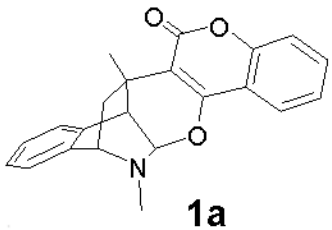
dyych073

exp4 std1h

SAMPLE		DEC. & VT	
date	Mar 4 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-594.1		
wp	4800.8		
vs	45		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	594.1		
rfp	0		
th	2		
ins	100.000		
nm cdc ph			



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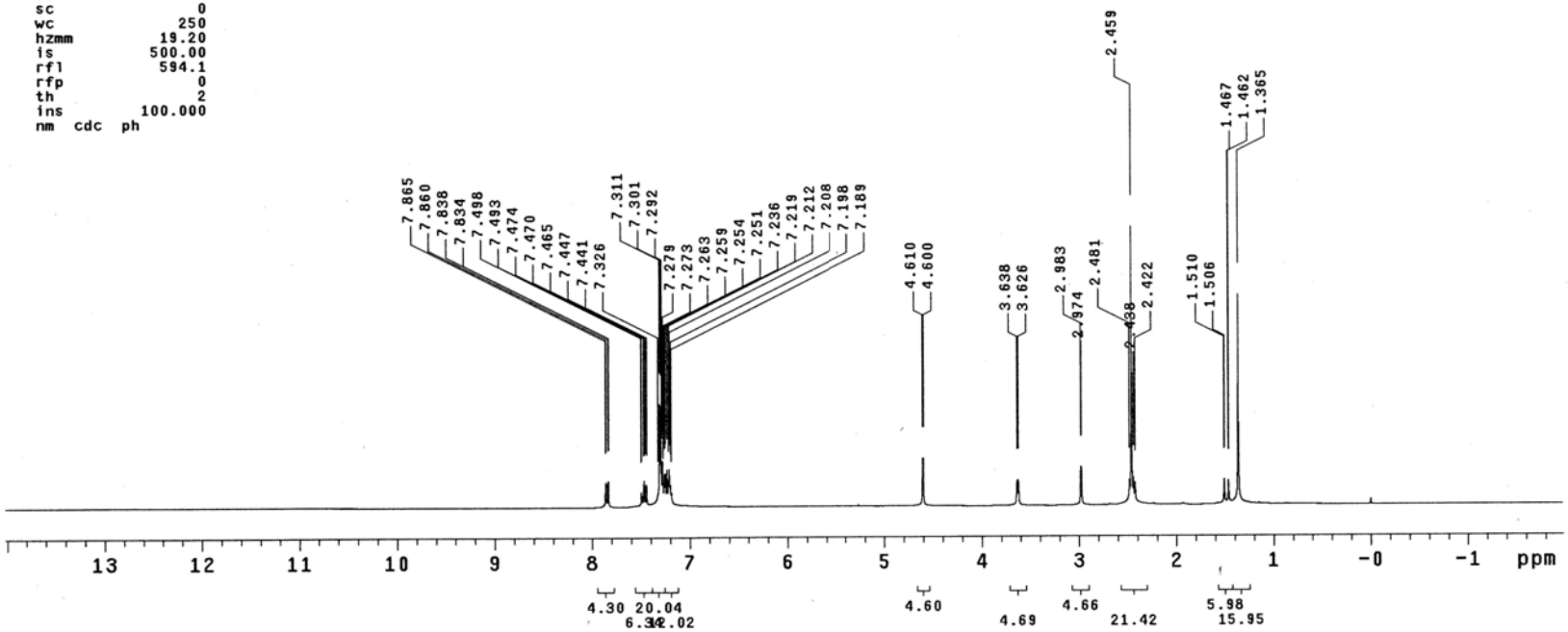
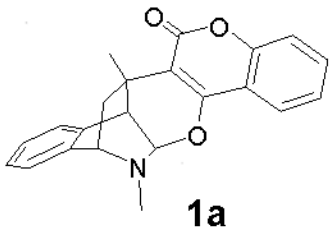


dyych073C

exp5 std13c

SAMPLE		DEC. & VT	
date	Mar 4 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-785.1		
wp	18859.0		
vs	27		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6594.8		
rfp	5809.7		
th	3		
ins	100.000		
nm no ph			



