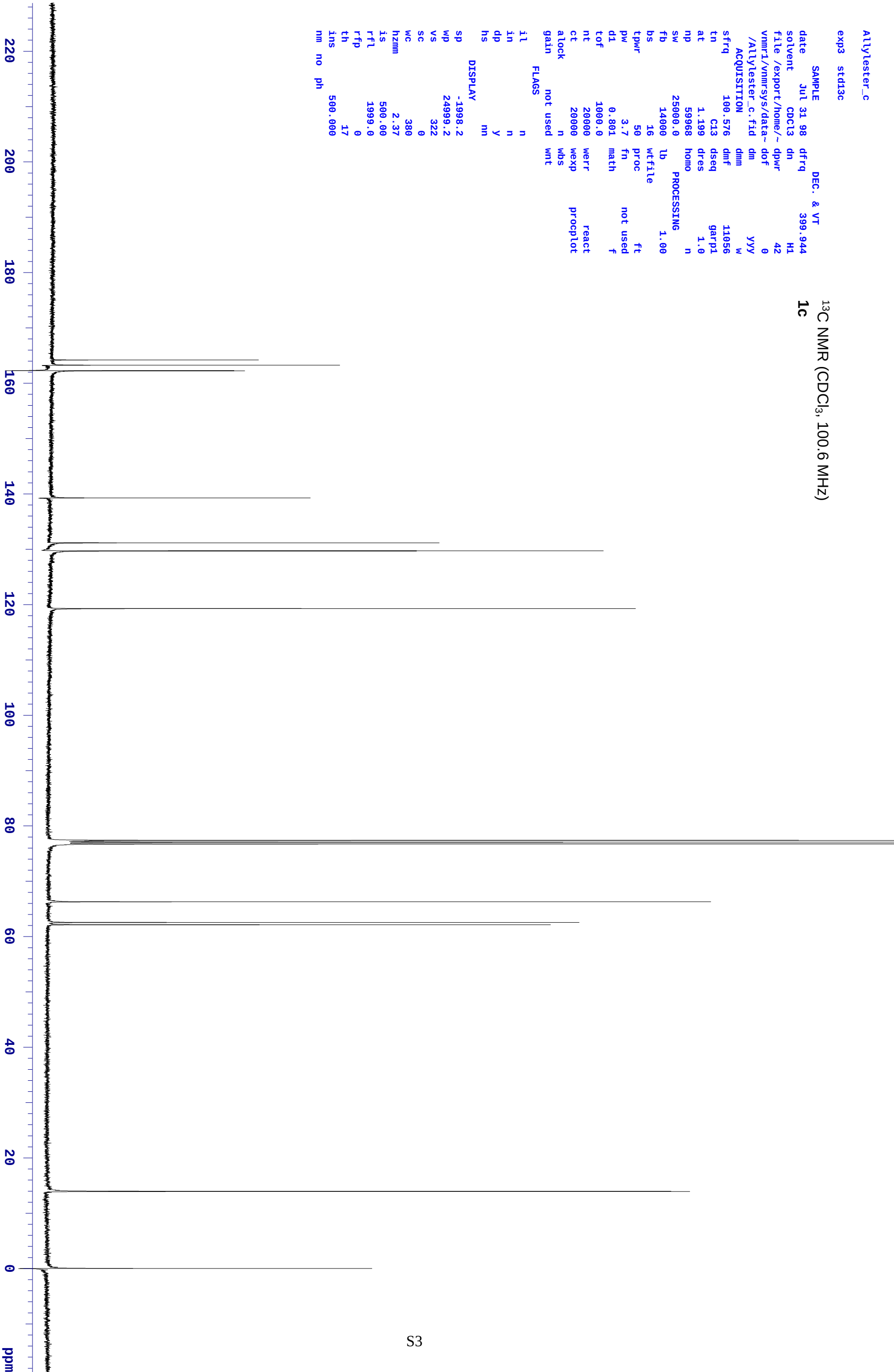
nm

no

ph

¹³C NMR (CDCl₃, 100.6 MHz)

1c

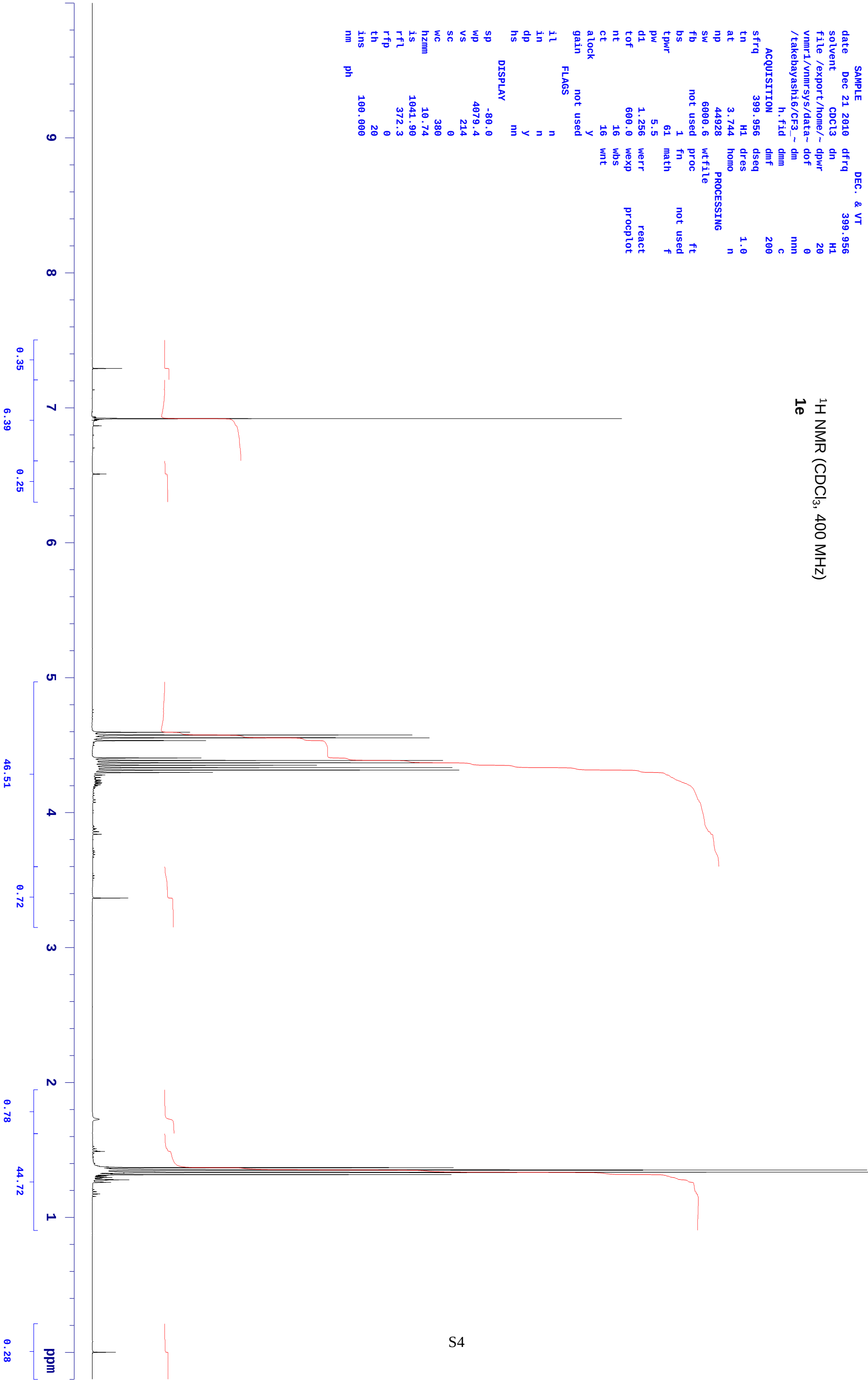


takebayashi6/CF3

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tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	6000.6	wtfile		
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bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	y			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.4			
vs	214			
sc	0			
wc	380			
h2mm	10.74			
is	1041.90			
rfl	372.3			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
1e



takebayashi6/CF3

exp11 std13c

SAMPLE

DEC. & VT

date

Dec 20 2010

dfrq

399.956

solvent

CDCl3

dn

H1

file

/export/home/~

dpwr

41

vnmr1/vnmrsys/data~

dof

0

/takebayashi6/CF3_~

dm

yyy

c.fid

dmn

w

ACQUISITION

dmf

10400

sfrq

100.579

dseq

garpl

tn

C13

dres

1.0

at

1.199

homo

n

np

59968

PROCESSING

sw

25000.0

lb

1.00

fb

not used

wfile

bs

16

proc

ft

tpwr

56

fn

not used

pw

5.0

math

f

d1

0.801

tof

1000.0

werr

react

nt

2048

wexp

procplot

ct

2048

wbs

alock

n

wnt

gain

not used

FLAGS

il

n

in

n

dp

y

hs

nn

DISPLAY

sp

-1395.0

wp

24999.2

vs

214

sc

0

wc

380

h2mm

2.57

is

500.00

rfl

9749.6

rfp

7753.8

th

6

ins

500.000

nm

no

ph

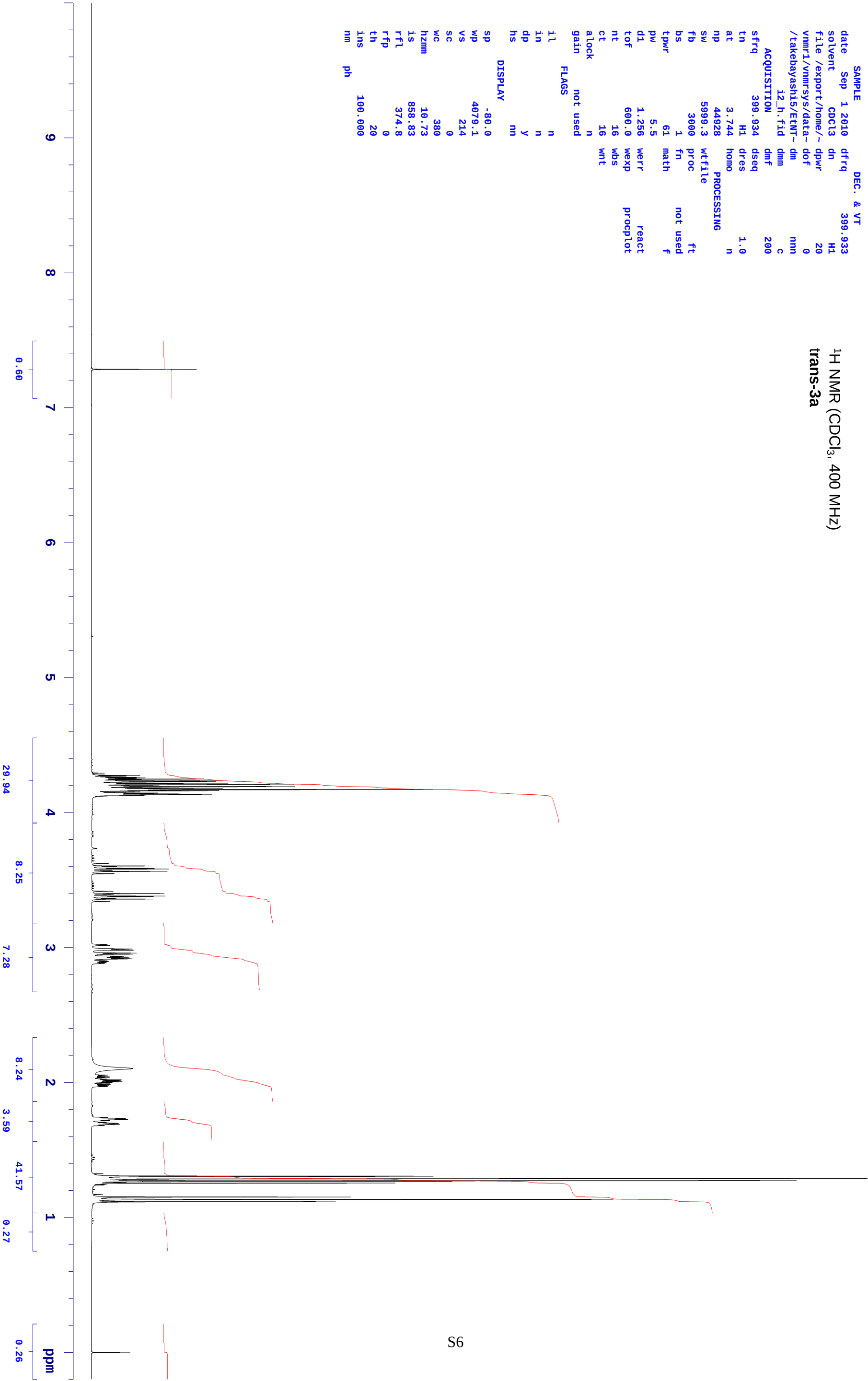
¹³C NMR (CDCl₃, 100.6 MHz)
1e



exp10 std1h

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tn	H1	dres	1.0		
at	3.744	homo	n		
np	44928	PROCESSING			
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fb	3000	proc	ft		
bs	1	fn	not used		
tpwr	61	math	f		
pw	5.5				
d1	1.256	werr	react		
tof	600.0	wexp	procp1ot		
nt	16	wbs			
ct	16	wnt			
alock	n				
gain	not used				
FLAGS					
il	n				
in	n				
dp	y				
hs	nn				
DISPLAY					
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wp	4079.1				
vs	214				
sc	0				
wc	380				
h2mm	10.73				
is	858.83				
rfl	374.8				
rfp	0				
th	20				
ins	100.000				
nm	ph				

¹H NMR (CDCl₃, 400 MHz)
trans-3a



exp10 std13c

SAMPLE

DEC. & VT

date

Sep 1 2010

dfrq

399.933

solvent

CDCl3

dn

H1

file

/export/home/~

dpwr

41

vmr1/vnmrsys/data~

dof

0

/takebayashi5/EtNT~

dm

yyy

i2.c.fid

dmn

w

ACQUISITION

sfrq

100.573

dseq

10400

tn

C13

dres

garpl

at

1.199

homo

1.0

np

59968

sw

25000.0

lb

PROCESSING

fb

14000

wtfile

1.00

bs

16

proc

ft

tpwr

57

fn

not used

pw

7.5

math

f

d1

0.801

tof

1000.0

werr

react

nt

1024

wexp

procplot

ct

1024

wbs

alock

n

wnt

gain

not used

FLAGS

il

n

in

n

dp

y

hs

nn

DISPLAY

sp

-1395.0

wp

24999.2

vs

214

sc

0

wc

380

h2mm

3.17

is

500.00

rfl

9749.1

rfp

7753.4

th

24

ins

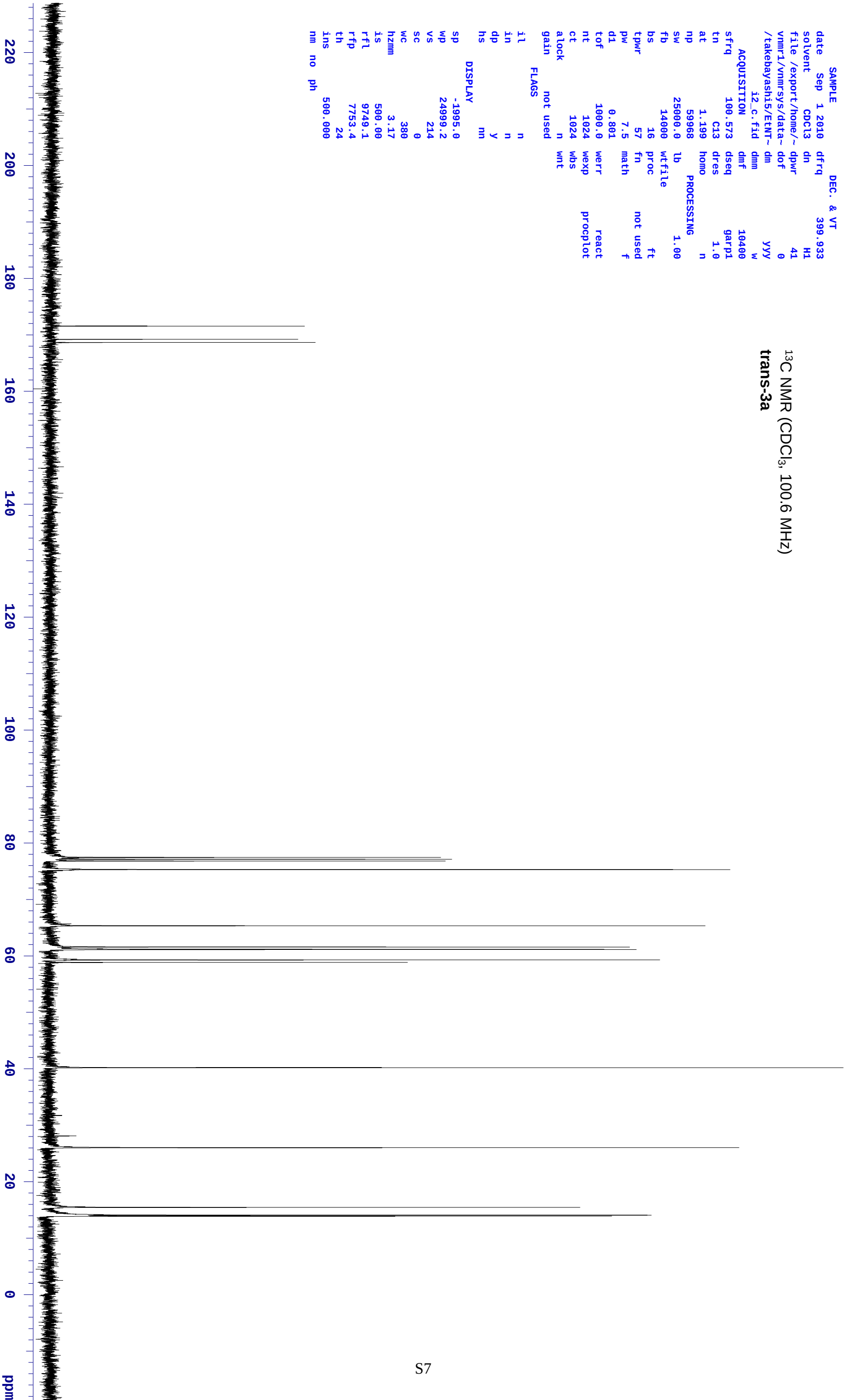
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nm

no

ph

¹³C NMR (CDCl₃, 100.6 MHz)
trans-3a

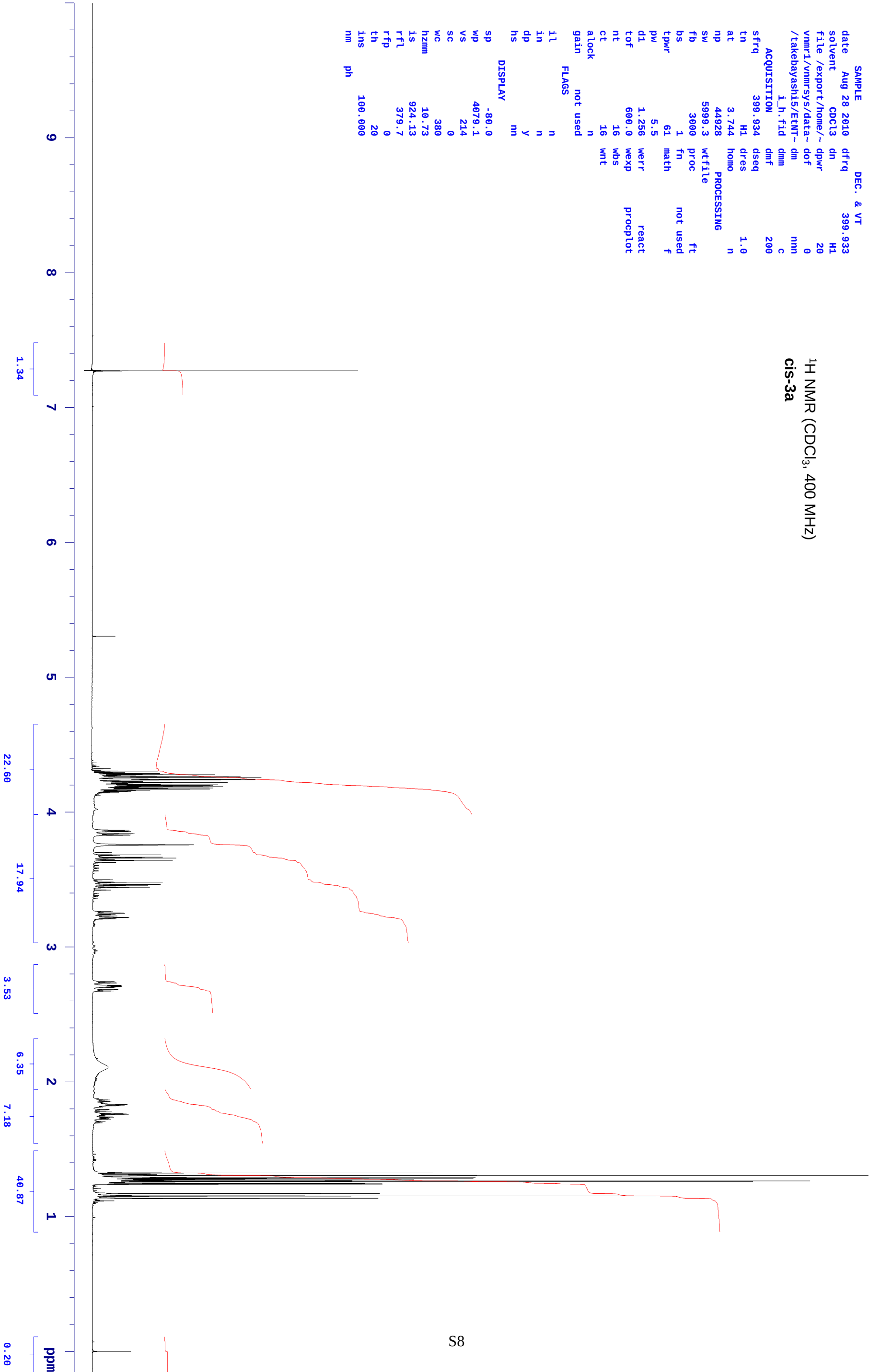


takebayash15/ETNT1

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/takebayash15/ETNT~	dm		nnn	
i_h.fid	dmm		c	
ACQUISITION				
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tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile		
fb	3000	proc	ft	
bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
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is	924.13			
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th	20			
ins	100.000			
nm	ph			