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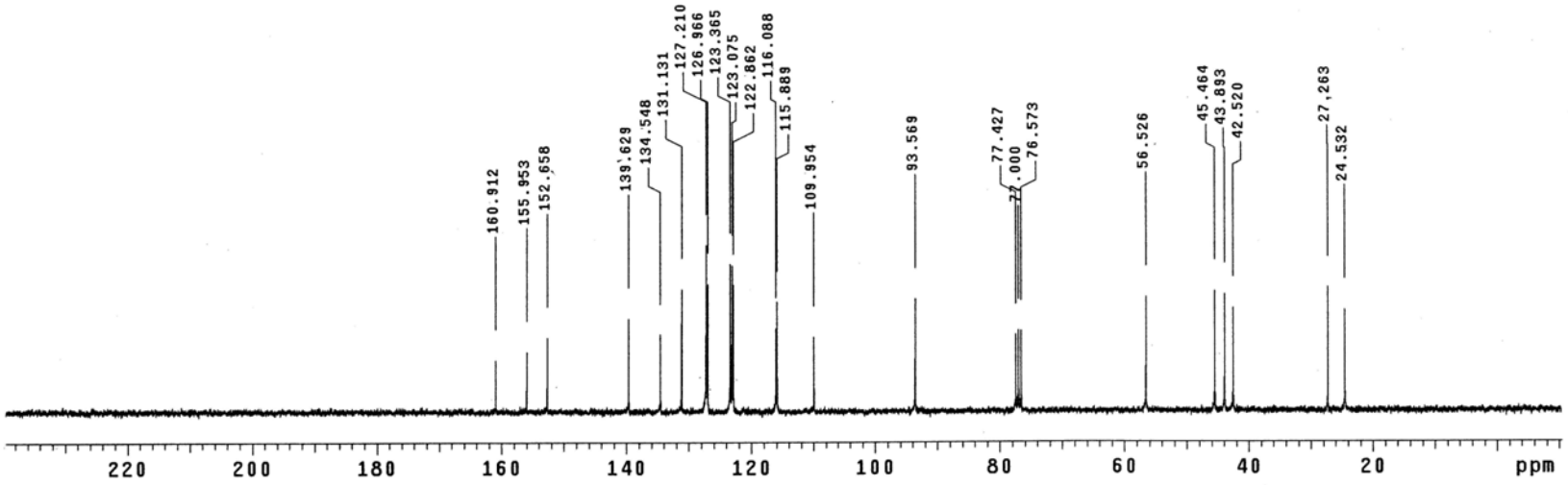
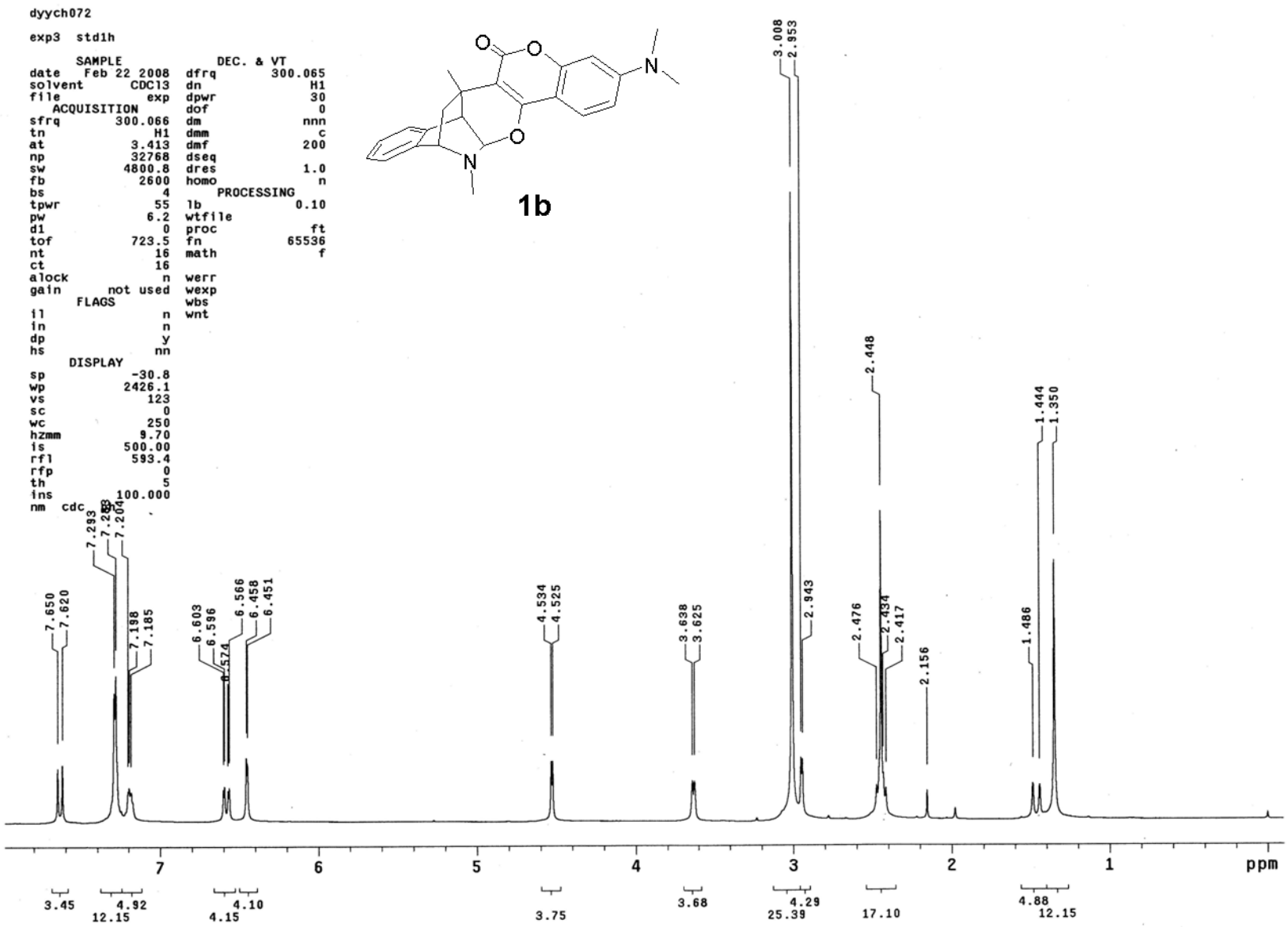
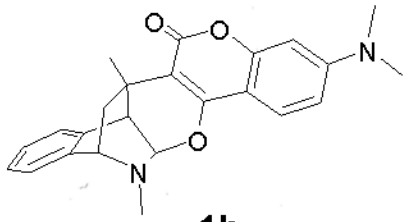



dyych072
exp3 std1h
SAMPLE
date Feb 22 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 300.066
tn H1
at 3.413
np 32768
sw 4800.8
fb 2600
bs 4
tpwr 55
pw 6.2
d1 0
tof 723.5
nt 16
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -30.8
wp 2426.1
vs 123
sc 0
wc 250
hzmm 9.70
is 500.00
rfl 593.4
rfp 0
th 5
ins 100.000
nm cdc
DEC. & VT
dfrq 300.065
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
dseq
dres 1.0
homo n
PROCESSING
lb 0.10
wtfile
proc ft
fn 65536
math f
werr
wexp
wbs
wnt
1b
7.650
7.620
7.293
7.288
7.284
7.204
7.198
7.185
6.603
6.596
6.574
6.566
6.458
6.451
4.534
4.525
3.638
3.625
3.008
2.953
2.943
2.476
2.448
2.434
2.417
2.156
1.486
1.444
1.350
7
6
5
4
3
2
1
ppm
3.45
12.15
4.92
4.15
4.10
3.75
3.68
25.39
4.29
17.10
4.88
12.15

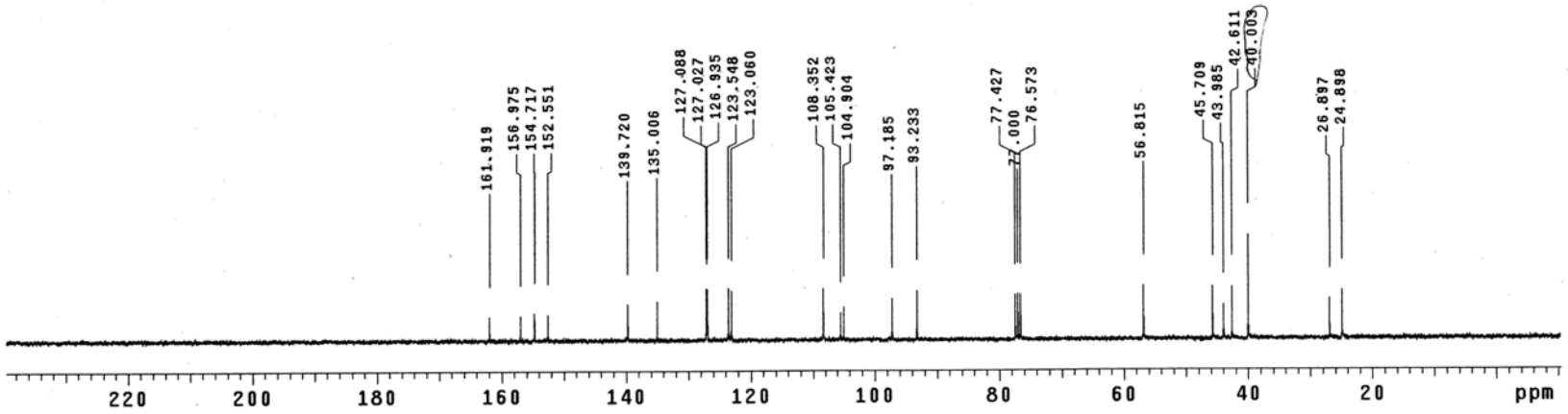
dyych072C

exp2 std13c

SAMPLE		DEC. & VT	
date	Feb 22 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	64	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-784.0		
wp	18859.0		
vs	17		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6593.7		
rfp	5809.7		
th	3		
ins	100.000		
nm no ph			



1b

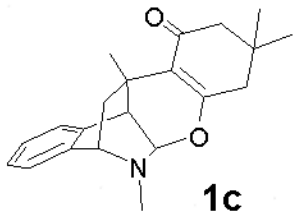


dyych081

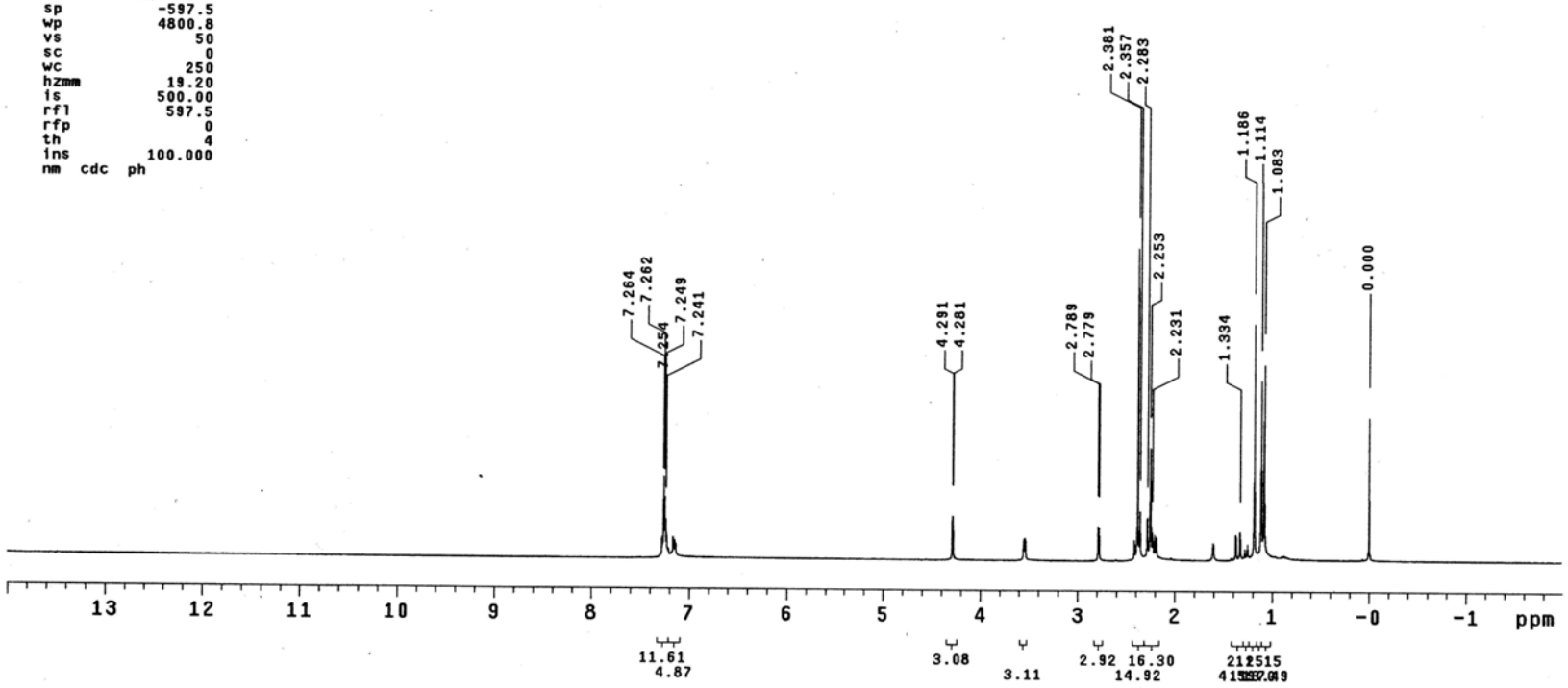
exp3 std1h

SAMPLE		DEC. & VT	
date	Mar 27 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	**PROCESSING**	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-597.5		
wp	4800.8		
vs	50		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	597.5		
rfp	0		
th	4		
ins	100.000		

nm cdc ph



1c

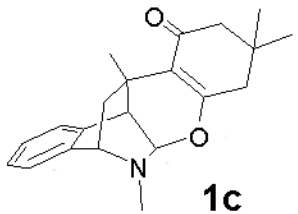


dyych081C

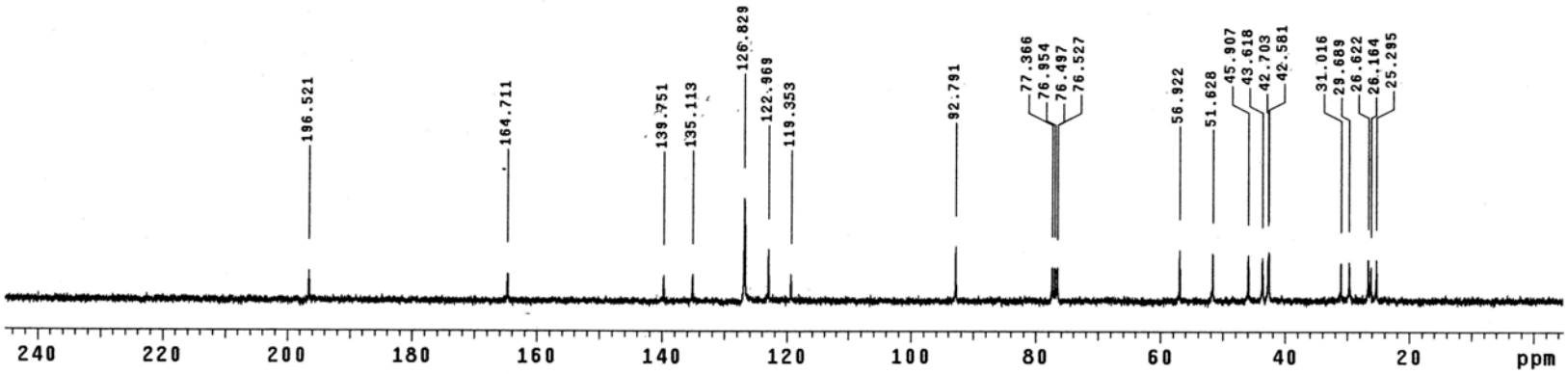
exp6 std13c

SAMPLE		DEC. & VT	
date	Apr 18 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	112		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-356.8		
wp	18859.0		
vs	16		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6166.6		
rfp	5809.7		
th	3		
ins	100.000		