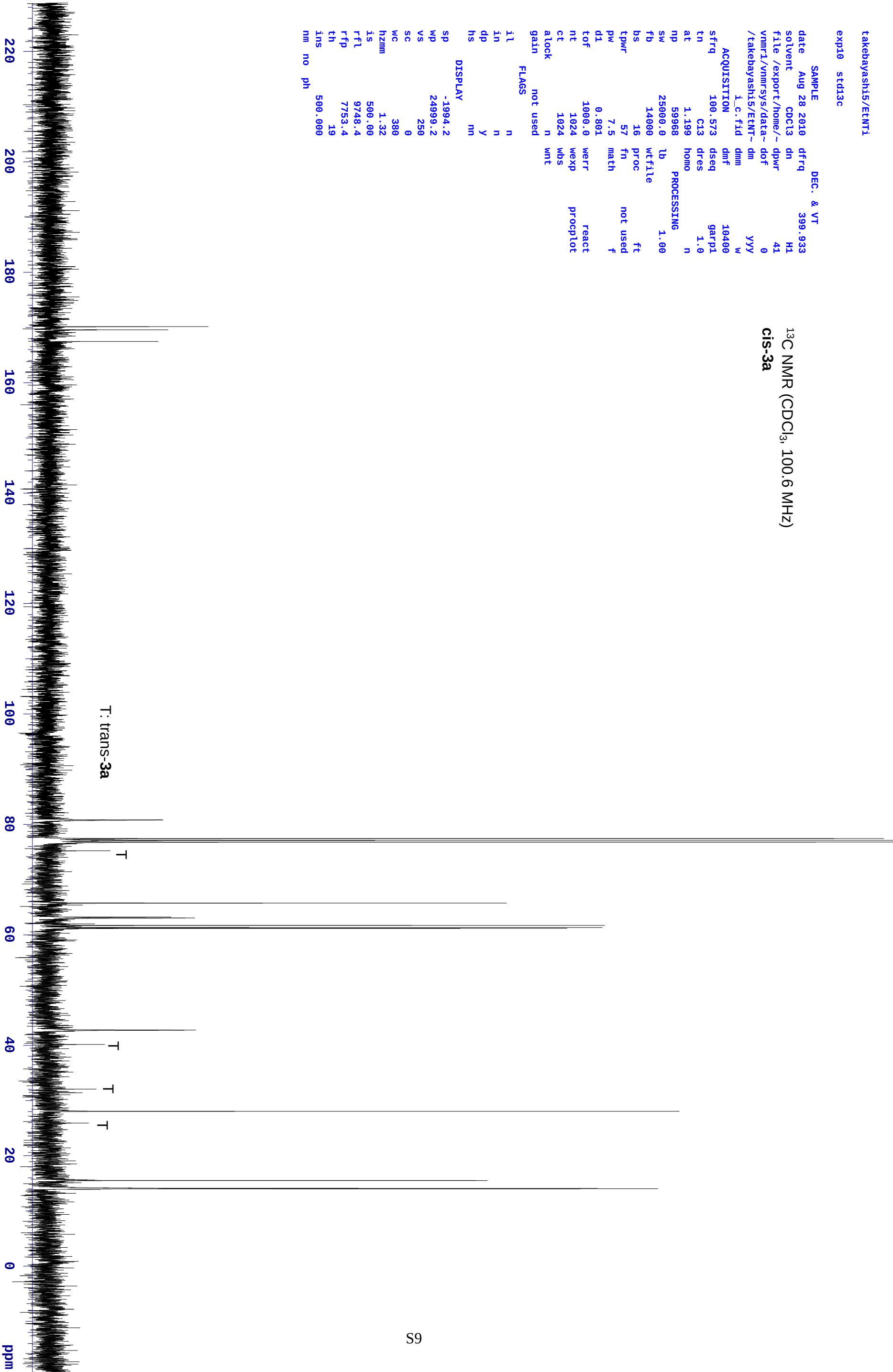
¹H NMR (CDCl₃, 400 MHz)
cis-3a



exp10 std13c

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	i_c.fid	dmm	w	
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tn	C13	dres	garpl	
at	1.199	homo	n	
np	59968	PROCESSING		
sw	25000.0	lb	1.00	
fb	14000	wtfile		
bs	16	proc	ft	
tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	1024	wexp	procplot	
ct	1024	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
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wp	24999.2			
vs	250			
sc	0			
wc	380			
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th	19			
ins	500.000			
nm	no	ph		

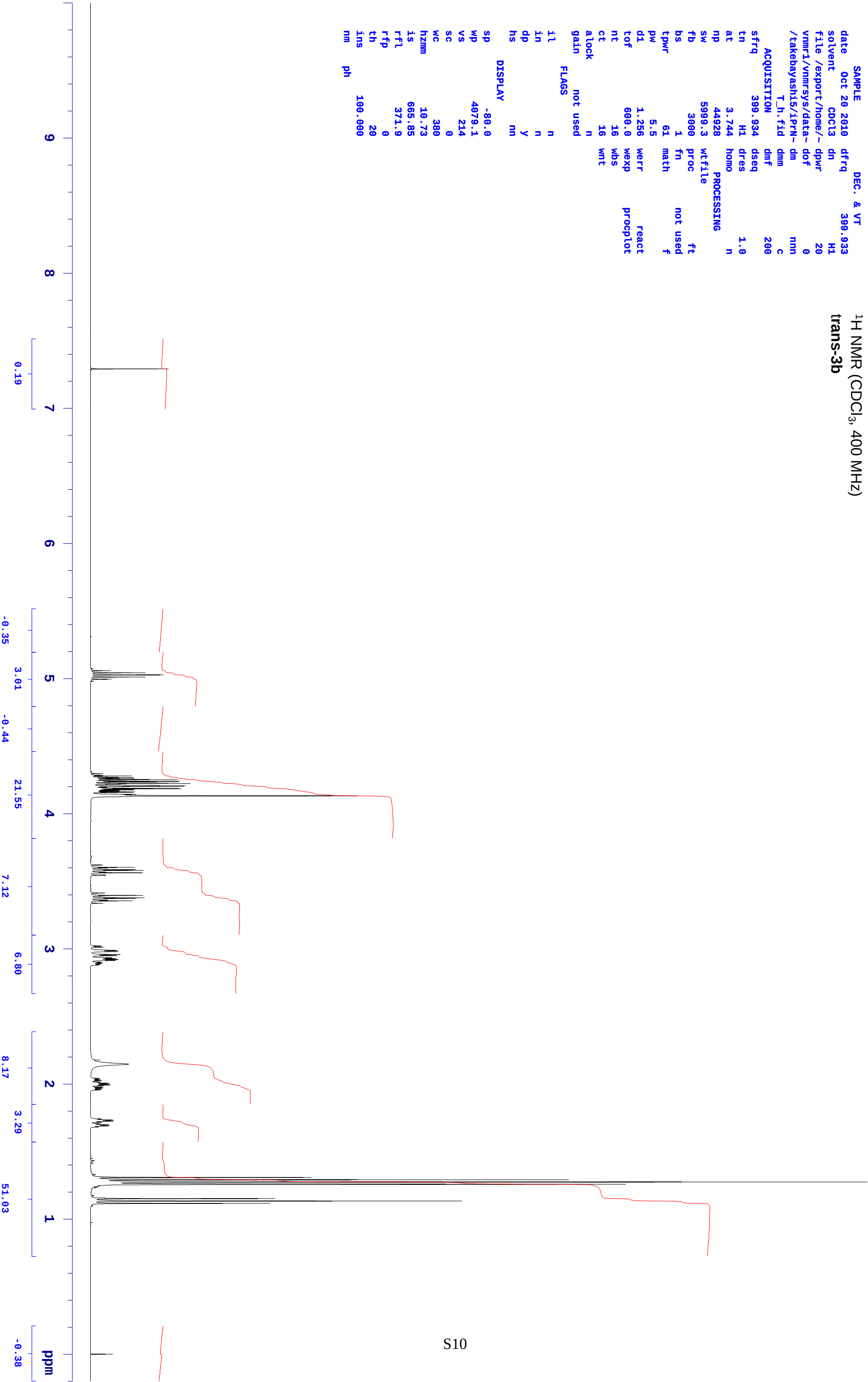
¹³C NMR (CDCl₃, 100.6 MHz)
cis-3a



exp10 std1h

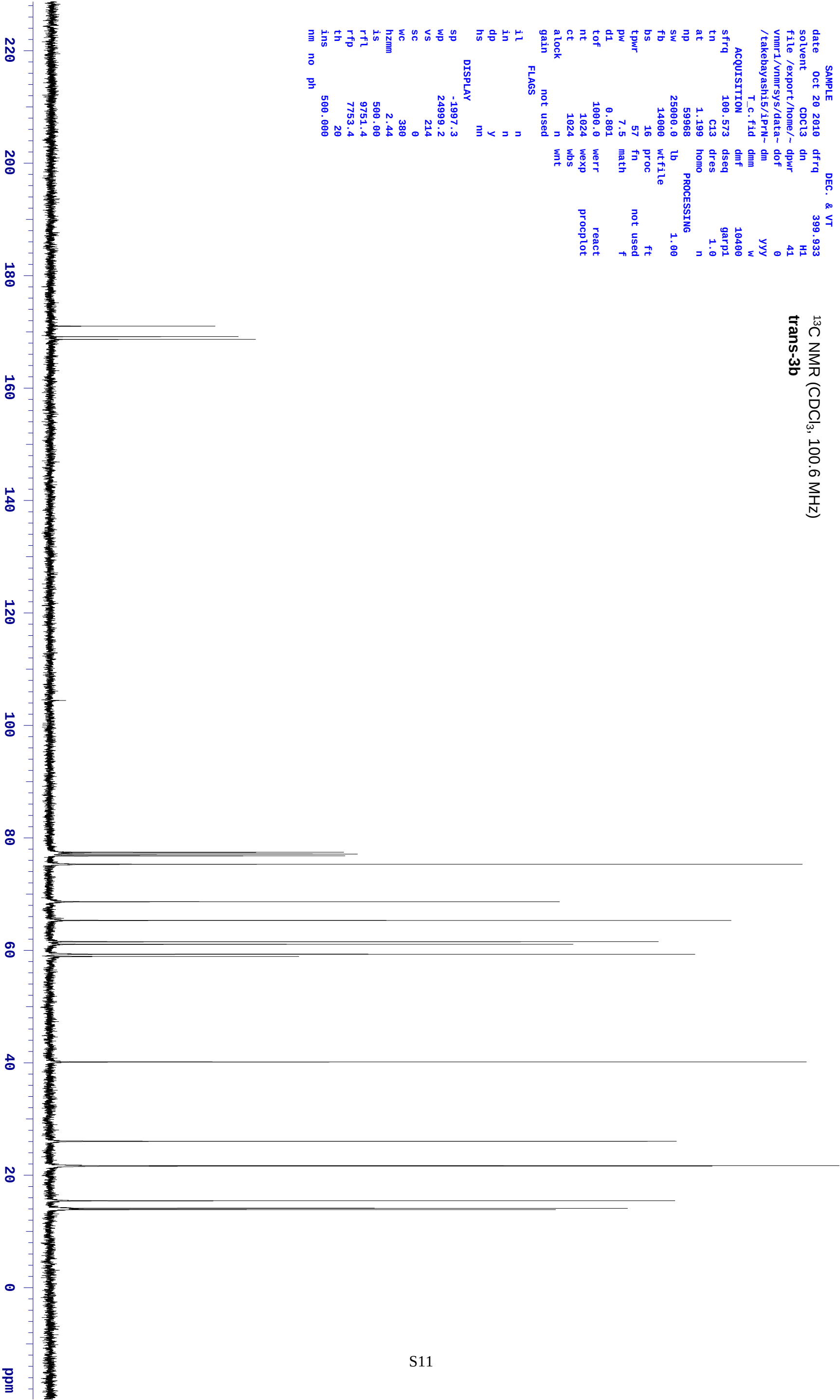
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T_h.fid	dmm		c	
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tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile	ft	
fb	3000	proc	not used	
bs	1	fn	f	
tpwr	61	math		
pw	5.5			
dl	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
h2mm	10.73			
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rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
trans-3b



SAMPLE			DEC. & VT	
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/takebayashi5/1PrN~	dm		yyy	
T_c.fid		dmm	w	
ACQUISITION				
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tn	C13	dres	garpl	
at	1.199	homo	n	
np	59968	PROCESSING		
sw	25000.0	lb	1.00	
fb	14000	wtfile		
bs	16	proc	ft	
tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	1024	wexp	procplot	
ct	1024	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-1997.3			
wp	24999.2			
vs	214			
sc	0			
wc	380			
h2mm	2.44			
is	500.00			
rfl	9751.4			
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th	20			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
trans-3b

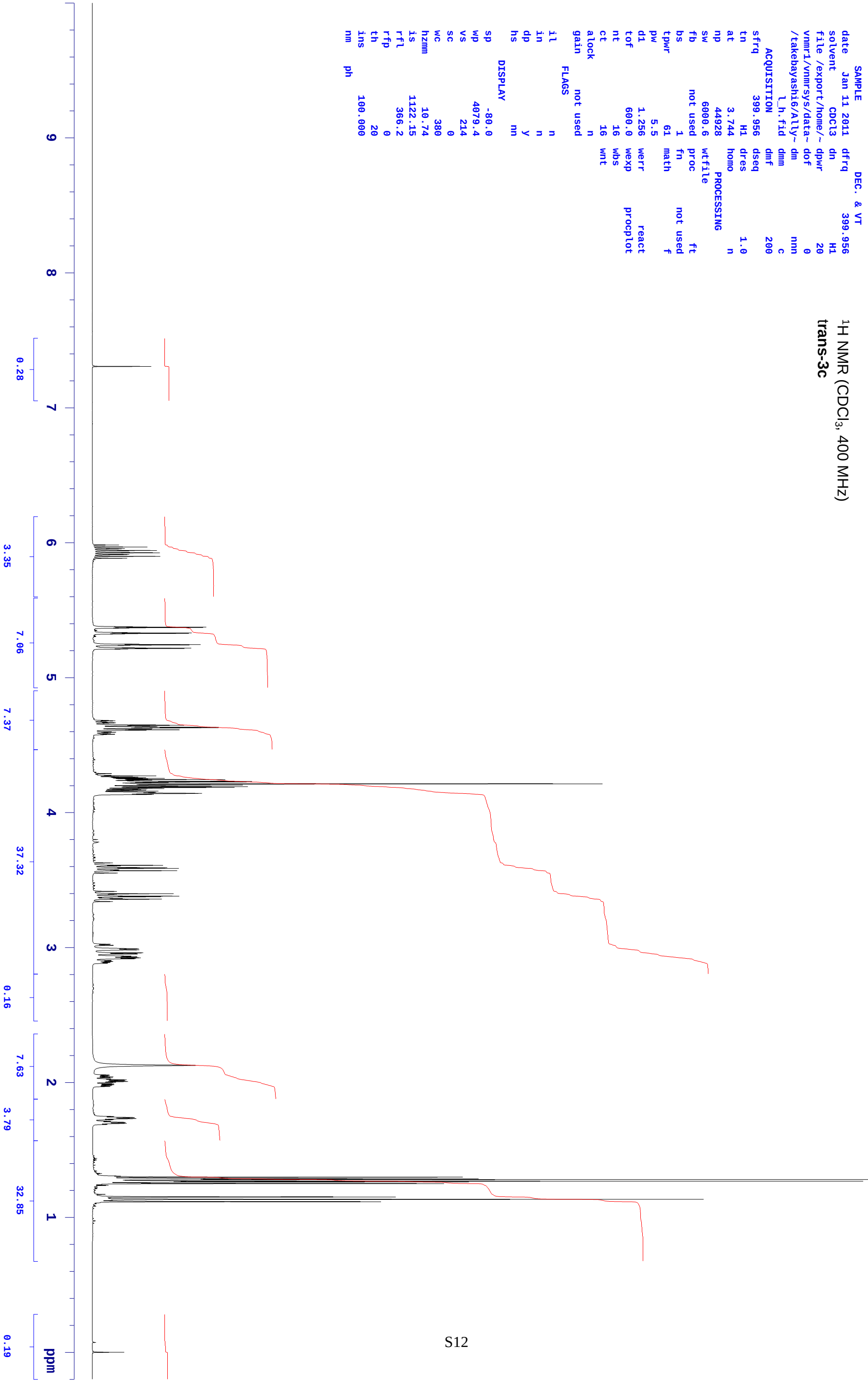


takebayashi6/Allyl

exp10 std1h

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at	3.744	homo	n	
np	44928	PROCESSING		
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fb	not used	proc	ft	
bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.4			
vs	214			
sc	0			
wc	380			
h2mm	10.74			
is	1122.15			
rfl	366.2			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
trans-3c

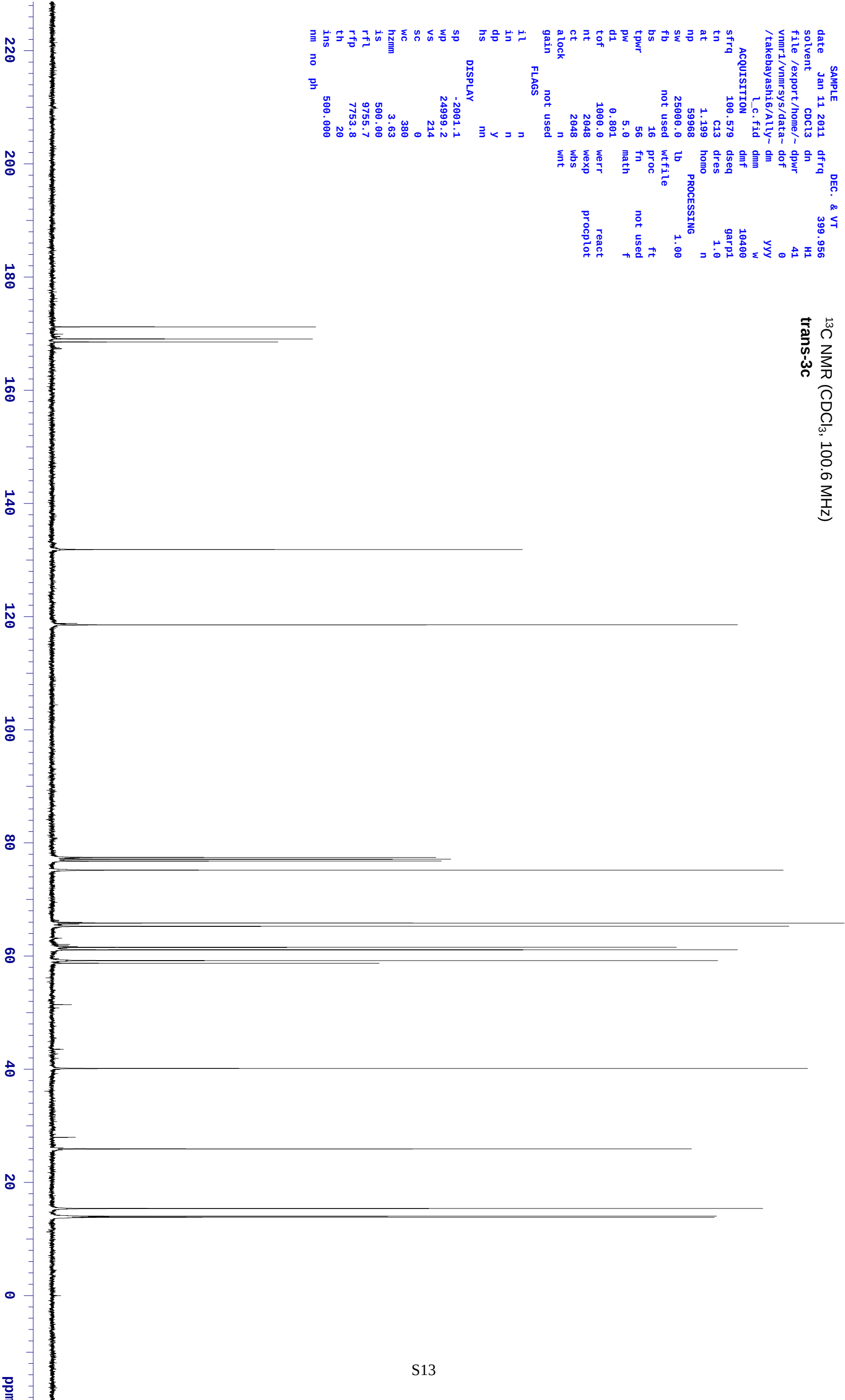


takebayashi6/Allyl

exp10 std13c

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	l_c.fid	dmm	w	
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sfrq	100.579	dseq	10400	
tn	C13	dres	garpl	
at	1.199	homo	1.0	
np	59968		n	
sw	25000.0	lb	PROCESSING	
fb	not used	wtfile	1.00	
bs	16	proc	ft	
tpwr	56	fn	not used	
pw	5.0	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	2048	wexp	procplot	
ct	2048	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-2001.1			
wp	24999.2			
vs	214			
sc	0			
wc	380			
h2mm	3.63			
is	500.00			
rfl	9755.7			
rfp	7753.8			
th	20			
ins	500.000			
nm	no	ph		