nm no ph



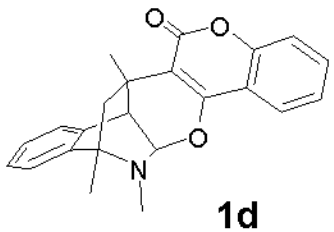
1c



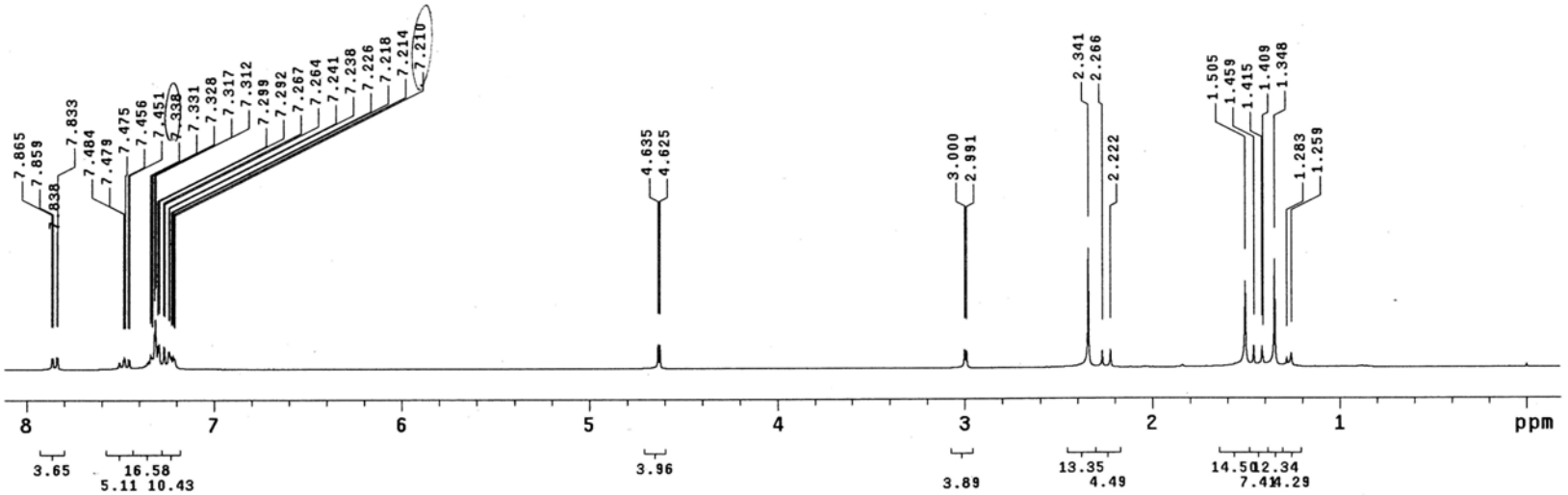
dyych060

exp6 std1h

SAMPLE		DEC. & VT	
date	Jan 4 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-54.5		
wp	2490.1		
vs	19		
sc	0		
wc	250		
hzmm	9.96		
is	500.00		
rfl	598.9		
rfp	0		
th	2		
ins	100.000		
nm cdc ph			



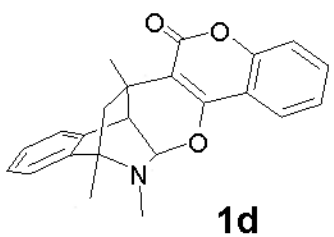
1d



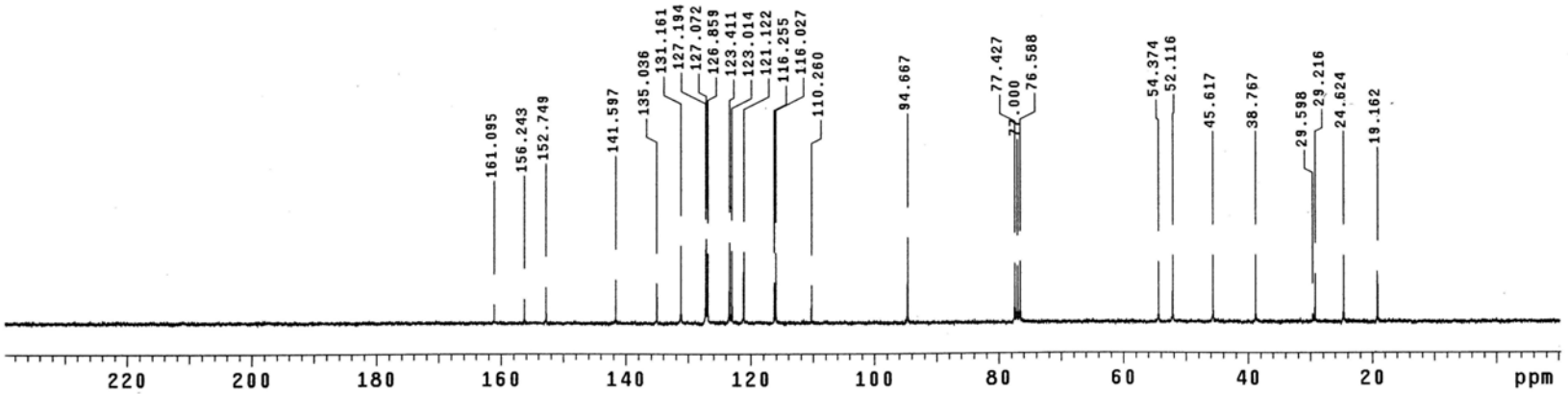
dyych060C

exp7 std13c

SAMPLE		DEC. & VT	
date	Jan 4 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	256	math	f
ct	256		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-779.3		
wp	18859.0		
vs	14		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6589.1		
rfp	5809.7		
th	1		
ins	100.000		
nm no ph			