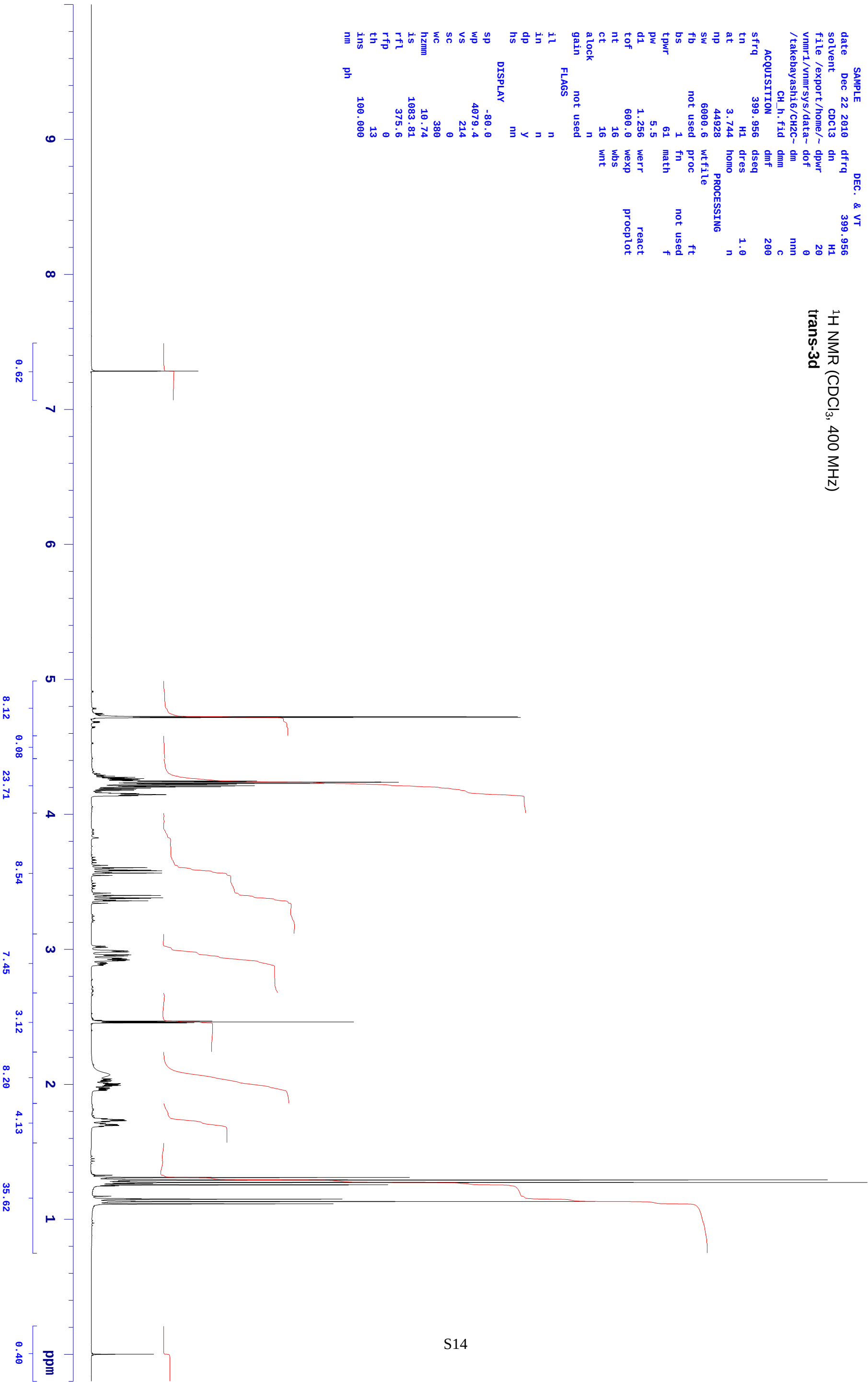
¹³C NMR (CDCl₃, 100.6 MHz)
trans-3c



takebayashi6/CH2CCH

exp10 std1h

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vnmr1/vnmrfs/data~	dof 0
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CH_h.fid	dmm C
ACQUISITION	
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tn H1	dres 1.0
at 3.744	homo n
np 44928	PROCESSING
sw 6000.6	wfile
fb not used	proc
bs 1	fn not used
tpwr 61	math f
pw 5.5	
d1 1.256	werr react
tof 600.0	wexp procplo
nt 16	wbs
ct 16	wnt
alock n	
gain not used	
FLAGS	
il n	
in n	
dp y	
hs nn	
DISPLAY	
sp -80.0	
wp 4079.4	
vs 214	
sc 0	
wc 380	
h2mm 10.74	
is 1083.81	
rfl 375.6	
rfp 0	
th 13	
ins 100.000	
nm	
ph	

¹H NMR (CDCl₃, 400 MHz)
trans-3d

takebayashi6/CH2CCH

exp10 std13c

SAMPLE

DEC. & VT

date

Dec 22 2010

dfrq

399.956

solvent

CDCl3

dn

H1

file

/export/home/~

dpwr

41

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dof

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/takebayashi6/CH2C~

dm

yyy

CH_c.fid

dmn

w

ACQUISITION

sfrq

100.579

dseq

10400

tn

C13

dres

garpl

at

1.199

homo

1.0

np

59968

PROCESSING

n

sw

25000.0

lb

1.00

fb

not used

wfile

bs

16

proc

ft

tpwr

56

fn

not used

pw

5.0

math

f

d1

0.801

tof

1000.0

werr

react

nt

2048

wexp

procplot

ct

2048

wbs

alock

n

wnt

gain

not used

FLAGS

il

n

in

n

dp

y

hs

nn

DISPLAY

sp

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wp

24999.2

vs

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h2mm

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rfl

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rfp

7753.8

th

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ins

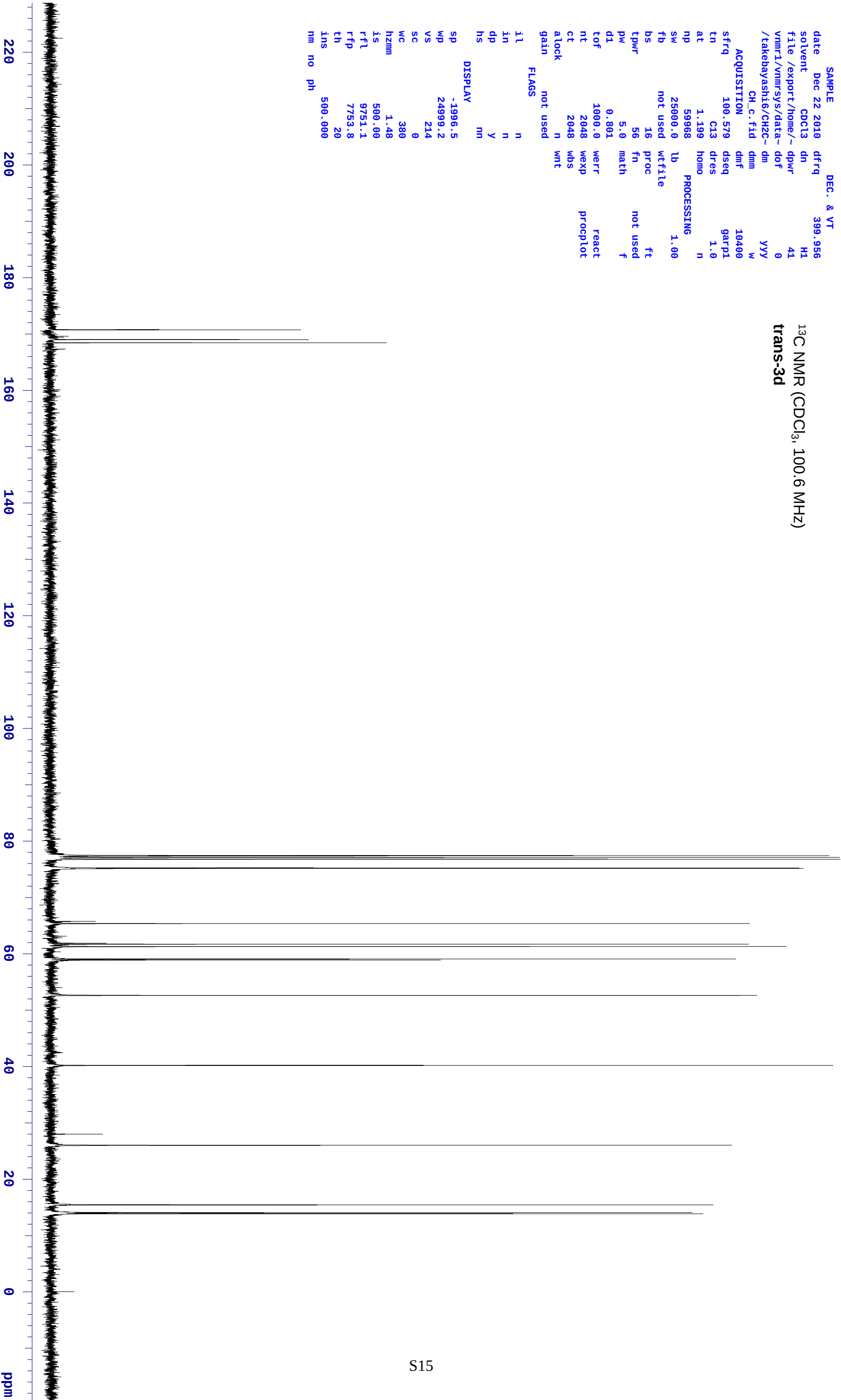
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nm

no

ph

¹³C NMR (CDCl₃, 100.6 MHz)
trans-3d

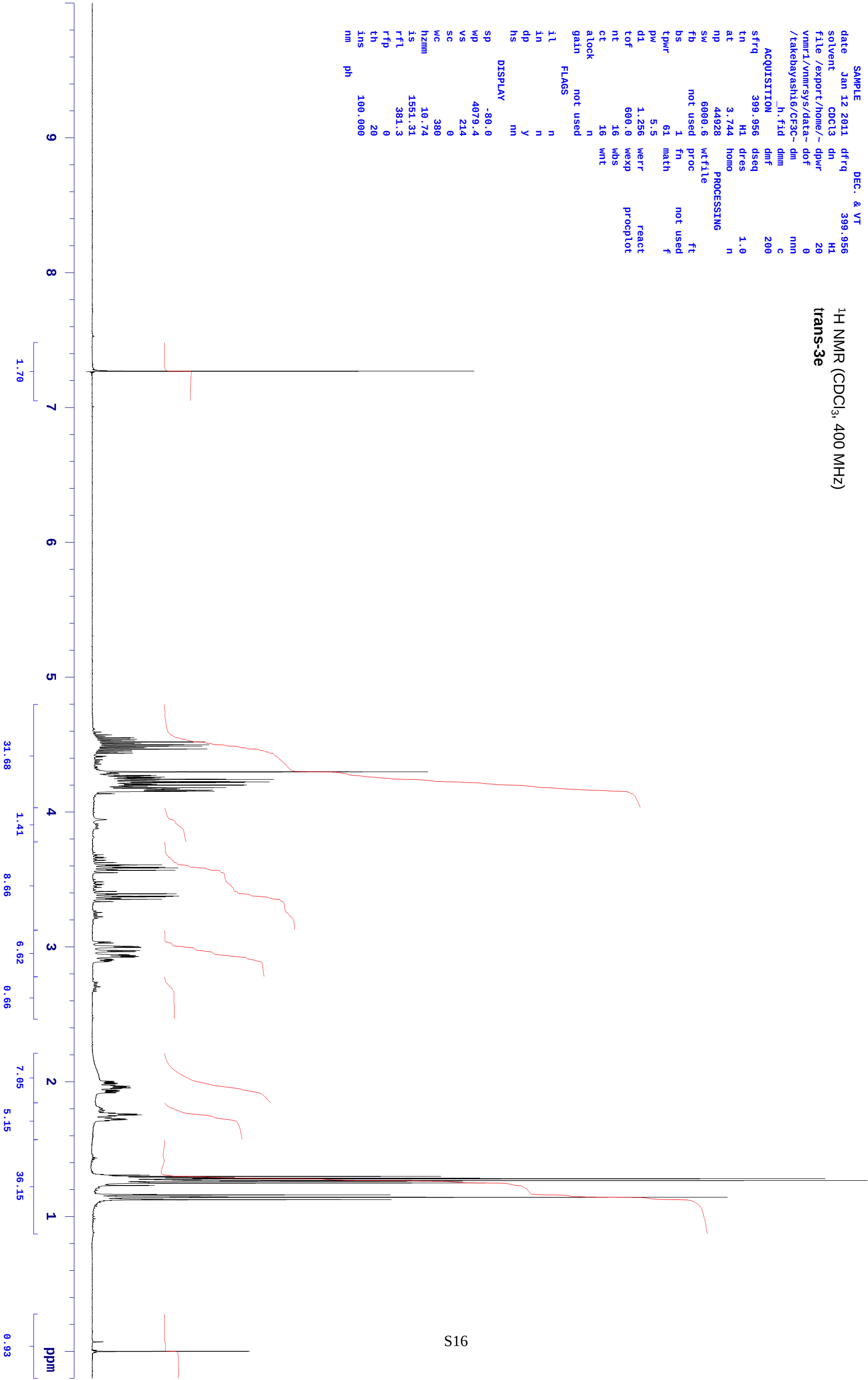


tkebayashi6/CF3C

exp10 std1h

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_h.fid		dmn	c	
ACQUISITION		dmf	200	
sfrq	399.956	dseq		
tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	6000.6	wtfile		
fb	not used	proc	ft	
bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.4			
vs	214			
sc	0			
wc	380			
h2mm	10.74			
is	1551.31			
rfl	381.3			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
trans-3e

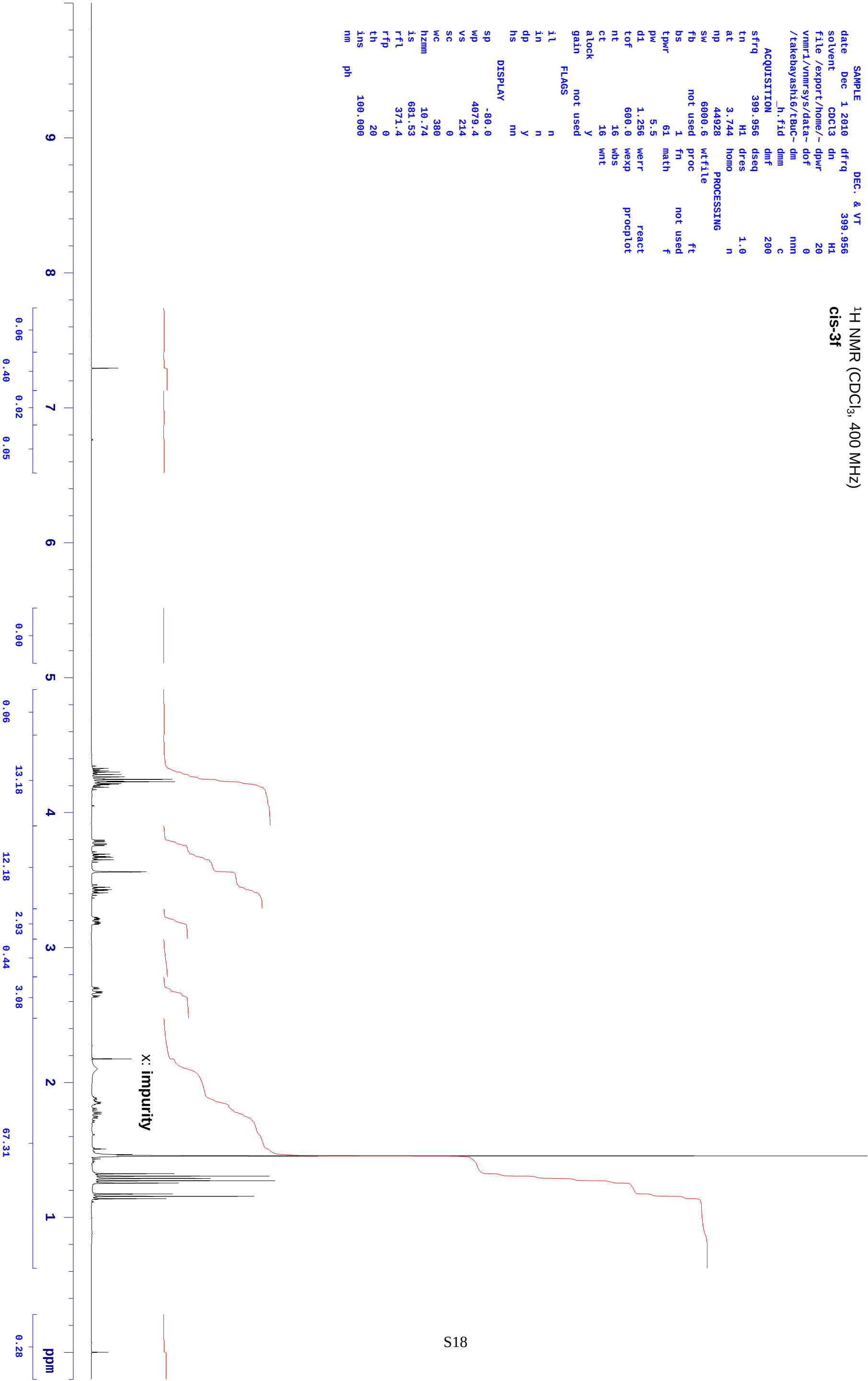


takebayashi6/tBUC

exp10 std1h

SAMPLE			DEC. & VT		
date	Dec 1 2010	dfreq	399.956		
solvent	CDCl3	dn	H1		
file	/export/home/~	dpwr	20		
vmr1/vnmrsys/data~	do		0		
/takebayashi6/tBUC~	dm		nnn		
	h.fid	dmn	c		
ACQUISITION					
sfrq	399.956	dseq	200		
tn	H1	dres	1.0		
at	3.744	homo	n		
np	44928	PROCESSING			
sw	6000.6	wtfile			
fb	not used	proc	ft		
bs	1	fn	not used		
tpwr	61	math	f		
pw	5.5				
d1	1.256	werr	react		
tof	600.0	wexp	procp1ot		
nt	16	wbs			
ct	16	wnt			
alock	y				
gain	not used				
FLAGS					
il	n				
in	n				
dp	y				
hs	nn				
DISPLAY					
sp	-80.0				
wp	4079.4				
vs	214				
sc	0				
wc	380				
h2mm	10.74				
is	681.53				
rfl	371.4				
rfp	0				
th	20				
ins	100.000				
nm	ph				

¹H NMR (CDCl₃, 400 MHz)
cis-3f

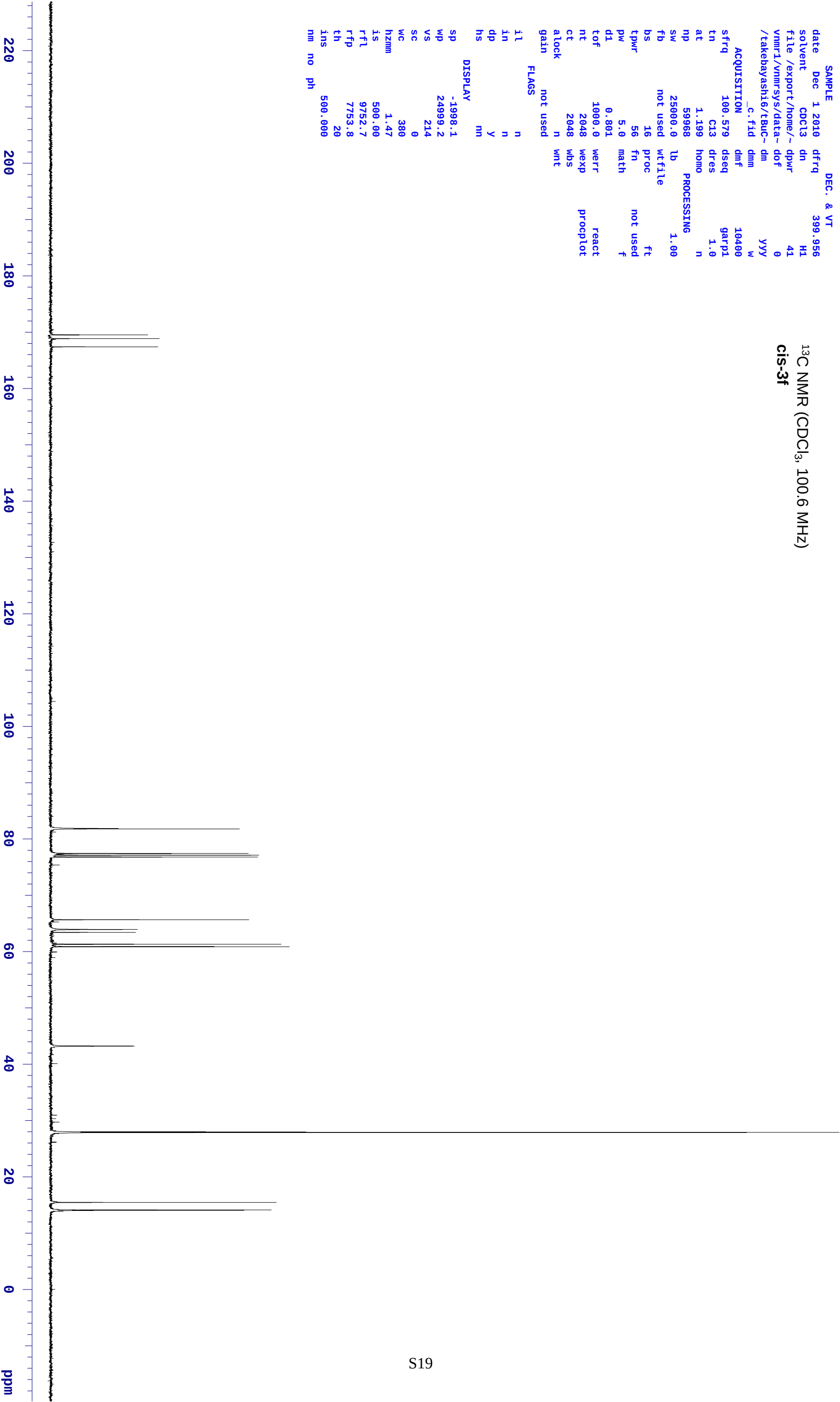


takebayashi6/tBUC

exp10 std13c

SAMPLE			DEC. & VT		
date	Dec 1 2010	dfrq	399.956		
solvent	CDCl3	dn	H1		
file	/export/home/~	dpwr	41		
vmr1/vnmrsys/data~	dof		0		
/takebayashi6/tBUC~	dm		yyy		
	~c.fid	dmm	w		
ACQUISITION					
sfrq	100.579	dmsq	10400		
tn	C13	dres	garpl		
at	1.199	homo	n		
np	59968	PROCESSING			
sw	25000.0	lb	1.00		
fb	not used	wfile			
bs	16	proc	ft		
tpwr	56	fn	not used		
pw	5.0	math	f		
d1	0.801				
tof	1000.0	werr	react		
nt	2048	wexp	procplot		
ct	2048	wbs			
alock	n	wnt			
gain	not used				
FLAGS					
il	n				
in	n				
dp	y				
hs	nn				
DISPLAY					
sp	-1398.1				
wp	24999.2				
vs	214				
sc	0				
wc	380				
h2mm	1.47				
is	500.00				
rfl	9752.7				
rfp	7753.8				
th	20				
ins	500.000				
nm	no	ph			

¹³C NMR (CDCl₃, 100.6 MHz)
cis-3f

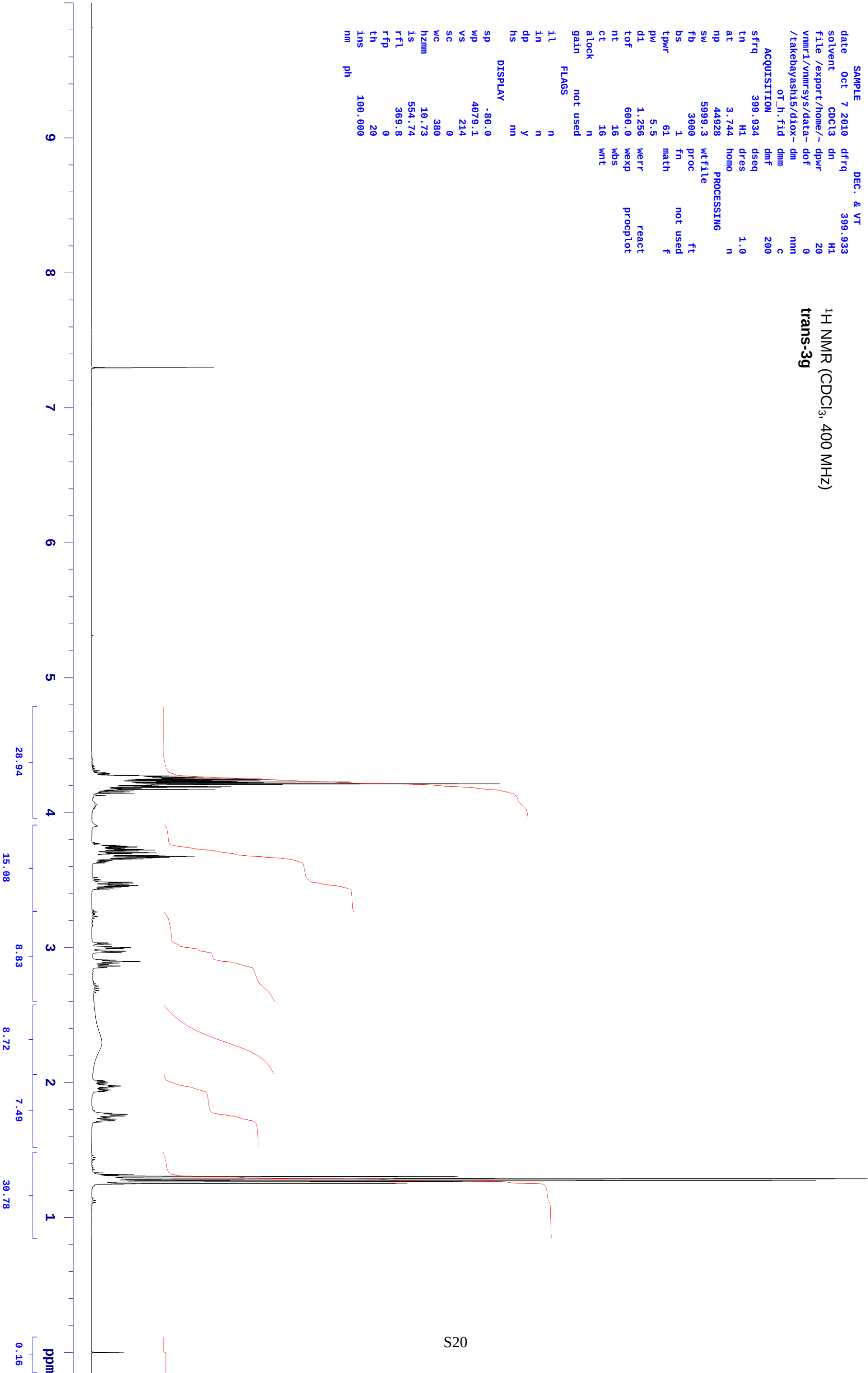


takebayashis/dioxoT

exp10 std1h

SAMPLE			DEC. & VT	
date	Oct 7 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	20	
vnmr1/vnmrsys/data~	dof		0	
/takebayashis/diox~	dm		nnn	
ot_h.fid	dmm		c	
ACQUISITION				
sfrq	399.934	dseq	200	
tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile		
fb	3000	proc	ft	
bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
h2mm	10.73			
is	554.74			
rfl	369.8			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
trans-3g

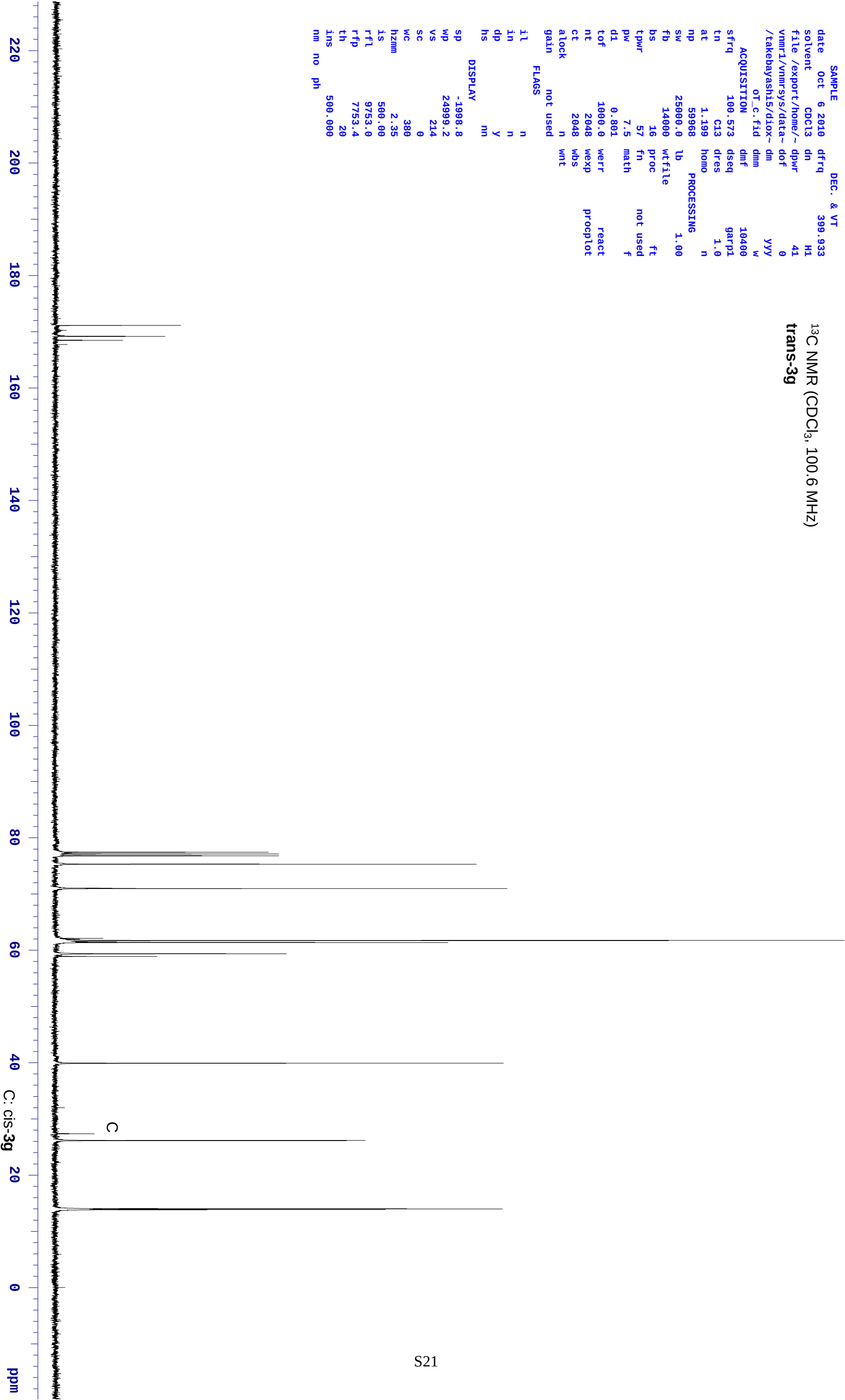


takebayashi5/dioxoT

exp10 std13c

SAMPLE			DEC. & VT	
date	Oct 6 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	41	
vmr1/vnmrsys/data~	dof		0	
/takebayashi5/diox~	dm		yyy	
ot_c.fid	dmm		w	
ACQUISITION				
sfrq	100.573	dmsf	10400	
tn	C13	dres	garpl	
at	1.199	homo	1.0	
np	59968	PROCESSING		
sw	25000.0	lb	1.00	
fb	14000	wtfile		
bs	16	proc	ft	
tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	2048	wexp	procplot	
ct	2048	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-1398.8			
wp	24999.2			
vs	214			
sc	0			
wc	380			
h2mm	2.35			
is	500.00			
rfl	9753.0			
rfp	7753.4			
th	20			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
trans-3g

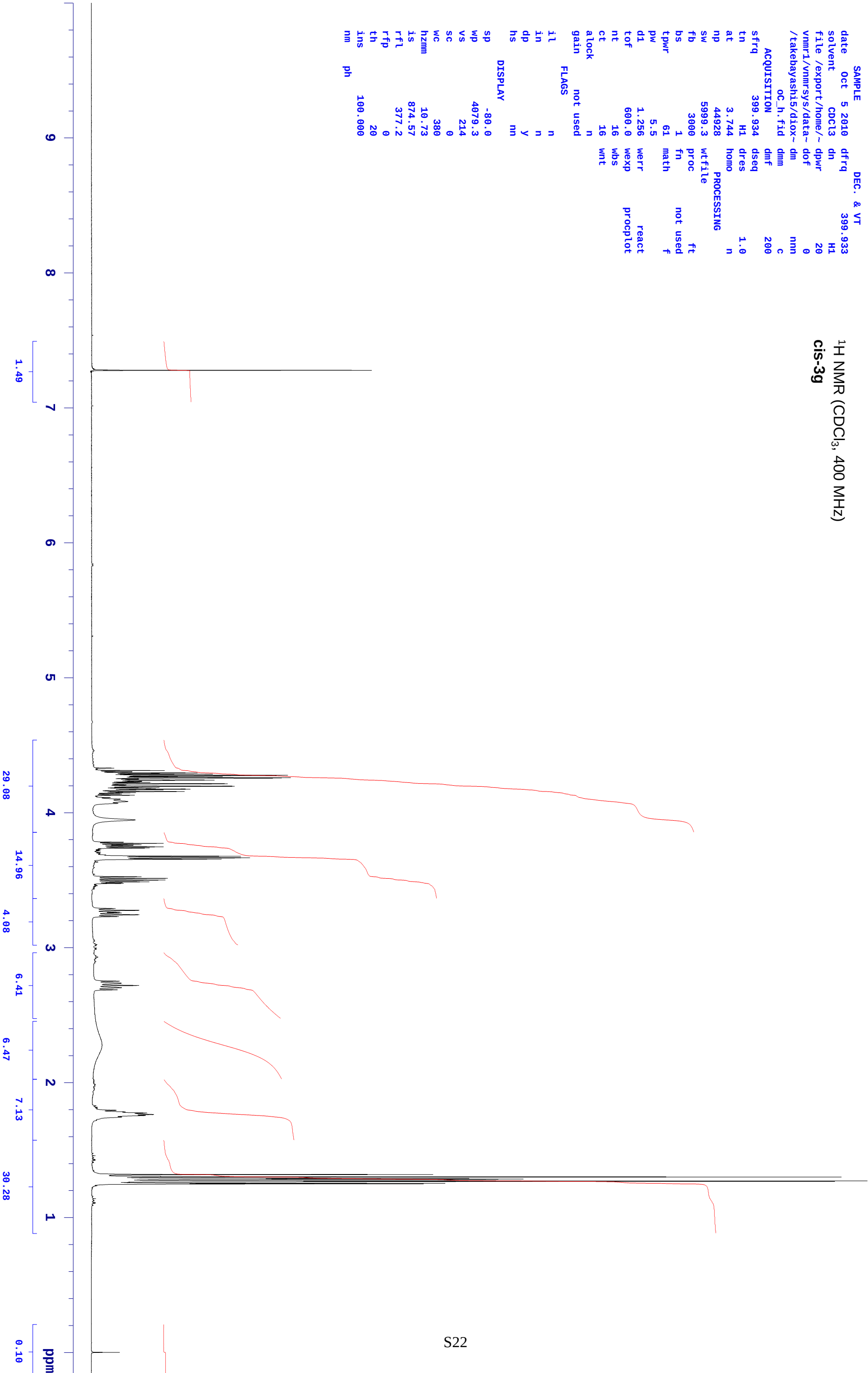


takebayash15/dioxoc

exp10 std1h

SAMPLE			DEC. & VT		
date	Oct 5 2010	dfrq	399.933		
solvent	CDCl3	dn	H1		
file	/export/home/~	dpwr	20		
vmr1/vnmrsys/data~	dof		0		
/takebayash15/diox~	dm		nnn		
oc_h.fid	dmn		c		
ACQUISITION					
sfrq	399.934	dseq	200		
tn	H1	dres	1.0		
at	3.744	homo	n		
np	44928	PROCESSING			
sw	5999.3	wtfile			
fb	3000	proc	ft		
bs	1	fn	not used		
tpwr	61	math	f		
pw	5.5				
dl	1.256	werr	react		
tof	600.0	wexp	procp1ot		
nt	16	wbs			
ct	16	wnt			
alock	n				
gain	not used				
FLAGS					
il	n				
in	n				
dp	y				
hs	nn				
DISPLAY					
sp	-80.0				
wp	4079.3				
vs	214				
sc	0				
wc	380				
hzmm	10.73				
is	874.57				
rfl	377.2				
rfp	0				
th	20				
ins	100.000				
nm	ph				

¹H NMR (CDCl₃, 400 MHz)
cis-3g

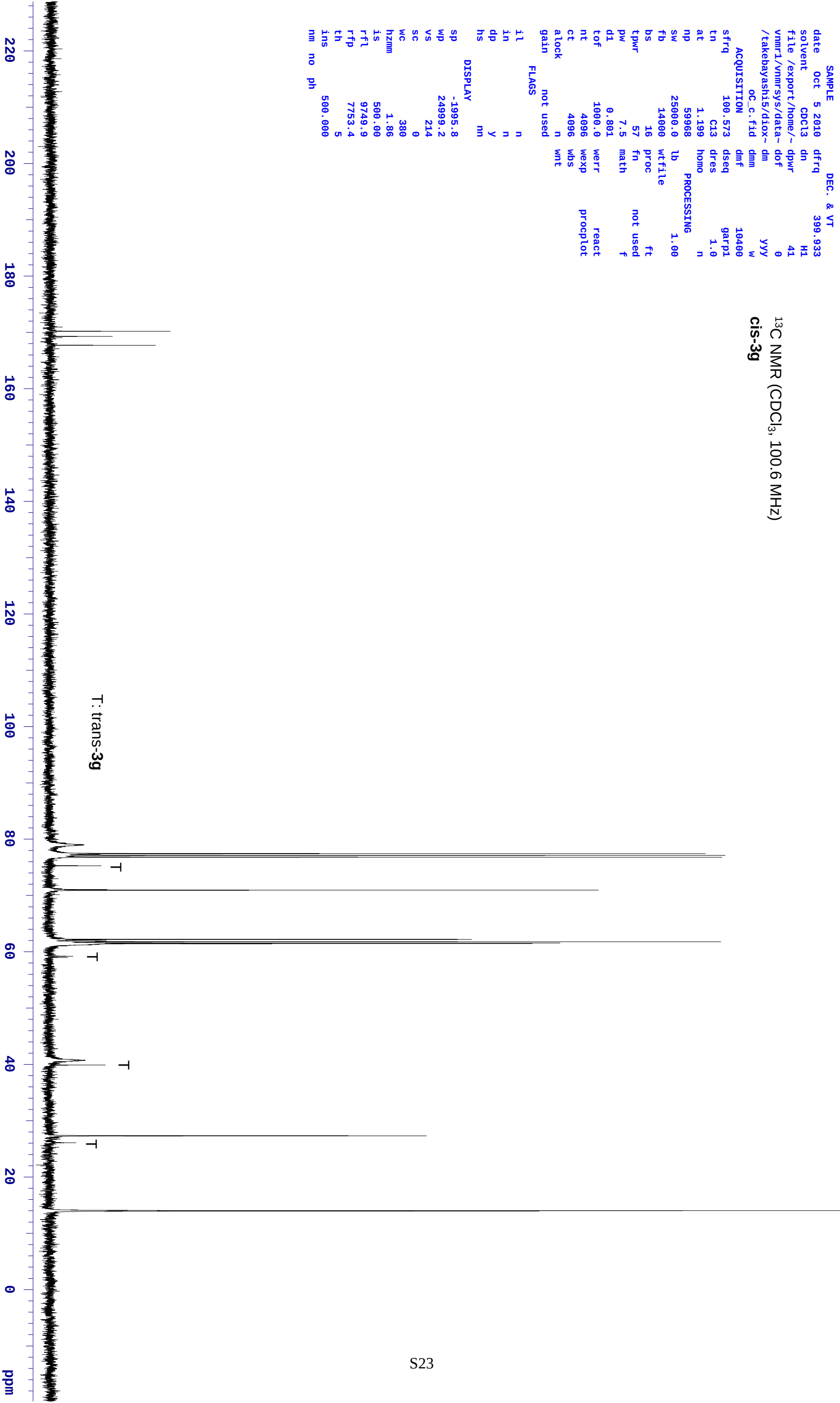


takebayashi5/dioxoc

exp10 std13c

SAMPLE			DEC. & VT	
date	Oct 5 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	41	
vmr1/vnmrsys/data~	dof		0	
/takebayashi5/diox~	dm		yyy	
oc_c.fid	dmm		w	
ACQUISITION				
sfrq	100.573	dmf	10400	
tn	C13	dseq	garpl	
at	1.199	dres	1.0	
np	59968	homo	n	
sw	25000.0	PROCESSING		
fb	14000	lb	1.00	
bs	16	wtfile		
tpwr	57	proc	ft	
pw	7.5	fn	not used	
math			f	
d1	0.801			
tof	1000.0	werr	react	
nt	4096	wexp	procp1ot	
ct	4096	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-1395.8			
wp	24999.2			
vs	214			
sc	0			
wc	380			
h2mm	1.86			
is	500.00			
rfl	9749.9			
rfp	7753.4			
th	5			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
cis-3g