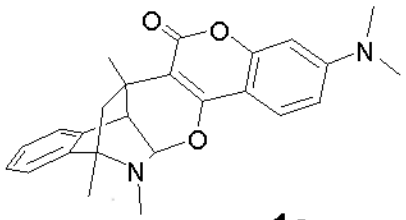
1d



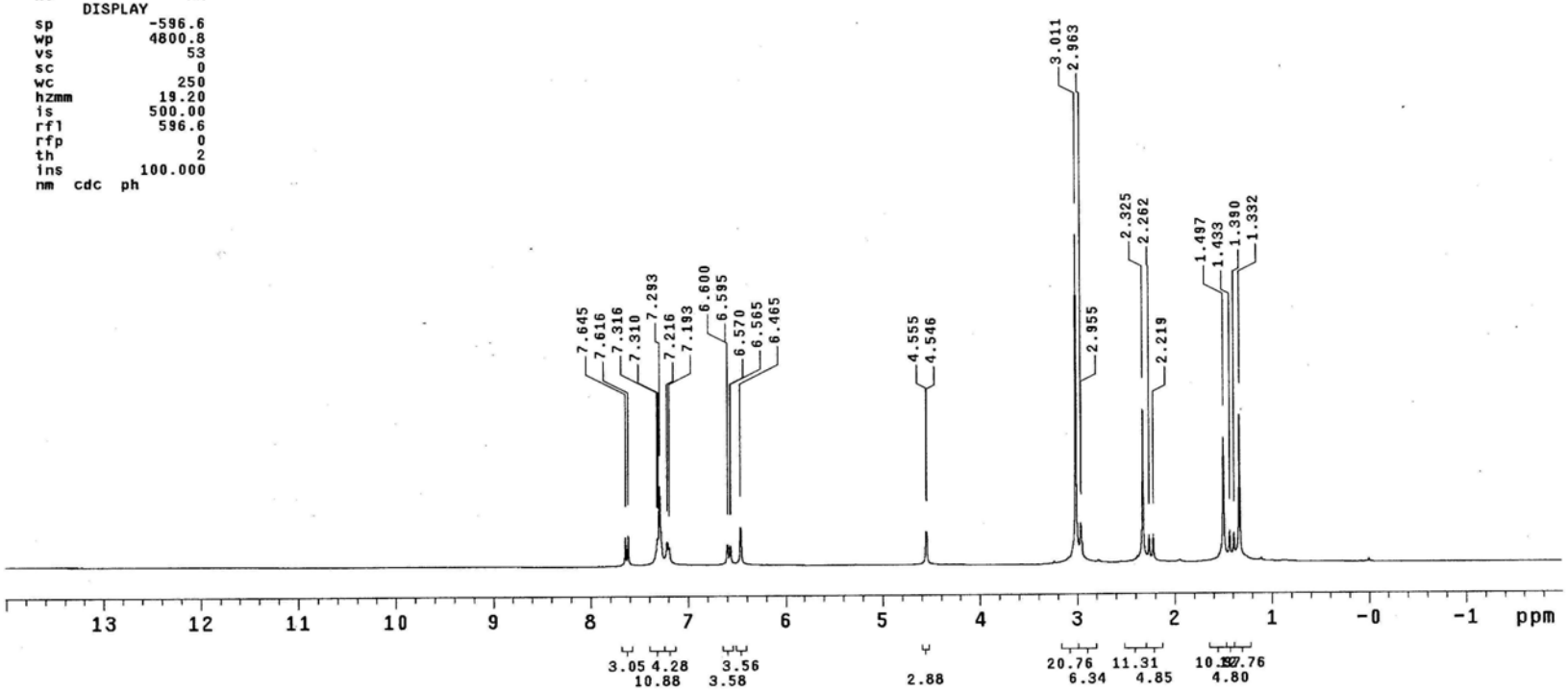
dyych055

exp4 std1h

SAMPLE		DEC. & VT	
date	Jan 4 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	-
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-596.6		
wp	4800.8		
vs	53		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	596.6		
rfp	0		
th	2		
ins	100.000		
nm	cdc ph		



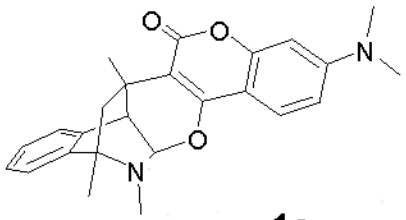
1e



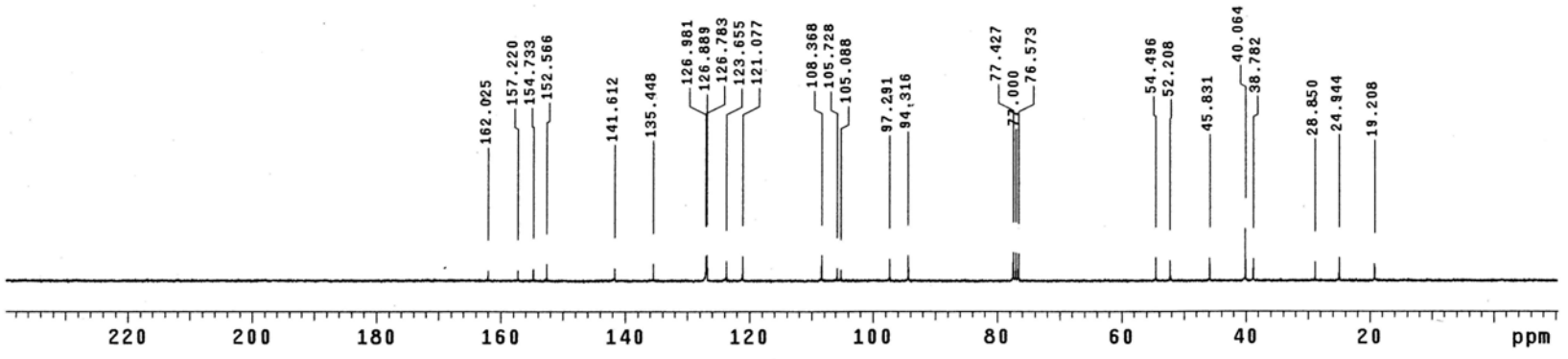
dyych055C

exp1 std13c

SAMPLE		DEC. & VT	
date	Jan 4 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-781.7		
wp	18859.0		
vs	8		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6591.4		
rfp	5809.7		
th	1		
ins	100.000		
nm no ph			