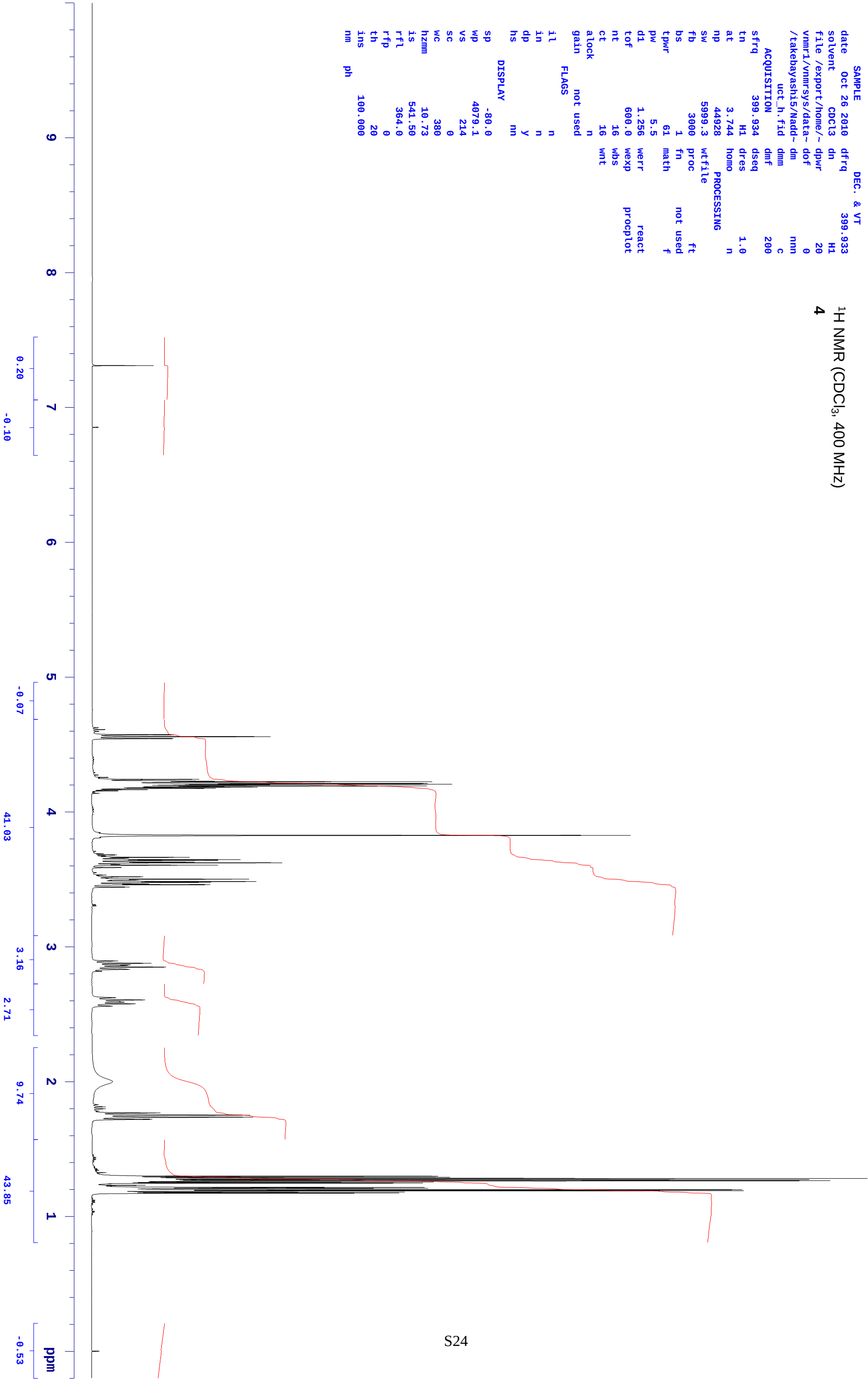
takebayashis/Nadduct

exp10 std1h

SAMPLE			DEC. & VT	
date	Oct 26 2010	dfreq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	20	
vmr1/vnmrsys/data~	dof		0	
/takebayashis/Nadd~	dm		nnn	
uct_h.fid	dmm		c	
ACQUISITION				
sfrq	399.934	dseq	200	
tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile		
fb	3000	proc	ft	
bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
h2mm	10.73			
is	541.50			
rfl	364.0			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)

4

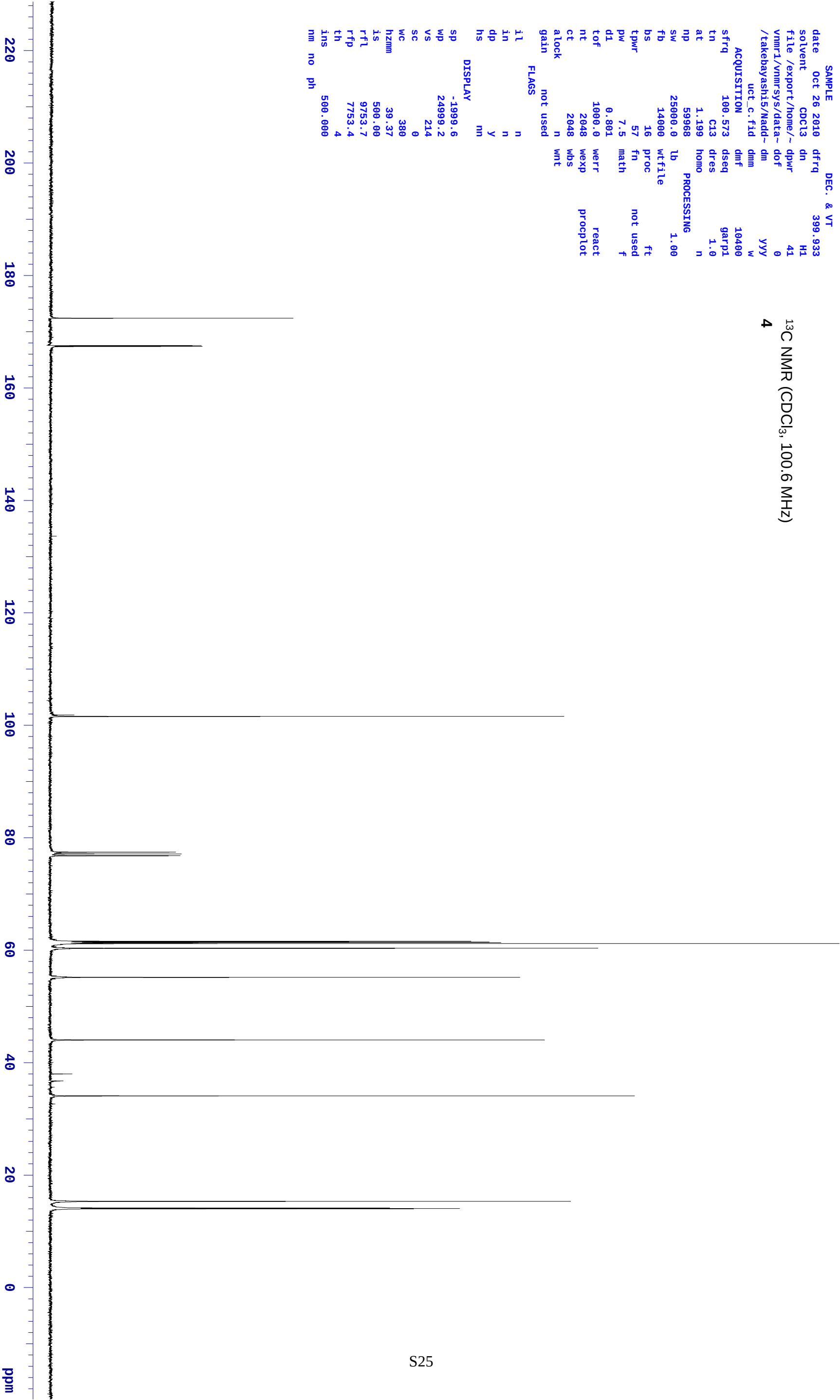


takebayashi5/Nadduct

exp10 std13c

SAMPLE			DEC. & VT	
date	Oct 26 2010	dfreq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	41	
vmnr1/vnmrsys/data~	dof		0	
/takebayashi5/Nadd~	dm		yyy	
uct_c.fid	dmm		w	
ACQUISITION				
sfrq	100.573	dmsf	10400	
tn	C13	dres	garpl	
at	1.199	homo	n	
np	59968	PROCESSING		
sw	25000.0	lb	1.00	
fb	14000	wtfile		
bs	16	proc	ft	
tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	2048	wexp	procplot	
ct	2048	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-1399.6			
wp	24999.2			
vs	214			
sc	0			
wc	380			
hzmm	39.37			
is	500.00			
rfl	9753.7			
rfp	7753.4			
th	4			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
4

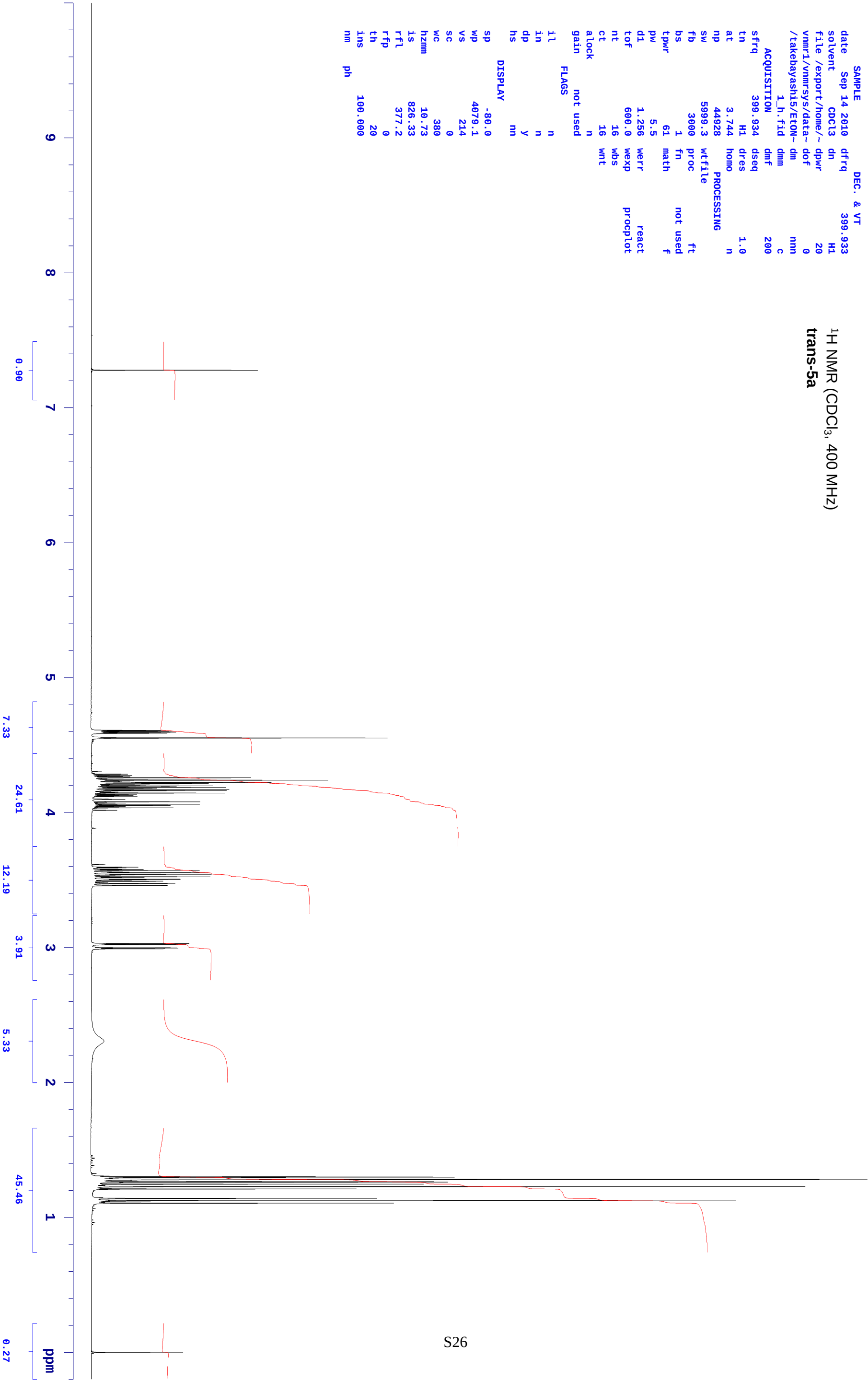


takebayash15/ETON1

exp10 std1h

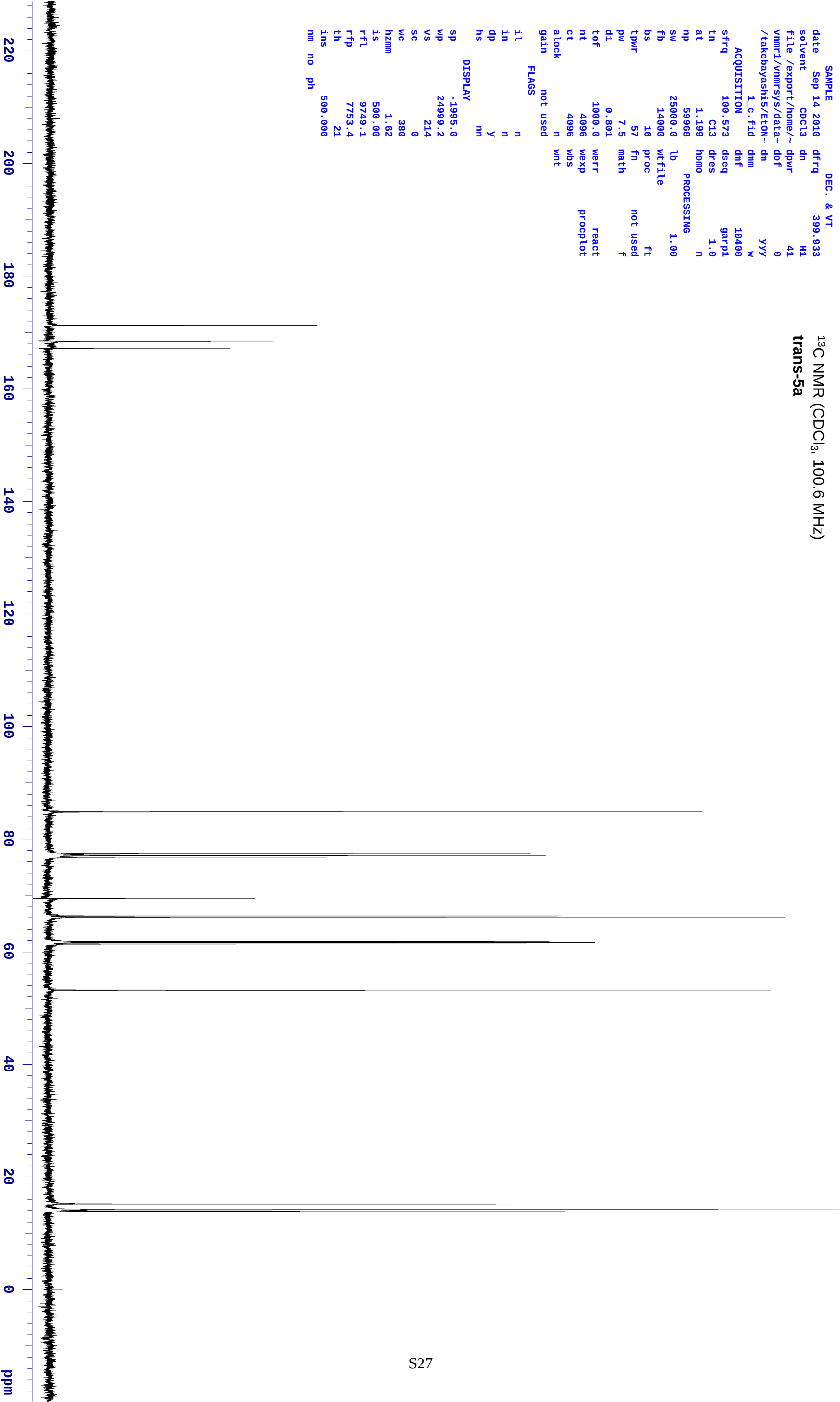
SAMPLE			DEC. & VT	
date	Sep 14 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	20	
vmr1/vnmrsys/data~	dof		0	
/takebayash15/ETON~	dm		nnn	
1_h.fid	dmm		c	
ACQUISITION		dmf	200	
sfrq	399.934	dseq		
tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile		
fb	3000	proc	ft	
bs	1	fn	not used	
tpwr	61	math	f	
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
h2mm	10.73			
is	826.33			
rfl	377.2			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
trans-5a



SAMPLE			DEC. & VT	
date	Sep 14 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	41	
vmr1/vnmrsys/data~	dof		0	
/takebayashi5/EtON~	dm	yyy		
	1_c.fid	dmm	w	
ACQUISITION				
sfrq	100.573	dmf	10400	
tn	C13	dseq	garpl	
at	1.199	homo	n	
np	59968	PROCESSING		
sw	25000.0	lb	1.00	
fb	14000	wfile		
bs	16	proc	ft	
tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	4096	wexp	procplot	
ct	4096	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-1395.0			
wp	24999.2			
vs	214			
sc	0			
wc	380			
h2mm	1.62			
is	500.00			
rfl	9749.1			
rfp	7753.4			
th	21			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
trans-5a

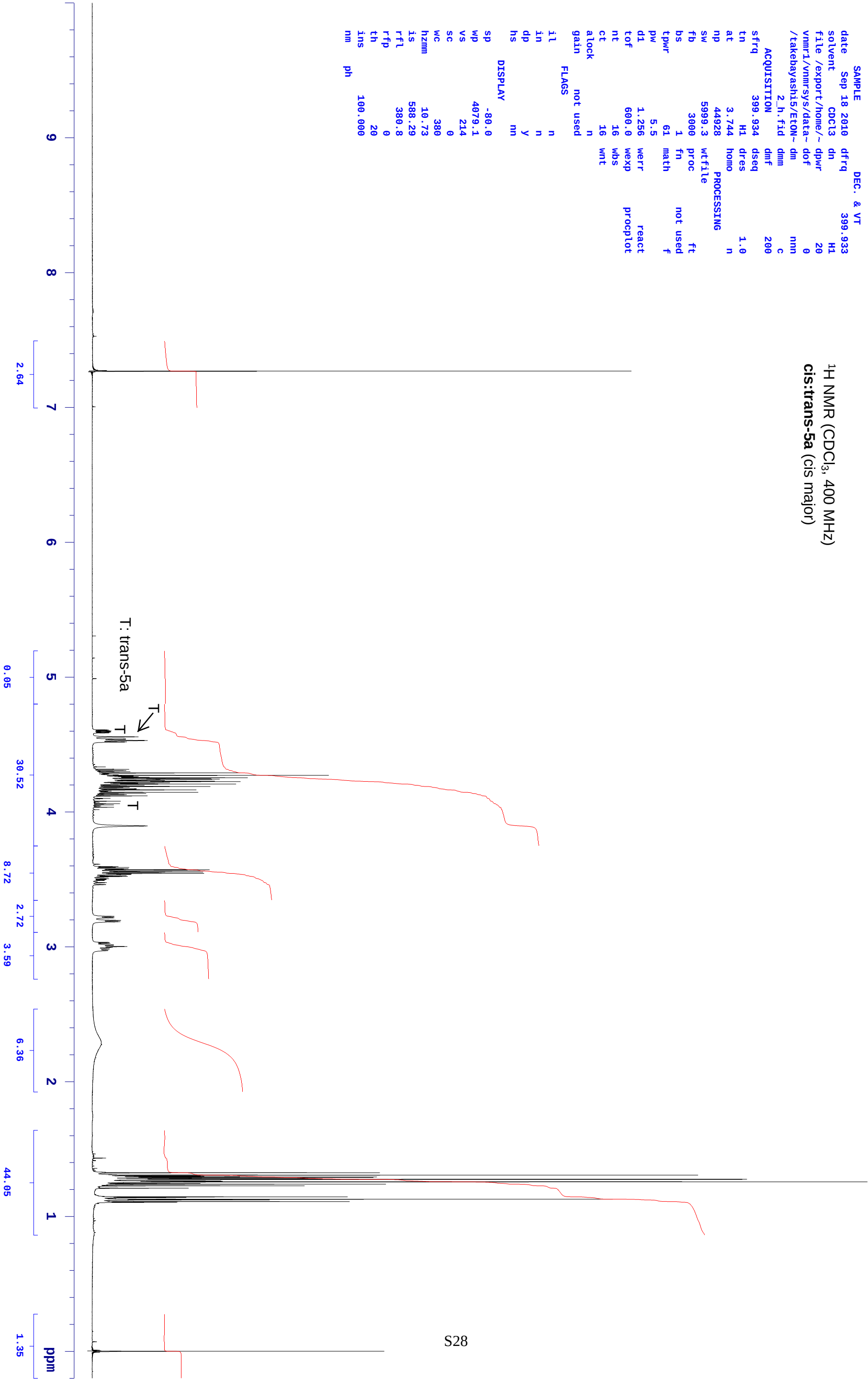


takebayash15/ETON2

exp10 std1h

SAMPLE			DEC. & VT	
date	Sep 18 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	20	
vmr1/vnmr1/sys/data~	do	dm	0	
/takebayash15/ETON~	dm	dm	nmn	
2_h.fid	dm	dm	c	
ACQUISITION				
sfrq	399.934	dseq	200	
tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile	ft	
fb	3000	proc	not used	
bs	1	fn	f	
tpwr	61	math		
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
hzmm	10.73			
is	588.29			
rfl	380.8			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
cis:trans-5a (cis major)

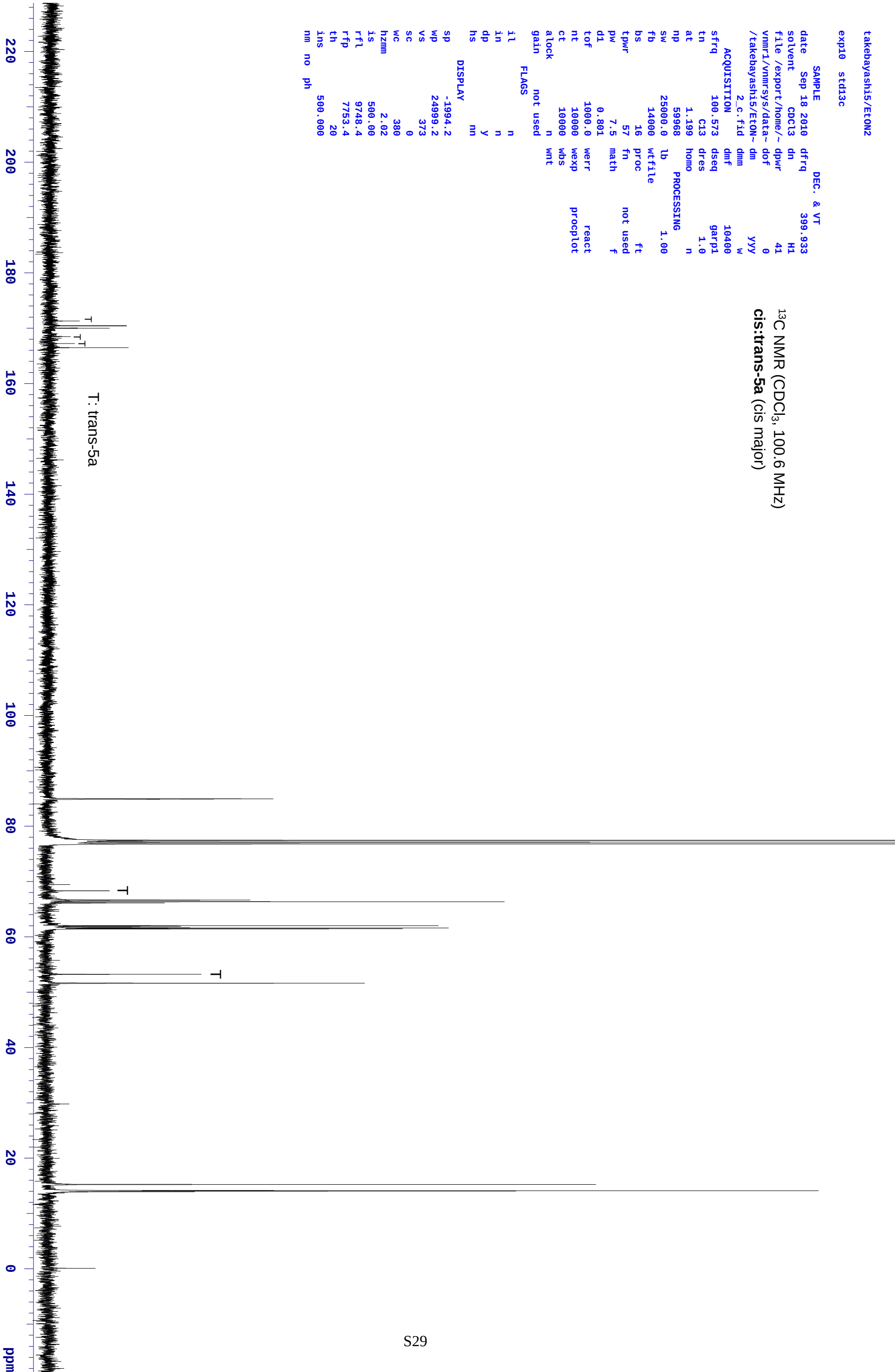


takebayashi5/EtON2

exp10 std13c

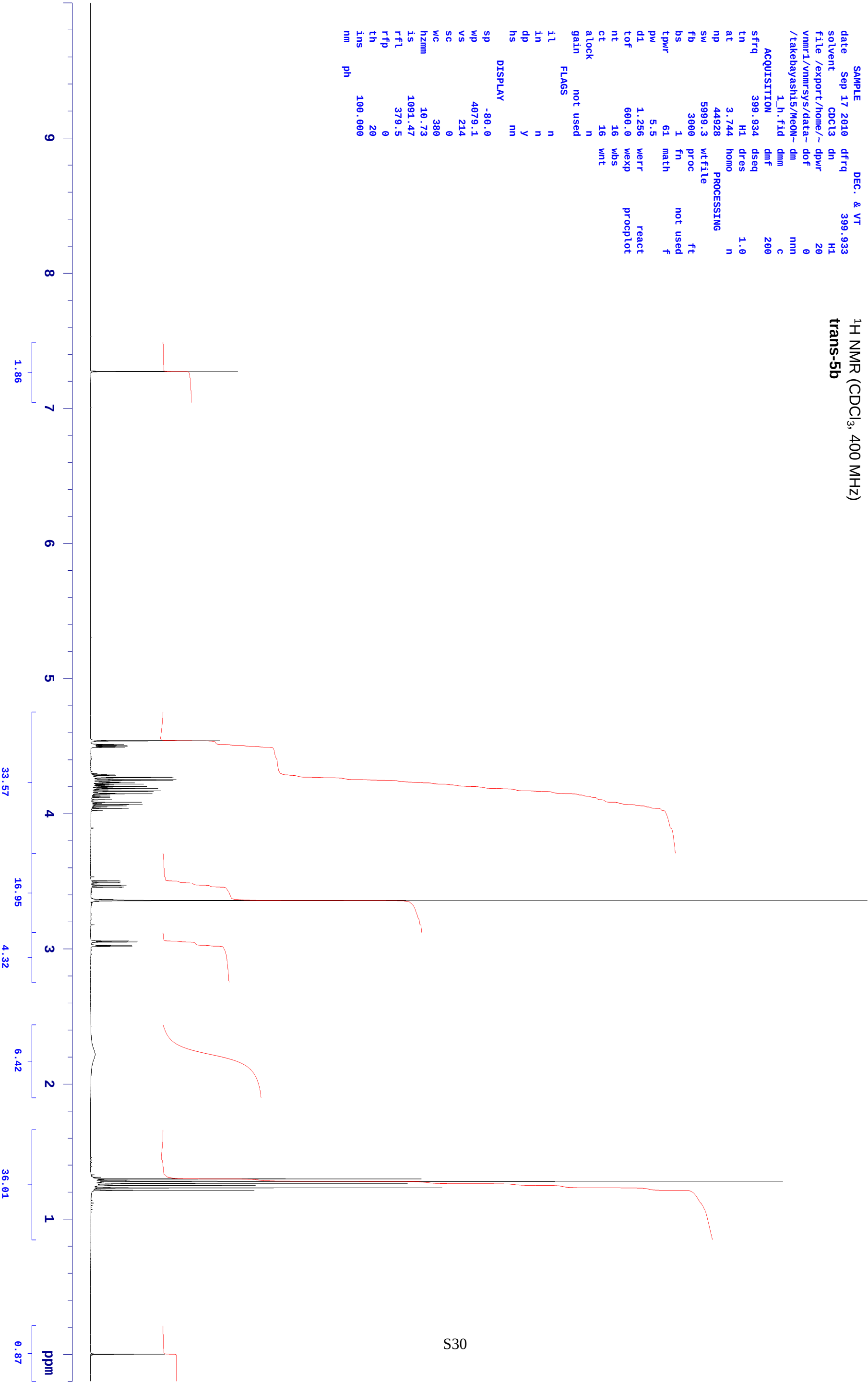
SAMPLE			DEC. & VT	
date	Sep 18 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	41	
vmr1/vnmrsys/data~	dof		0	
/takebayashi5/EtON~	dm		yyy	
2.c.fid dnm w				
ACQUISITION				
sfrq	100.573	dmf	10400	
tn	C13	dseq	garpl	
at	1.199	homo	1.0	
np	59968	PROCESSING		
sw	25000.0	lb	1.00	
fb	14000	wtfile		
bs	16	proc	ft	
tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
tof	1000.0	werr	react	
nt	10000	wexp	procp1ot	
ct	10000	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-1394.2			
wp	24999.2			
vs	373			
sc	0			
wc	380			
h2mm	2.02			
is	500.00			
rfl	9748.4			
rfp	7753.4			
th	20			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
cis:trans-5a (cis major)



SAMPLE			DEC. & VT	
date	Sep 17 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	20	
vmr1/vnmr5/data~	dof		0	
/takebayashi5/MeON~	dm		nnn	
	1_h.fid	dmm	c	
ACQUISITION				
sfrq	399.934	dseq	200	
tn	H1	dres	1.0	
at	3.744	homo	n	
np	44928	PROCESSING		
sw	5999.3	wtfile	ft	
fb	3000	proc	not used	
bs	1	fn	f	
tpwr	61	math		
pw	5.5			
d1	1.256	werr	react	
tof	600.0	wexp	procp1ot	
nt	16	wbs		
ct	16	wnt		
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nn			
DISPLAY				
sp	-80.0			
wp	4079.1			
vs	214			
sc	0			
wc	380			
h2mm	10.73			
is	1091.47			
rfl	379.5			
rfp	0			
th	20			
ins	100.000			
nm	ph			

¹H NMR (CDCl₃, 400 MHz)
trans-5b



takebayashi5/MeON1

exp10 std13c

SAMPLE

date Sep 17 2010

dfreq 399.933

solvent CDCl3

dn H1

file /export/home/~

dpwr 41

vmr1/vnmrsys/data~

dof 0

/takebayashi5/MeON~

dm

yyy

w

ACQUISITION

sfrq 100.573

dseq 10400

tn C13

dres 1.0

at 1.199

homo n

np 59968

PROCESSING

sw 25000.0

lb 1.00

fb 14000

wfile

bs 16

proc

ft

tpwr 57

fn

not used

f

pw 7.5

math

d1 0.801

tof 1000.0

werr

react

nt 4096

wexp

procplot

ct 4096

wbs

alock n

wnt

gain not used

FLAGS

il n

in n

dp y

hs nn

DISPLAY

sp -1395.0

wp 24999.2

vs 214

sc 0

wc 380

h2mm 2.19

is 500.00

rfl 9749.1

rfp 7753.4

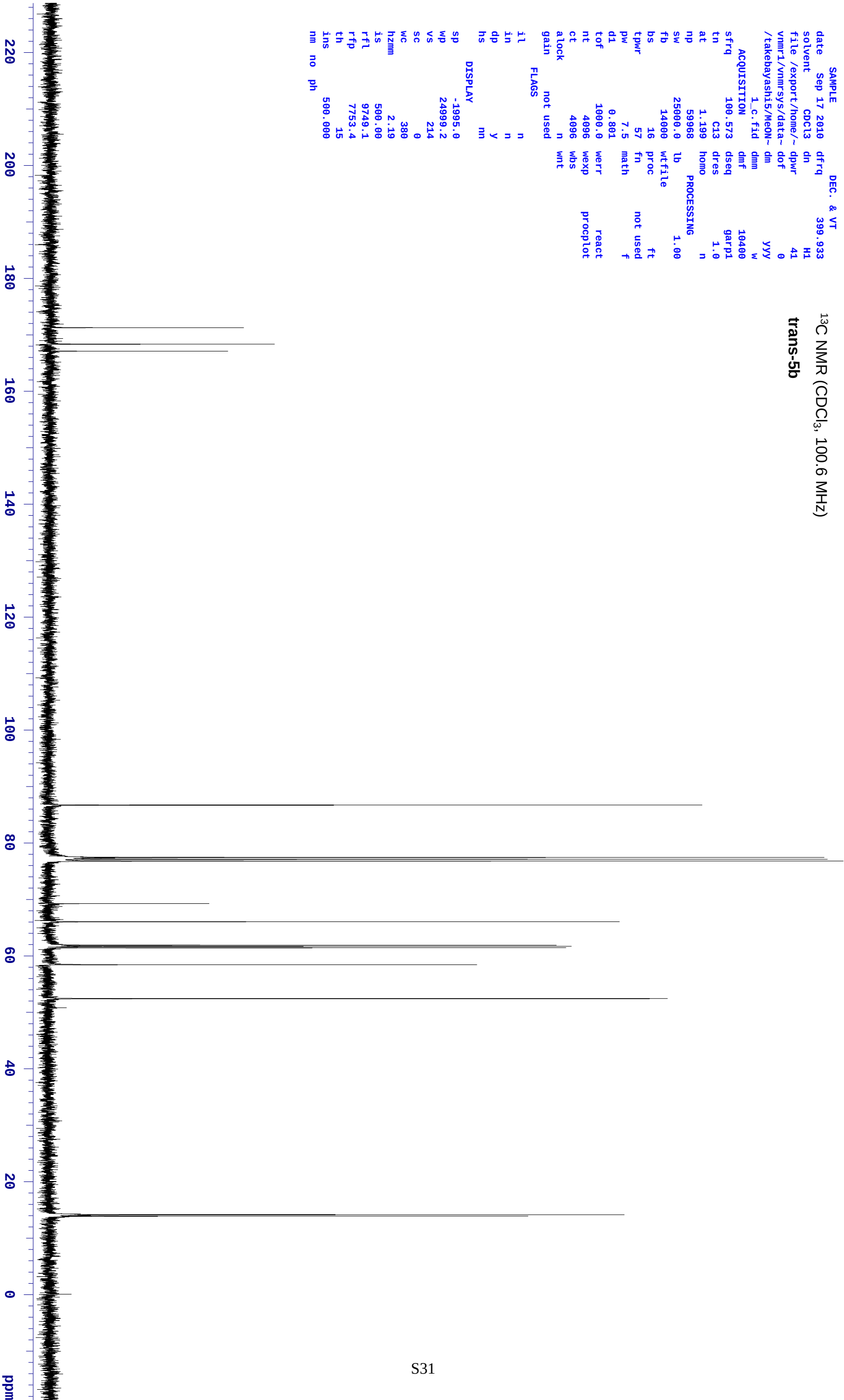
th 15

ins 500.000

nm no ph

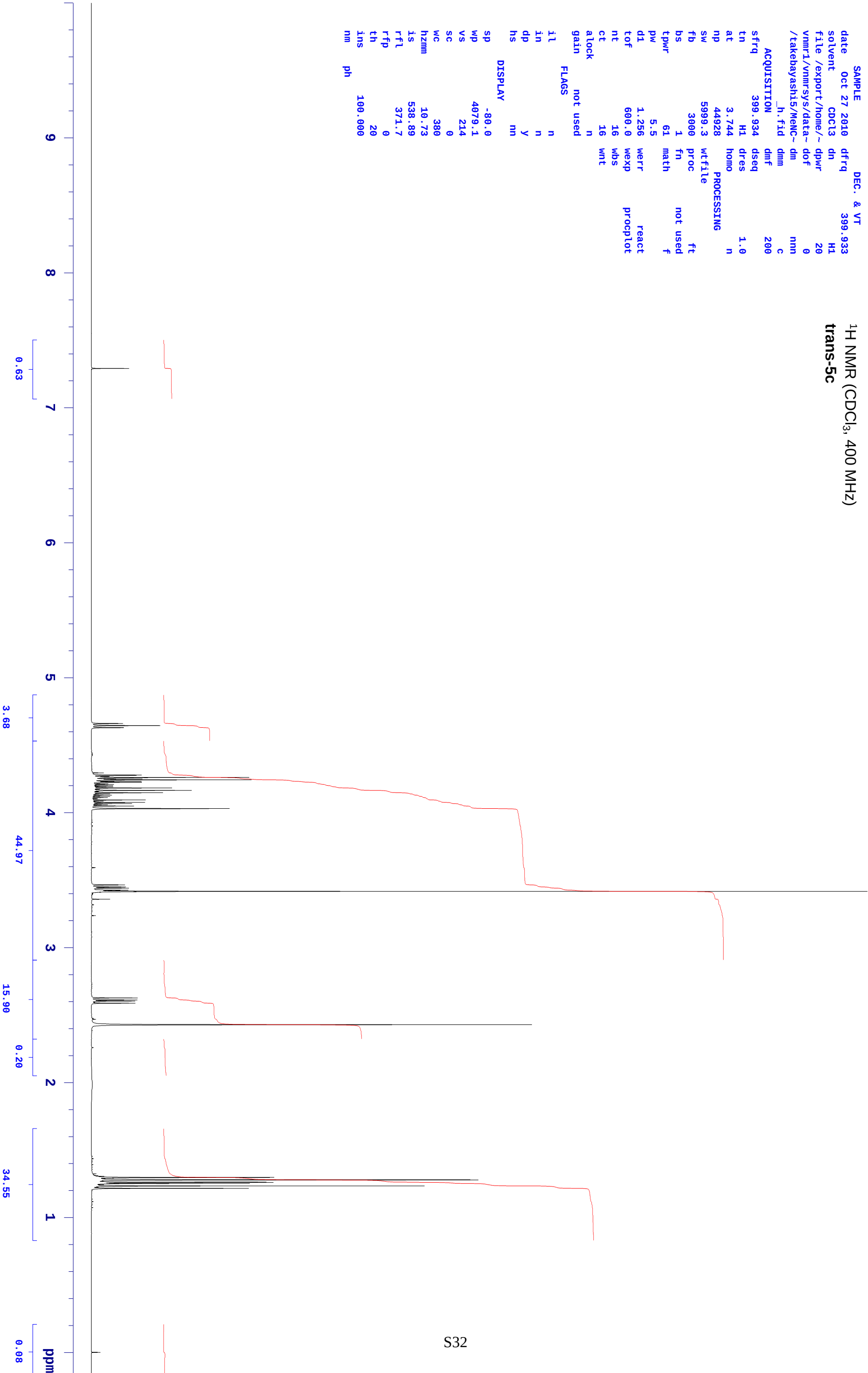
¹³C NMR (CDCl₃, 100.6 MHz)

trans-5b



SAMPLE			DEC. & VT		
date	Oct 27 2010	dfrq	399.933		
solvent	CDCl3	dn	H1		
file	/export/home/~	dpwr	20		
vmr1/vnmrsys/data~	dof		0		
/takebayashi5/MenC~	dm		nnn		
_h.fid			dmn		
ACQUISITION			dmf		
sfrq	399.934	dseq	200		
tn	H1	dres	1.0		
at	3.744	homo	n		
np	44928	PROCESSING			
sw	5999.3	wtfile			
fb	3000	proc	ft		
bs	1	fn	not used		
tpwr	61	math	f		
pw	5.5				
d1	1.256	werr	react		
tof	600.0	wexp	procp1ot		
nt	16	wbs			
ct	16	wnt			
alock	n				
gain	not used				
FLAGS					
il	n				
in	n				
dp	y				
hs	nn				
DISPLAY					
sp	-80.0				
wp	4079.1				
vs	214				
sc	0				
wc	380				
h2mm	10.73				
is	538.89				
rfl	371.7				
rfp	0				
th	20				
ins	100.000				
nm	ph				

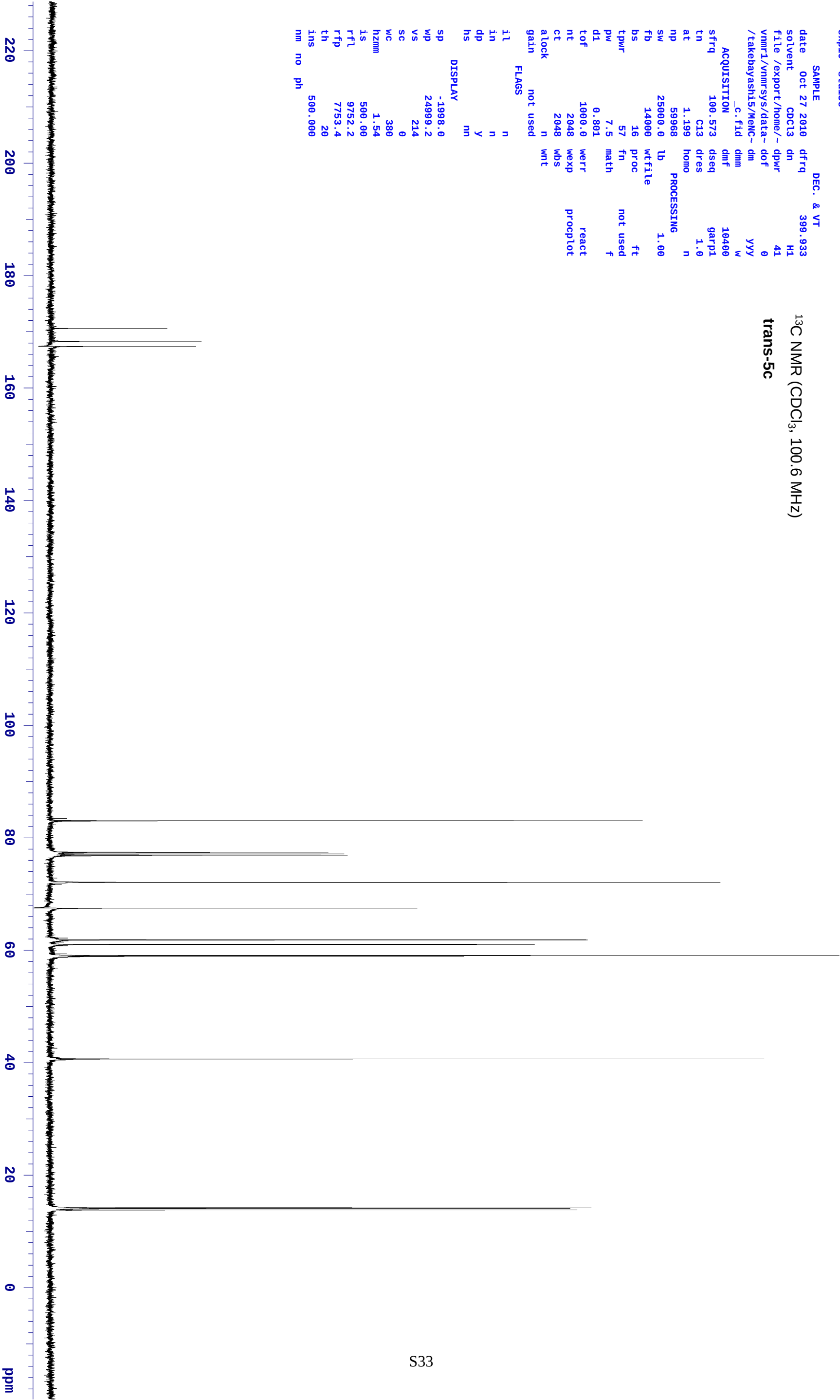
¹H NMR (CDCl₃, 400 MHz)
trans-5c



exp10 std13c

SAMPLE			DEC. & VT	
date	Oct 27 2010	dfrq	399.933	
solvent	CDCl3	dn	H1	
file	/export/home/~	dpwr	41	
vnmr1/vnmrsys/data~	do f		0	
/takebayashi5/MenC~	dm		yyy	
_C.fid				
ACQUISITION				
sfrq	100.573	dseq	10400	
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tof	1000.0	werr	react	
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alock	n	wnt		
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
hs	nm			
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vs	214			
sc	0			
wc	380			
hzm	1.54			
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nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
trans-5c