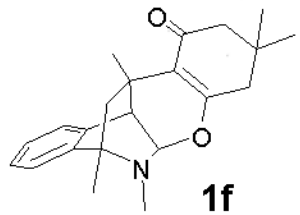
1e



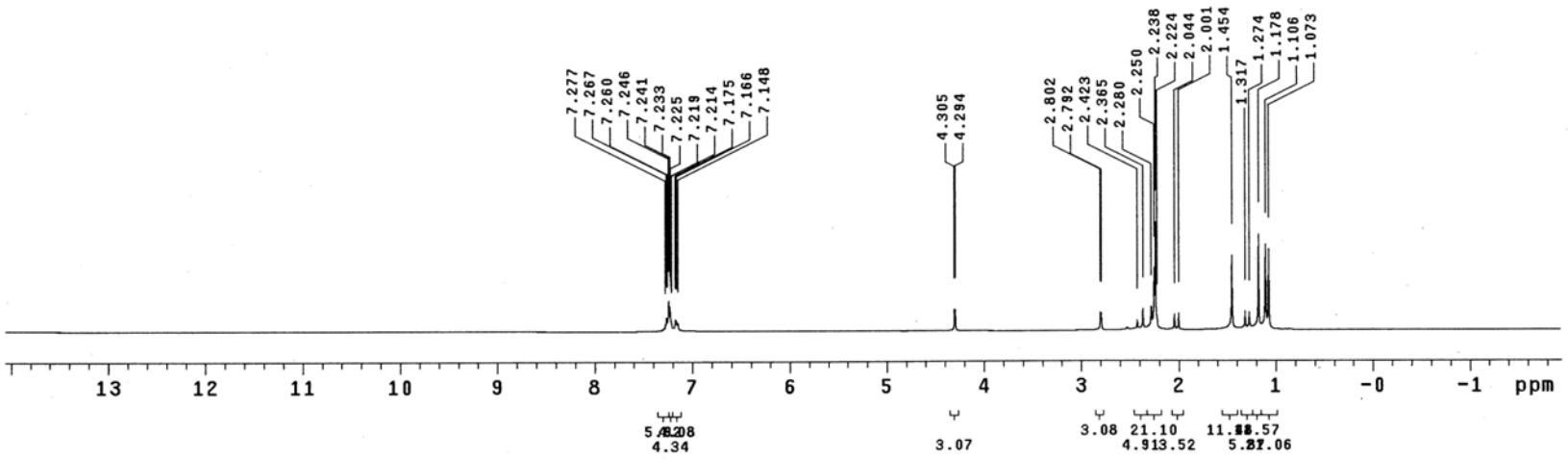
dyych061

exp1 std1h

SAMPLE		DEC. & VT	
date	Jan 17 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-582.4		
wp	4800.8		
vs	17		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	582.4		
rfp	0		
th	1		
ins	100.000		
nm cdc ph			



1f

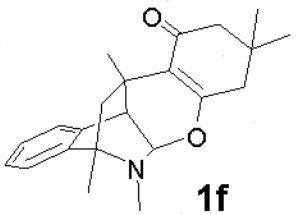


dyych061C

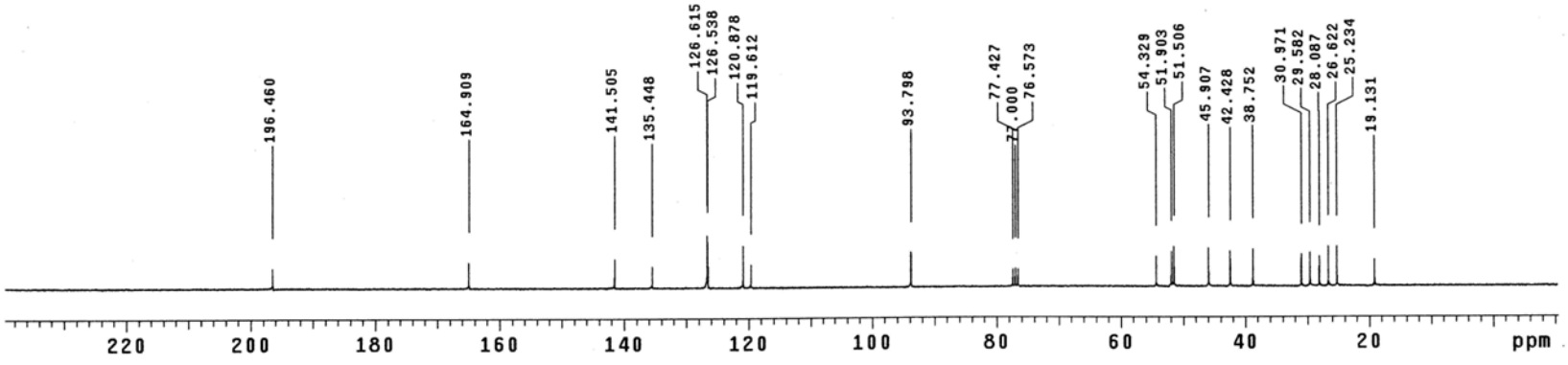
exp2 std13c

SAMPLE		DEC. & VT	
date	Jan 17 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-788.6		
wp	18859.0		
vs	8		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6598.3		
rfp	5809.7		
th	2		
ins	100.000		