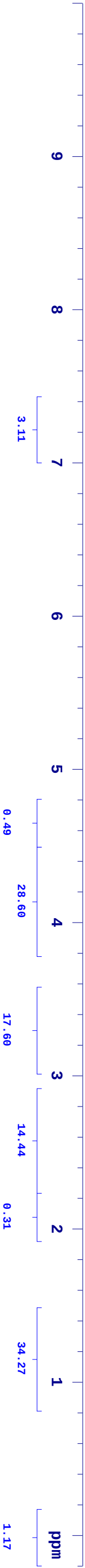
takebayash15/MeN1

exp10 std1h

¹H NMR (CDCl₃, 400 MHz)

cis-5c

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nm	ph			

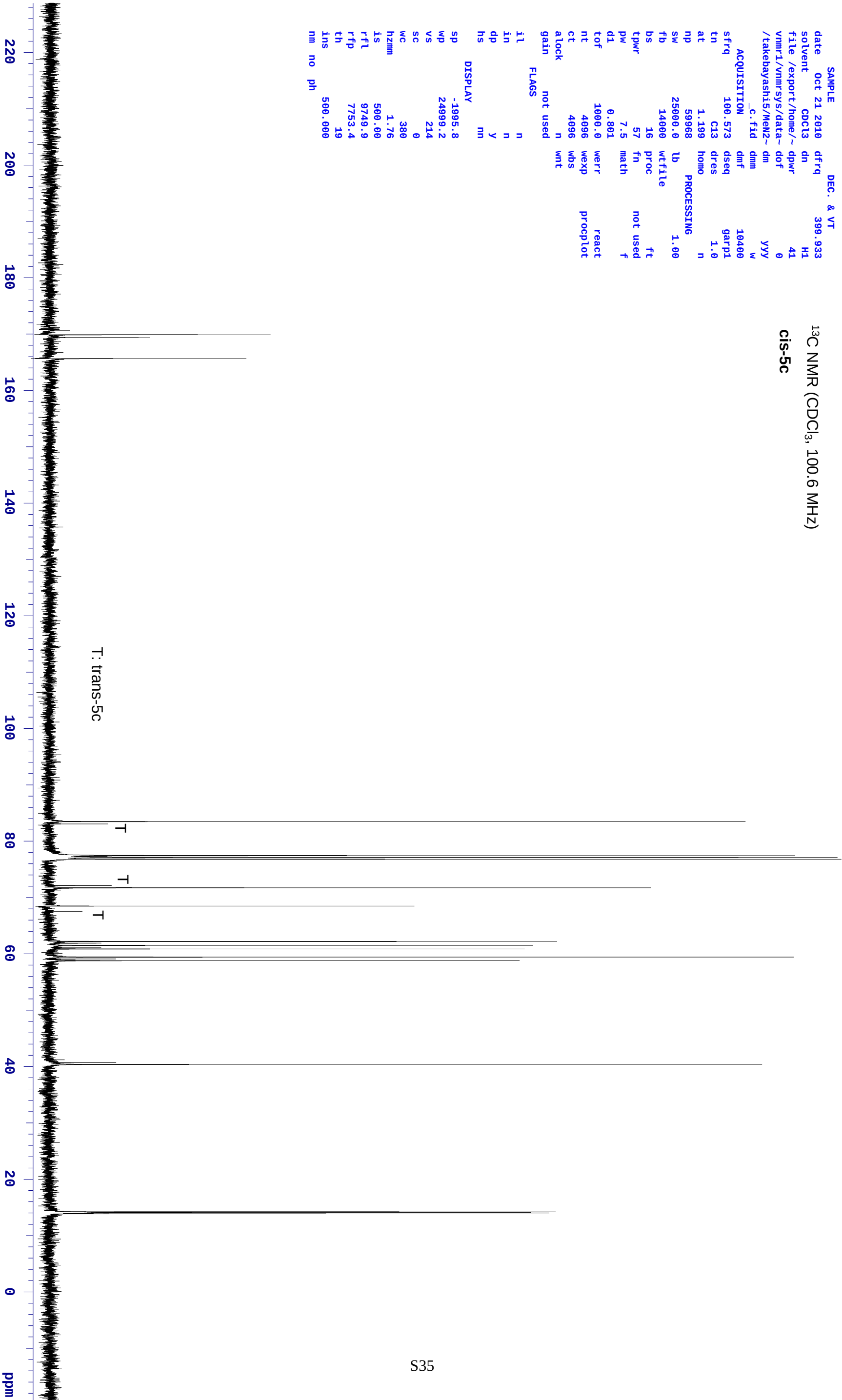


takebayashi5/Men2

exp10 std13c

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	__c.fid	dmm	w	
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tpwr	57	fn	not used	
pw	7.5	math	f	
d1	0.801			
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ct	4096	wbs		
alock	n	wnt		
gain	not used			
FLAGS				
il	n			
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rfl	9749.9			
rfp	7753.4			
th	19			
ins	500.000			
nm	no	ph		

¹³C NMR (CDCl₃, 100.6 MHz)
cis-5c



II. Selected NOEs and HMBC correlations

Atom numberings and NOEs of compounds **3** and **5** were graphically described in Figures S1 and S2.

Trans-3a: Selected NOEs are between H-6b and H-5a, H-2, between H-5a and OCHHCH₃, between H-5b and H-6a, and between H-4 and H-5a, H-5b. Selected HMBC correlations are between H-6a,b and C-2, C-4, and between H-2,4 and C-2, C-3, C-4, C-6.

Cis-3a: Selected NOEs are between H-6a and H-2, H-4, and between H-4 and H-2, H-5b. Selected HMBC correlations are between H-2 and C-3, C-4, C-6.

Trans-3b: Selected NOEs are between H-6b and H-5a, H-2, between H-5a and OCHHCH₃, between H-5b and H-6a, and between H-4 and H-5a, H-5b. Selected HMBC correlations are between H-6a,b and C-2, C-4, between H-2 and C-4, C-3, C-6, and between H-4 and δ C-2, C-3, C-6.

Trans-3c: Selected NOEs are between H-6b and H-5a, H-2, between H-5a and OCHHCH₃, between H-5b and H-6a, and between H-4 and H-5a, H-5b. Selected HMBC correlations are between H-6a,b and C-2, C-4, and between H-2 and C-4, C-3, C-6.

Trans-3d: Selected NOEs are between H-6b and H-5a, H-2, between H-5a and OCHHCH₃, between H-5b and H-6a, and between H-4 and H-5a, H-5b. Selected HMBC correlations are between H-6a,b and C-2, C-4, between H-2 and C-4, C-3, C-6, and between H-4 and C-2.

Trans-3e: Selected NOEs are between H-6b and H-5a, H-2, between H-5a and OCHHCH₃, between H-5b and H-6a, and between H-4 and H-5a, H-5b. Selected HMBC correlations are between H-6a,b and C-2, C-4, and between H-2 and C-4, C-3, C-6.

Cis-3f: Selected NOEs are between H-6a and H-2, H-4 and between H-4 and H-2, H-5b. Selected HMBC correlations are between H-2 and C-4, C-3, C-6, and between H-4 and C-3.

Trans-3g: Selected NOEs are between H-6b and H-5a, H-2, between H-5a and OCHHCH₂OH, between H-5b and H-6a, and between H-4 and H-5a, H-5b. Selected HMBC correlations are between H-6a,b and C-2, C-4, and between H-2,4 and C-3, C-4, C-6.

Cis-3g: Selected NOEs are between H-6a and H-2, H-4 and between H-2 and H-4. Selected HMBC correlations are between H-6a,b and C-2, C-4.

4: Selected NOEs are between $CH-N$ and NCH_2 , NH , and between $CH(OEt)_2$ and $CH(OCH_2CH_3)_2$. Selected HMBC correlations are between $CH-N$ and NCH_2 , between NCH_2 and $CH-N$, between $CH(OEt)_2$ and $CH(OCH_2CH_3)_2$, and between $CH(OCH_2CH_3)_2$ and $CH(OEt)_2$.

Trans-5a: Selected NOEs are between H-5a and H-2, OCH_2CH_3 , and between H-5b and H-4. Selected HMBC correlations are between H-5a,b and C-2, C-3, C-4, between H-2 and C-4, C-3, C-5 and between H-4 and C-2.

Cis-5a: Selected NOEs are between H-5b and H-2, H-4, between H-5a and OCH_2CH_3 , and between H-2 and H-4. Selected HMBC correlations are between H-5a and C-2, C-4, and between H-2 and C-3.

Trans-5b: Selected NOEs are between H-5a and H-2, OCH_3 , and between H-5b and H-4. Selected HMBC correlations are between H-5a,b and C-2, C-3, C-4, between H-2 and C-4, C-3, and between H-4 and C-5, C-2.

Trans-5c: Selected NOEs are between H-2 and H-5a, NCH_3 , between NCH_3 and H-5a, and between H-4 and H-5b. Selected HMBC correlations are between H-5a and C-4, between H-5b and δ C-2, C-3, between H-2 and C-4, C-3, and between H-4 and C-5, C-3.

Cis-5c: Selected NOEs are between H-5b and H-2, H-4. Selected HMBC correlations are between δ H-5a and C-2, C-3, C-4, and between H-2 and C-3, C-4.

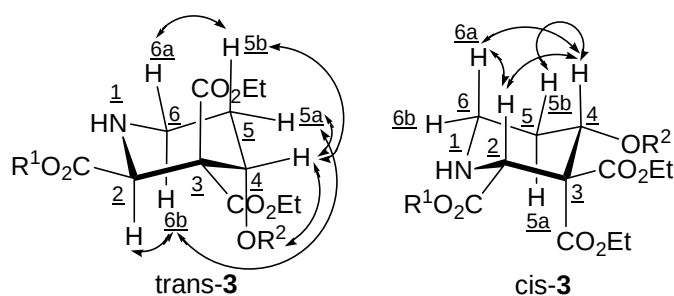


Figure S1. NOEs for *trans*-3a-g and *cis*-3a, f, g.

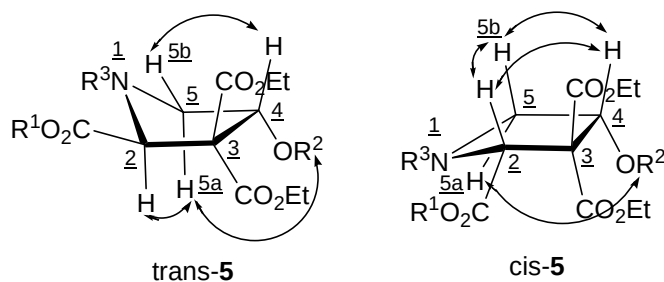


Figure S2. NOEs for *trans*-5a-c and *cis*-5a,c. Some peaks (e.g. between H-2 and H-4 for *cis*-5c) were overlapped and not clearly identified.

III. Discussion for observed 2,4-*trans* selectivity of the six-membered ring using the calculations of model compounds

2,4-*Cis* stereoselectivity (1,3-equatorial conformation) can be expected for the cyclohexane-like heterocyclic six-membered ring. In order to explain observed 2,4-*trans* selectivity of the six-membered ring, structures of the model compounds, trimethyl esters with methoxy group shown in Figure S3 were optimized by B3LYP/6-31G*^{S1, S2} and their energies ΔG° were compared. Their structures are shown in Figure S4. *Trans*-3M and is only 0.71 kcal/mol stable than 1,3-*cis* (the equilibrium constant K (*trans/cis*) = 3.3 at 298 K (25 °C)). 1TiCl₄-coordinated structures, *trans*-XM and *cis*-XM have the similar small energy difference 0.87 kcal/mol (K (*trans/cis*) = 4.3). On the other hand, 2TiCl₄-coordinated structure *trans*-ZM is 3.51 kcal/mol more stable than *cis*-ZM (K (*trans/cis*) = 384). Calculations of various 1TiCl₄- or 2TiCl₄-coordinated structures including *trans*-YM, *cis*-YM, and other bidentate and monodentate TiCl₄-coordinated structures have also been examined. However, they are much less stable than *trans,cis*-XM and *trans,cis*-ZM, or they could not be optimized. Although the estimation is only for the model compounds, it is suggested that multiple functional groups and the coordination of TiCl₄ may play an important role in the preferred conformation.

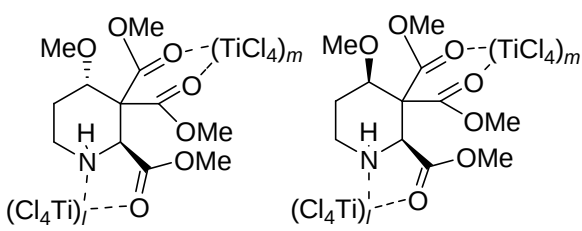
	
trans- 3M ($l=m=0$)	cis- 3M ($l=m=0$)
0 kcal/mol	+0.71 kcal/mol
3M-1TiCl₄ trans- XM ($l=1,m=0$)	cis- XM ($l=1,m=0$)
0 kcal/mol	+0.87 kcal/mol
(-5.26 kcal/mol)	(-4.39 kcal/mol)
trans- YM ($l=0,m=1$)	cis- YM ($l=0,m=1$)
+8.80 kcal/mol	+8.48 kcal/mol
(+3.54 kcal/mol)	(+3.22 kcal/mol)
3M-2TiCl₄ trans- ZM ($l=m=1$)	cis- ZM ($l=m=1$)
0 kcal/mol	+3.51 kcal/mol
(-0.55 kcal/mol)	(+2.96 kcal/mol)

Figure S3. The model compounds, trimethyl esters with methoxy group optimized by B3LYP/6-31G* and their relative energies ΔG° . ΔG° is the difference of Gibbs free energies ($T = 298.15$ K, $P = 1$ atm) relative to that of *trans*-**3M**, *trans*-**XM**, and *trans*-**ZM**, respectively. Those in the parentheses is relative to the Gibbs free energies of *trans*-**3M** + $n\text{TiCl}_4$ ($n=l+m=1$ for *trans/cis*-**XM**, *trans/cis*-**YM**, and $n=l+m=2$ for *trans/cis*-**ZM**) (all the constituent molecules separated).

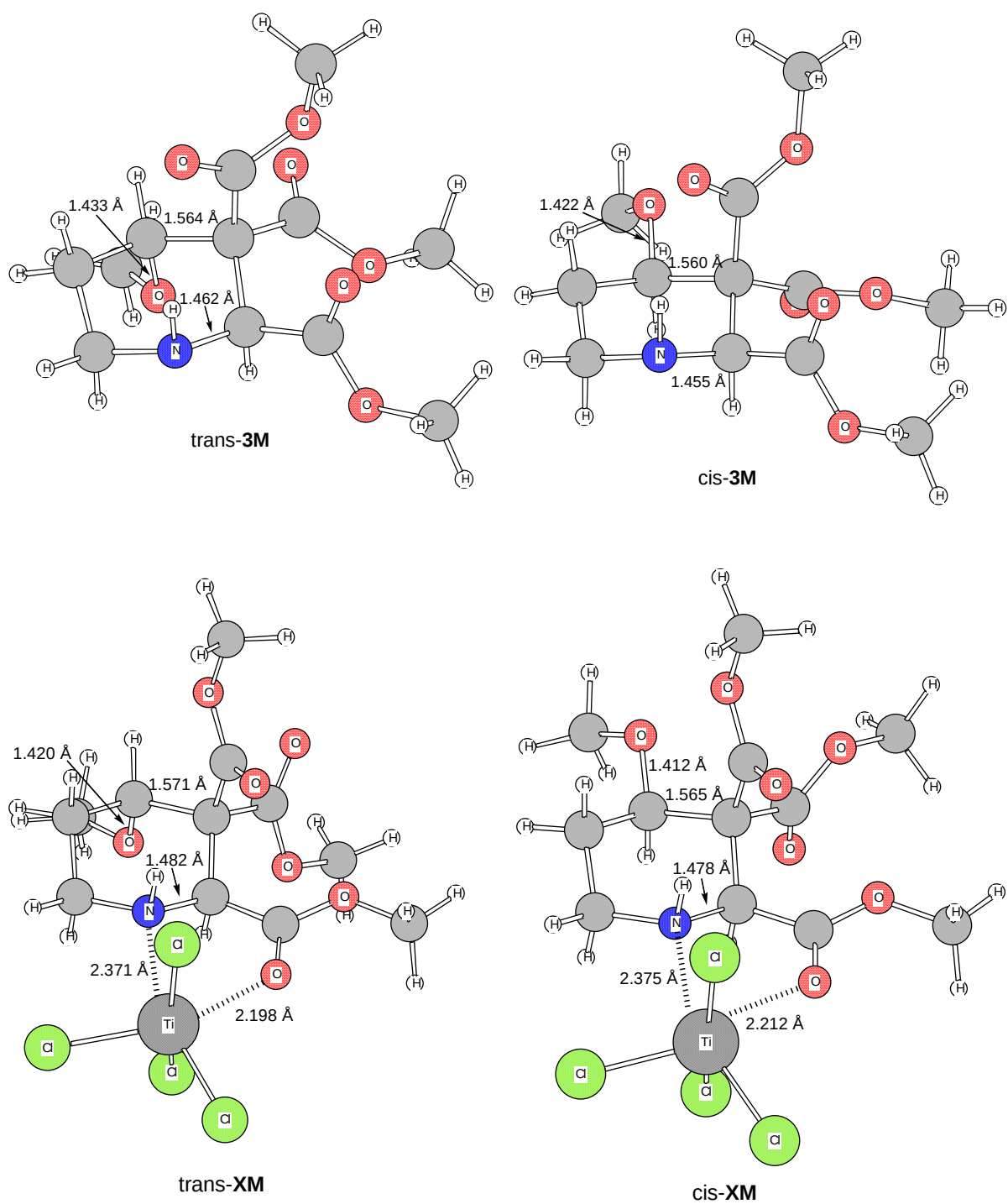


Figure S4. continued.

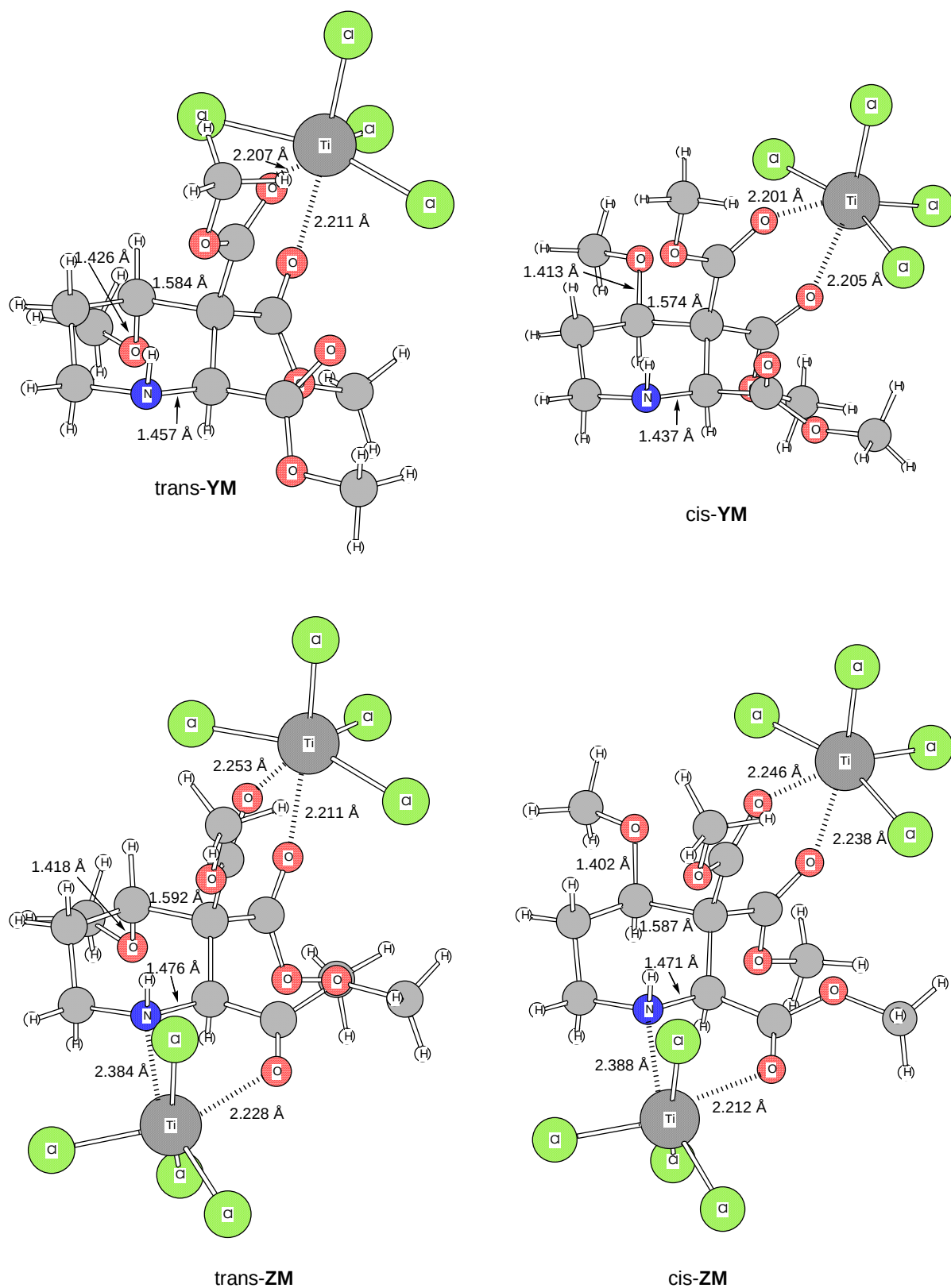


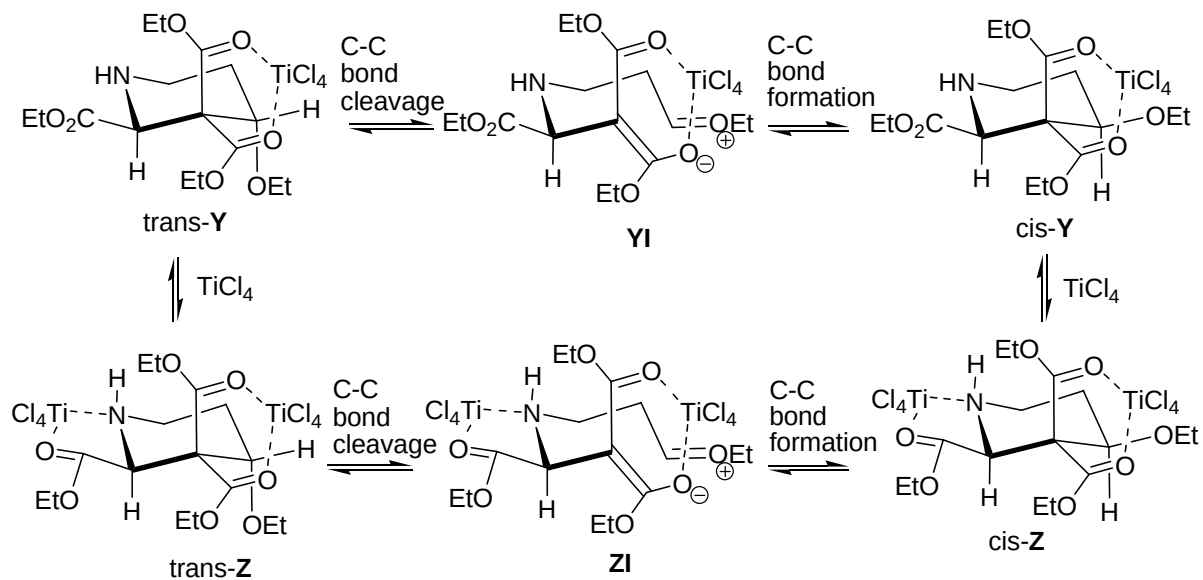
Figure S4. B3LYP/6-31G*-optimized structures^{S1, S2} of the model compounds in Scheme 3.