nm no ph



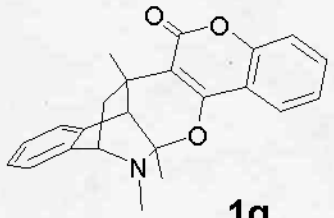
1f



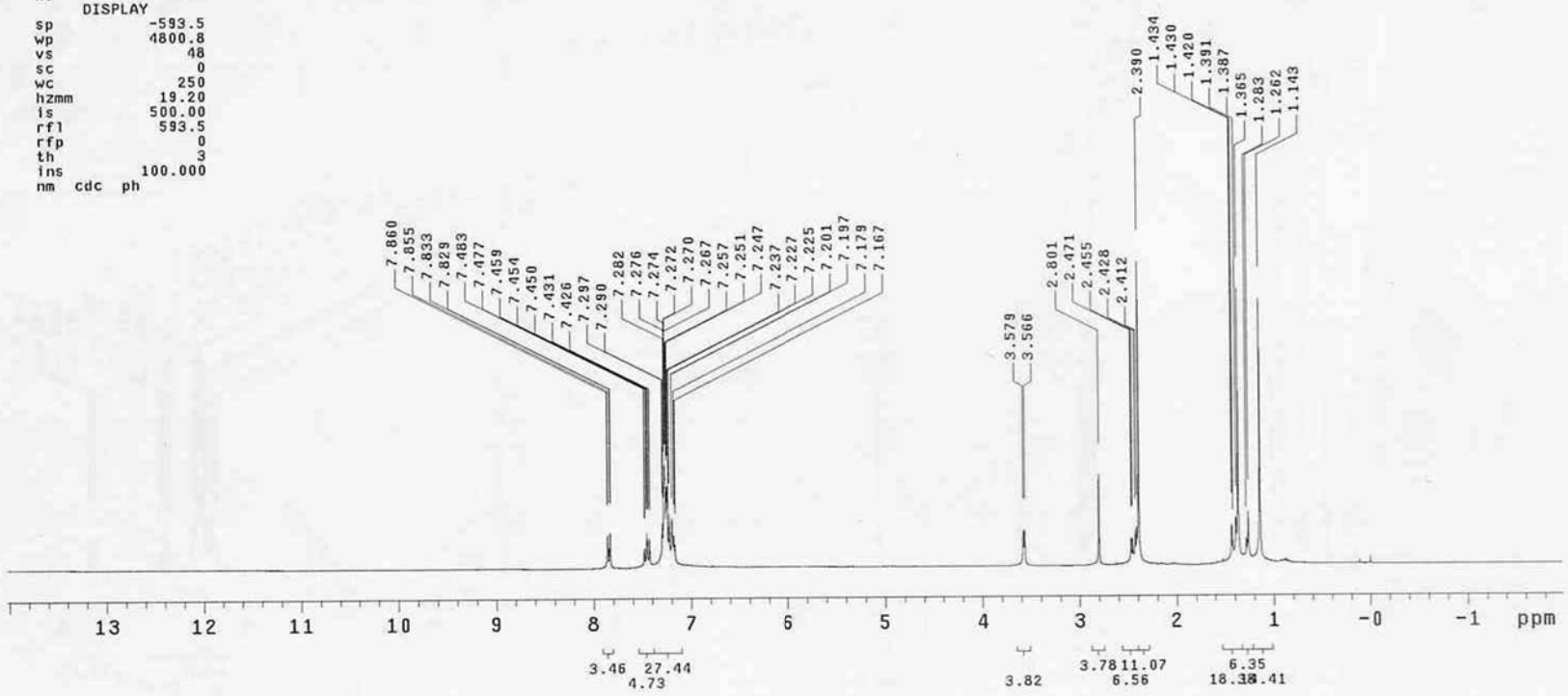
dyych063

exp2 std1h

SAMPLE		DEC. & VT	
date	Jan 17 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-593.5		
wp	4800.8		
vs	48		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	593.5		
rfp	0		
th	3		
ins	100.000		
nm	cdc ph		



1g

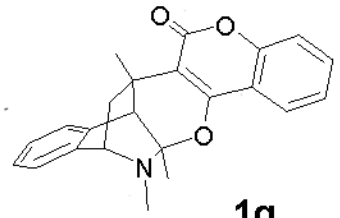


dyych063C

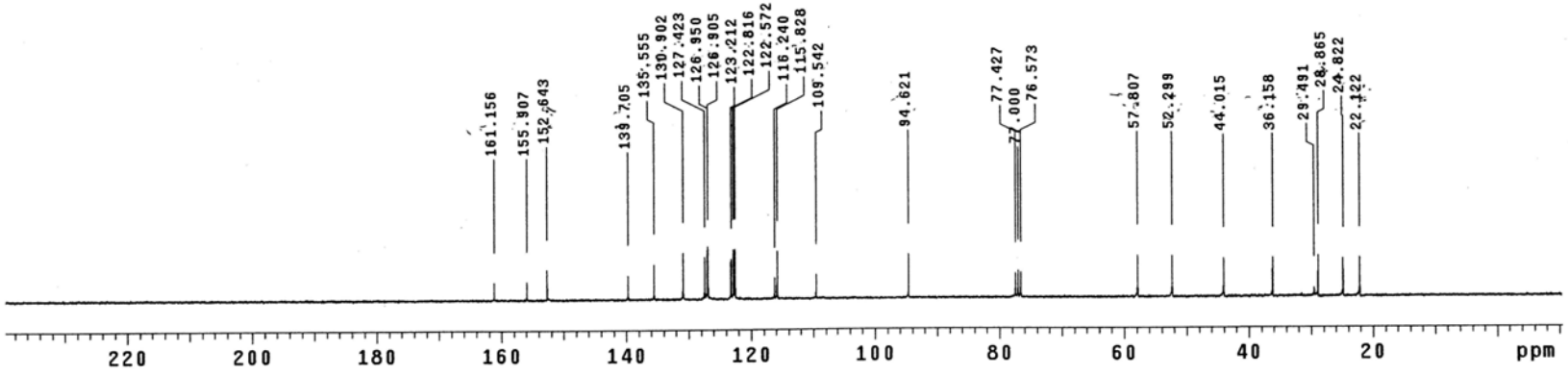
exp3 std13c

SAMPLE		DEC. & VT	
date	Jan 17 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-787.4		
wp	18859.0		
vs	8		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6597.1		
rfp	5809.7		
th	1		
ins	100.000		

nm no ph



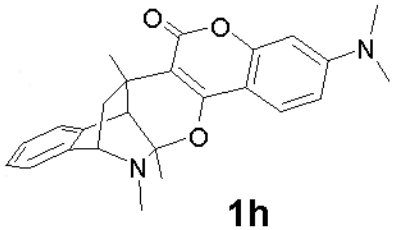
1g



dyych062

exp6 std1h

SAMPLE		DEC. & VT	
date	Jan 14 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-595.9		
wp	4800.8		
vs	113		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	595.9		
rfp	0		
th	4		
ins	100.000		
nm cdc ph			

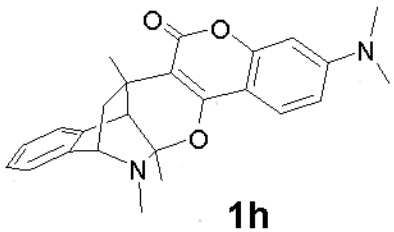


1h

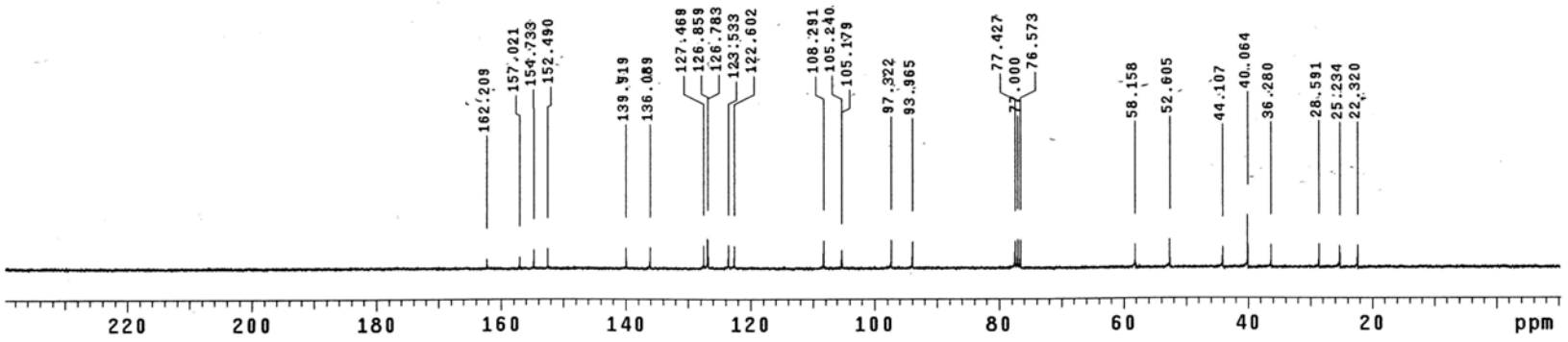
dyych062C

exp2 std13c

SAMPLE		DEC. & VT	
date	Jan 14 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	**PROCESSING**	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-781.7		
wp	18859.0		
vs	8		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6591.4		
rfp	5809.7		
th	1		
ins	100.000		
nm no ph			