References

- ^{S1} (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1998**, *37*, 785.
- ^{S2} Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Foresman, K. Raghavachari, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

IV.

Scheme S1. The other possible isomerization route via oxocarbenium ion intermediates **YI** and **ZI**.



V. Cartesian coordinates of the optimized geometries of Figure S4

trans-3M (EA1.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.336419	1.555401	-0.155985
2	6	0	-0.520733	0.085221	0.251630
3	6	0	0.245108	-0.933800	-0.679219
4	6	0	1.763045	-0.834173	-0.569484
5	8	0	2.373534	-0.853536	0.480547
6	8	0	2.350112	-0.806056	-1.776322
7	7	0	-0.091943	-2.330450	-0.409584
8	6	0	-1.527538	-2.593109	-0.571089
9	6	0	-2.410289	-1.688023	0.302966
10	6	0	-2.048867	-0.212493	0.098622
11	6	0	-0.057497	-0.104639	1.702428
12	1	0	-2.590135	0.427275	0.805746
13	8	0	-0.275754	-1.099362	2.365533
14	8	0	-1.084654	2.450763	0.168489
15	8	0	0.760508	1.739178	-0.914415
16	8	0	0.630372	0.953152	2.157420
17	6	0	1.229233	0.789979	3.455150
18	6	0	1.017574	3.095749	-1.314664
19	6	0	3.787041	-0.816537	-1.760379
20	1	0	0.184394	-2.545528	0.548608
21	1	0	-0.049220	-0.706523	-1.705782
22	1	0	-1.706873	-3.648178	-0.338069
23	1	0	-1.777456	-2.444917	-1.627937
24	1	0	-2.287127	-1.949318	1.357697
25	1	0	-3.469199	-1.822447	0.045980
26	8	0	-2.371297	0.177926	-1.241949
27	1	0	1.180567	3.724937	-0.436018
28	1	0	0.173833	3.489461	-1.886566
29	1	0	1.915468	3.052114	-1.931285
30	1	0	4.158124	-1.718444	-1.266500
31	1	0	4.170635	0.061289	-1.233432
32	1	0	4.090440	-0.799969	-2.807484
33	1	0	1.963413	-0.018304	3.419973
34	1	0	0.466664	0.562112	4.203528
35	1	0	1.711865	1.742829	3.672574
36	6	0	-3.603636	0.866910	-1.363685
37	1	0	-4.448683	0.264826	-0.997129
38	1	0	-3.750942	1.061993	-2.429410
39	1	0	-3.576857	1.820507	-0.819578

cis-3M (EE2.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066536	-1.213314	-0.964263
2	6	0	0.430457	0.052112	-0.173947
3	6	0	-0.675087	1.159539	-0.445774
4	6	0	-2.044461	0.794746	0.129226
5	8	0	-2.267968	0.605953	1.304354
6	8	0	-2.987302	0.770742	-0.831854
7	7	0	-0.337653	2.481638	0.058460
8	6	0	0.921164	2.971277	-0.509314
9	6	0	2.103552	2.020562	-0.262654
10	6	0	1.789658	0.590360	-0.718520
11	6	0	0.588009	-0.205229	1.331321
12	8	0	0.752176	0.677692	2.149188
13	8	0	0.707786	-1.675861	-1.883271
14	8	0	-1.124282	-1.711522	-0.576983
15	8	0	0.588047	-1.509036	1.640047
16	6	0	0.774396	-1.810874	3.034148
17	6	0	-1.569400	-2.878194	-1.288009
18	6	0	-4.320143	0.493308	-0.370594
19	1	0	-0.253340	2.416059	1.073090
20	1	0	-0.776567	1.235192	-1.534348
21	1	0	1.127070	3.958636	-0.082441
22	1	0	0.766390	3.117635	-1.587796
23	1	0	2.347171	1.999002	0.803503

24	1	0	2.994857	2.372199	-0.798436
25	1	0	1.711737	0.560588	-1.813784
26	1	0	-0.848067	-3.690809	-1.171493
27	1	0	-1.690704	-2.656437	-2.351485
28	1	0	-2.525484	-3.146096	-0.837948
29	1	0	-4.642271	1.251777	0.347448
30	1	0	-4.360901	-0.489109	0.107487
31	1	0	-4.948442	0.515476	-1.261428
32	1	0	-0.027626	-1.364872	3.627117
33	1	0	1.737269	-1.426746	3.379779
34	1	0	0.746399	-2.898637	3.100503
35	8	0	2.805983	-0.304553	-0.283896
36	6	0	3.780282	-0.612977	-1.265325
37	1	0	4.315445	0.284103	-1.612441
38	1	0	3.324652	-1.120627	-2.125180
39	1	0	4.500693	-1.284021	-0.789818

trans-XM (EA3Ti.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.039087	-0.582519	-0.740514
2	6	0	2.005975	0.116021	0.175426
3	6	0	0.546978	-0.029810	-0.327746
4	6	0	-0.040713	-1.431332	-0.375427
5	8	0	-1.259990	-1.594079	-0.286796
6	8	0	0.791845	-2.422721	-0.585806
7	7	0	-0.420838	0.775138	0.453513
8	6	0	-0.077601	2.218859	0.428342
9	6	0	1.337826	2.460102	0.962143
10	6	0	2.384408	1.640135	0.192524
11	6	0	2.113064	-0.484166	1.589373
12	1	0	3.368877	1.728820	0.667880
13	8	0	1.281391	-1.243794	2.046340
14	8	0	4.134162	-0.931693	-0.363140
15	8	0	2.591128	-0.710127	-1.994879
16	8	0	3.190940	-0.068297	2.254942
17	6	0	3.380784	-0.645581	3.565416
18	6	0	3.515425	-1.300411	-2.927929
19	6	0	0.217458	-3.755070	-0.636845
20	1	0	-0.397326	0.445426	1.422048
21	1	0	0.511628	0.340833	-1.357249
22	1	0	-0.822076	2.746704	1.026649
23	1	0	-0.175428	2.558081	-0.606041
24	1	0	1.389426	2.206695	2.029489
25	1	0	1.582813	3.525643	0.888152
26	8	0	2.465385	2.042335	-1.166946
27	1	0	3.776858	-2.313535	-2.612851
28	1	0	4.423760	-0.696885	-2.992263
29	1	0	2.991251	-1.313830	-3.882987
30	1	0	-0.514563	-3.812577	-1.444074
31	1	0	-0.258908	-3.981989	0.318360
32	1	0	1.062095	-4.416663	-0.821627
33	1	0	3.513184	-1.726164	3.479528
34	1	0	2.518994	-0.433928	4.202263
35	1	0	4.282304	-0.175988	3.956743
36	22	0	-2.638642	0.100485	-0.044387
37	17	0	-3.522550	2.111488	0.374290
38	17	0	-2.005858	0.634447	-2.209003
39	17	0	-2.570655	-0.524504	2.183743
40	17	0	-4.378181	-1.158942	-0.604300
41	6	0	3.238782	3.210631	-1.394344
42	1	0	2.784485	4.106767	-0.949676
43	1	0	3.285791	3.343765	-2.477245
44	1	0	4.258258	3.095735	-0.997822

cis-XM (Cis3Tib.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.793219	0.740842	-1.000383

2	6	0	-1.895840	-0.173788	-0.142008
3	6	0	-0.400126	0.083320	-0.496665
4	6	0	0.163391	1.461352	-0.201223
5	8	0	1.363723	1.611695	0.030074
6	8	0	-0.676222	2.464318	-0.309696
7	7	0	0.522061	-0.876041	0.145771
8	6	0	0.216802	-2.279052	-0.232139
9	6	0	-1.248370	-2.638514	0.046312
10	6	0	-2.193106	-1.633601	-0.621209
11	6	0	-2.080836	0.067383	1.365813
12	8	0	-1.237234	0.638653	2.034621
13	8	0	-2.735766	0.744006	-2.209892
14	8	0	-3.619548	1.498952	-0.273328
15	8	0	-3.216580	-0.415916	1.859075
16	6	0	-3.438617	-0.177829	3.264724
17	6	0	-4.495620	2.359209	-1.028706
18	6	0	-0.135832	3.793861	-0.087205
19	1	0	0.417339	-0.771369	1.158417
20	1	0	-0.295016	-0.037660	-1.581607
21	1	0	0.898448	-2.924437	0.324507
22	1	0	0.457569	-2.385769	-1.294851
23	1	0	-1.445890	-2.667168	1.125617
24	1	0	-1.448472	-3.644394	-0.339942
25	1	0	-1.991014	-1.620462	-1.703378
26	1	0	-5.144005	1.762785	-1.674592
27	1	0	-3.911296	3.049454	-1.641770
28	1	0	-5.081588	2.898974	-0.285378
29	1	0	0.653607	3.997556	-0.812470
30	1	0	0.259400	3.859634	0.927729
31	1	0	-0.980809	4.466194	-0.224918
32	1	0	-3.507488	0.895519	3.456941
33	1	0	-2.623055	-0.598691	3.857071
34	1	0	-4.381793	-0.673358	3.491804
35	22	0	2.760879	-0.101942	-0.023385
36	17	0	3.651932	-2.151259	-0.027170
37	17	0	2.272313	-0.124208	-2.292346
38	17	0	2.535697	-0.006678	2.271475
39	17	0	4.506048	1.258943	-0.167851
40	8	0	-3.560708	-1.915543	-0.409771
41	6	0	-4.104075	-2.858815	-1.321393
42	1	0	-3.633111	-3.847719	-1.228162
43	1	0	-4.003056	-2.513181	-2.360528
44	1	0	-5.163998	-2.952004	-1.074440

trans-YM (Trans2Tij.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.431090	0.164161	-1.208626
2	6	0	-1.257723	0.485582	0.043695
3	6	0	-2.751543	0.022548	-0.107833
4	6	0	-2.829885	-1.504701	-0.139185
5	8	0	-1.940750	-2.236134	0.251942
6	8	0	-3.990342	-1.931895	-0.642833
7	7	0	-3.680757	0.555420	0.879705
8	6	0	-3.657736	2.021598	0.915587
9	6	0	-2.255176	2.592961	1.171589
10	6	0	-1.233984	2.065665	0.156383
11	6	0	-0.539690	-0.122413	1.253930
12	1	0	-0.218218	2.368180	0.432349
13	8	0	0.652146	-0.408260	1.301853
14	8	0	0.787575	0.304685	-1.281715
15	8	0	-1.142380	-0.250913	-2.234959
16	8	0	-1.308736	-0.249481	2.326981
17	6	0	-0.691070	-0.860915	3.491602
18	6	0	-0.409332	-0.567068	-3.449540
19	6	0	-4.160627	-3.362659	-0.688669
20	1	0	-3.442775	0.190681	1.799058
21	22	0	2.464493	-0.230266	0.055808
22	17	0	2.346925	1.988116	0.736320
23	17	0	3.930193	0.127918	-1.574410
24	17	0	3.769491	-0.871693	1.735387
25	17	0	1.874612	-2.357443	-0.590787
26	1	0	-3.086208	0.390371	-1.081029
27	1	0	-4.358097	2.354795	1.688324
28	1	0	-4.034443	2.387821	-0.046377

29	1	0	-1.922901	2.342398	2.186274
30	1	0	-2.266962	3.687890	1.106021
31	8	0	-1.530989	2.527334	-1.159672
32	1	0	0.351349	-1.318088	-3.233404
33	1	0	0.056452	0.339857	-3.839150
34	1	0	-1.163258	-0.946834	-4.137081
35	1	0	-4.117584	-3.782930	0.319108
36	1	0	-3.379307	-3.819290	-1.301064
37	1	0	-5.143664	-3.521915	-1.130865
38	1	0	0.171848	-0.273553	3.808445
39	1	0	-0.382147	-1.877572	3.243471
40	1	0	-1.470070	-0.860365	4.252604
41	6	0	-0.897911	3.758954	-1.497076
42	1	0	-1.233045	4.580737	-0.849529
43	1	0	-1.186921	3.981755	-2.526624
44	1	0	0.194072	3.671719	-1.430841

cis-YM (Cis1Tib.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.528178	-0.127785	1.389870
2	6	0	-1.511365	-0.287080	0.225194
3	6	0	-2.588649	0.921990	0.279792
4	6	0	-1.954345	2.250066	-0.139519
5	8	0	-1.867161	2.605053	-1.295263
6	8	0	-1.533228	2.947403	0.920162
7	7	0	-3.767826	0.726226	-0.517156
8	6	0	-4.462587	-0.527968	-0.252040
9	6	0	-3.566070	-1.769323	-0.399002
10	6	0	-2.298004	-1.632038	0.449416
11	6	0	-0.770456	-0.317180	-1.113590
12	8	0	0.441098	-0.252567	-1.285232
13	8	0	0.689578	-0.008949	1.338262
14	8	0	-1.159103	-0.104605	2.557792
15	8	0	-1.593969	-0.396879	-2.148333
16	6	0	-0.982373	-0.332744	-3.464941
17	6	0	-0.333351	0.073628	3.737181
18	6	0	-0.926743	4.230260	0.626983
19	1	0	-3.543149	0.845617	-1.501378
20	22	0	2.317862	-0.111921	-0.144922
21	17	0	2.048018	-2.370761	0.125625
22	17	0	3.866129	0.113872	1.439525
23	17	0	3.536688	-0.243458	-1.999120
24	17	0	1.885456	2.153351	-0.323474
25	1	0	-2.878494	0.984339	1.331471
26	1	0	-5.322608	-0.593335	-0.925521
27	1	0	-4.864247	-0.479756	0.769978
28	1	0	-3.292212	-1.928020	-1.445055
29	1	0	-4.115290	-2.657067	-0.062316
30	1	0	-2.593805	-1.637985	1.509259
31	1	0	0.190592	1.029091	3.678793
32	1	0	0.389597	-0.740493	3.810980
33	1	0	-1.032404	0.058506	4.571984
34	1	0	-1.645562	4.865829	0.104864
35	1	0	-0.035082	4.086351	0.016758
36	1	0	-0.669080	4.651334	1.598087
37	1	0	-0.261553	-1.143314	-3.579921
38	1	0	-0.488082	0.632304	-3.585496
39	1	0	-1.812161	-0.439465	-4.161978
40	8	0	-1.340915	-2.643010	0.208901
41	6	0	-1.638547	-3.922279	0.747561
42	1	0	-2.480347	-4.403874	0.232104
43	1	0	-1.868263	-3.856570	1.821660
44	1	0	-0.739361	-4.524721	0.608936

trans-ZM (Trans1Ti2j.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.323870	0.734085	1.154747

2	6	0	-0.397684	0.648885	-0.073145
3	6	0	1.083423	0.415581	0.346667
4	6	0	1.396192	-0.952741	0.930209
5	8	0	2.554232	-1.362181	0.985891
6	8	0	0.360624	-1.623877	1.375246
7	7	0	2.091166	0.663458	-0.702961
8	6	0	1.985751	2.045606	-1.232356
9	6	0	0.590785	2.288460	-1.815522
10	6	0	-0.518681	2.070220	-0.779024
11	6	0	-0.934358	-0.411614	-1.044192
12	1	0	-1.508095	2.117431	-1.248590
13	8	0	-2.115921	-0.646868	-1.251187
14	8	0	-2.545214	0.638968	1.100605
15	8	0	-0.689856	0.966917	2.281299
16	8	0	0.028695	-1.035603	-1.703800
17	6	0	-0.361774	-2.068956	-2.656436
18	6	0	-1.504807	1.118692	3.475057
19	6	0	0.596000	-2.933170	1.969024
20	1	0	1.922076	0.014208	-1.472848
21	22	0	-4.061524	-0.377860	-0.146865
22	17	0	-4.110177	1.632236	-1.271586
23	17	0	-5.667798	0.094559	1.294835
24	17	0	-5.134318	-1.534313	-1.697279
25	17	0	-3.228606	-2.223847	0.985062
26	1	0	1.300918	1.129034	1.148139
27	1	0	2.760364	2.169529	-1.990809
28	1	0	2.200618	2.735524	-0.412393
29	1	0	0.425187	1.635938	-2.682749
30	1	0	0.517308	3.316898	-2.186310
31	8	0	-0.434618	3.015359	0.274729
32	1	0	-2.096622	0.215964	3.632836
33	1	0	-2.161358	1.982502	3.358878
34	1	0	-0.789510	1.273795	4.280579
35	1	0	1.178428	-2.813807	2.884112
36	1	0	1.135509	-3.562463	1.259848
37	1	0	-0.399477	-3.321827	2.173236
38	1	0	-0.934041	-1.616024	-3.467593
39	1	0	-0.964730	-2.821829	-2.147628
40	1	0	0.581415	-2.479998	-3.010773
41	22	0	4.191477	-0.226115	-0.010663
42	17	0	5.345611	1.169170	-1.302432
43	17	0	3.908363	1.247098	1.736607
44	17	0	3.676212	-1.712670	-1.738880
45	17	0	5.733038	-1.489084	0.943403
46	6	0	-1.107919	4.247985	0.012856
47	1	0	-0.653140	4.789784	-0.826679
48	1	0	-1.002781	4.849085	0.917914
49	1	0	-2.170624	4.076016	-0.197826

cis-ZM (Cis1Ti2b.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.292154	0.562376	1.387571
2	6	0	-0.345756	0.910507	0.219412
3	6	0	1.113833	0.417085	0.539665
4	6	0	1.317369	-1.083512	0.675007
5	8	0	2.423593	-1.589181	0.492047
6	8	0	0.262415	-1.751901	1.060858
7	7	0	2.166312	0.917963	-0.358298
8	6	0	2.227087	2.398578	-0.340544
9	6	0	0.876994	3.002154	-0.736244
10	6	0	-0.267831	2.494252	0.149033
11	6	0	-0.926067	0.362731	-1.095153
12	8	0	-2.098321	0.105656	-1.314224
13	8	0	-2.404558	0.064494	1.315811
14	8	0	-0.755705	0.899949	2.551509
15	8	0	0.004537	0.206304	-2.028015
16	6	0	-0.421122	-0.347453	-3.309819
17	6	0	-1.553753	0.645723	3.739725
18	6	0	0.411694	-3.187949	1.285739
19	1	0	1.946881	0.616062	-1.308646
20	22	0	-3.926123	-0.570278	-0.197974
21	17	0	-4.491245	1.634017	-0.134420
22	17	0	-5.348347	-1.221222	1.373560
23	17	0	-4.999280	-1.030598	-2.078948

24	17	0	-2.705032	-2.547835	-0.173676
25	1	0	1.354653	0.807990	1.535415
26	1	0	3.014589	2.708004	-1.029405
27	1	0	2.533973	2.702040	0.665839
28	1	0	0.651192	2.780336	-1.785410
29	1	0	0.928604	4.092769	-0.643425
30	1	0	-0.085092	2.827584	1.182949
31	1	0	-1.753888	-0.423568	3.824638
32	1	0	-2.494033	1.195552	3.676616
33	1	0	-0.941125	0.999459	4.567015
34	1	0	1.099245	-3.345696	2.118289
35	1	0	0.797757	-3.655022	0.379429
36	1	0	-0.593972	-3.533981	1.508213
37	1	0	-1.082261	0.363584	-3.807458
38	1	0	-0.940665	-1.291191	-3.142002
39	1	0	0.504238	-0.493398	-3.863464
40	22	0	4.169108	-0.348267	-0.062558
41	17	0	5.474120	1.309572	-0.771678
42	17	0	3.964542	0.448733	2.102666
43	17	0	3.576724	-1.059346	-2.194299
44	17	0	5.572528	-1.991140	0.387254
45	8	0	-1.532142	2.912858	-0.289480
46	6	0	-1.878847	4.261303	0.007165
47	1	0	-1.289613	4.976079	-0.581875
48	1	0	-1.741887	4.476229	1.076771
49	1	0	-2.933875	4.362121	-0.248869