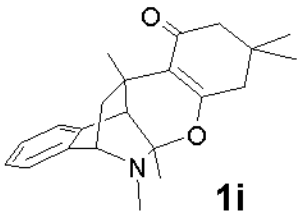
1h



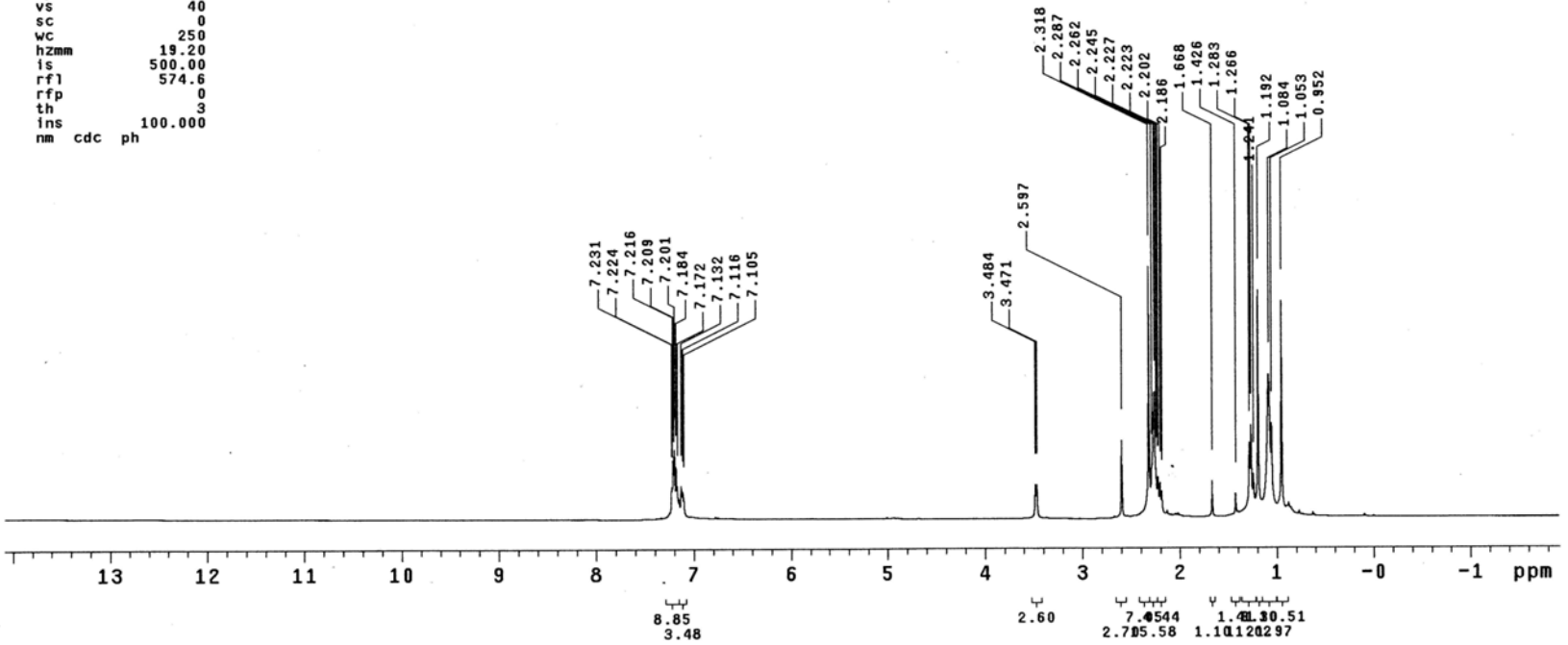
dyych064

exp6 std1h

SAMPLE		DEC. & VT	
date	Jan 18 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-574.6		
wp	4800.8		
vs	40		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	574.6		
rfp	0		
th	3		
ins	100.000		
nm cdc ph			



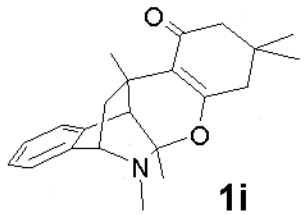
1i



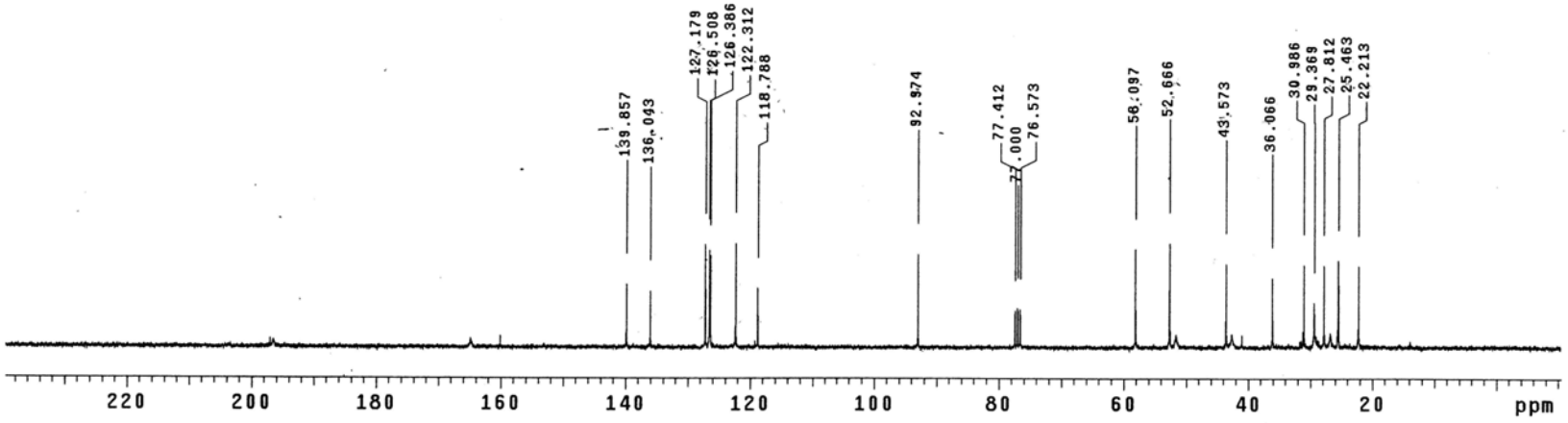
dyych064C

exp7 std13c

SAMPLE		DEC. & VT	
date	Jan 18 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	64		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-789.7		
wp	18859.0		
vs	17		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6599.5		
rfp	5809.7		
th	5		
ins	100.000		
nm no ph			



1i

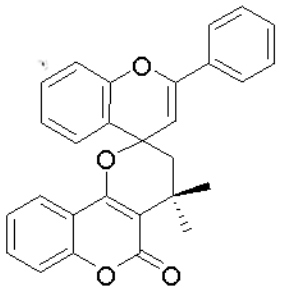


dyyjr098

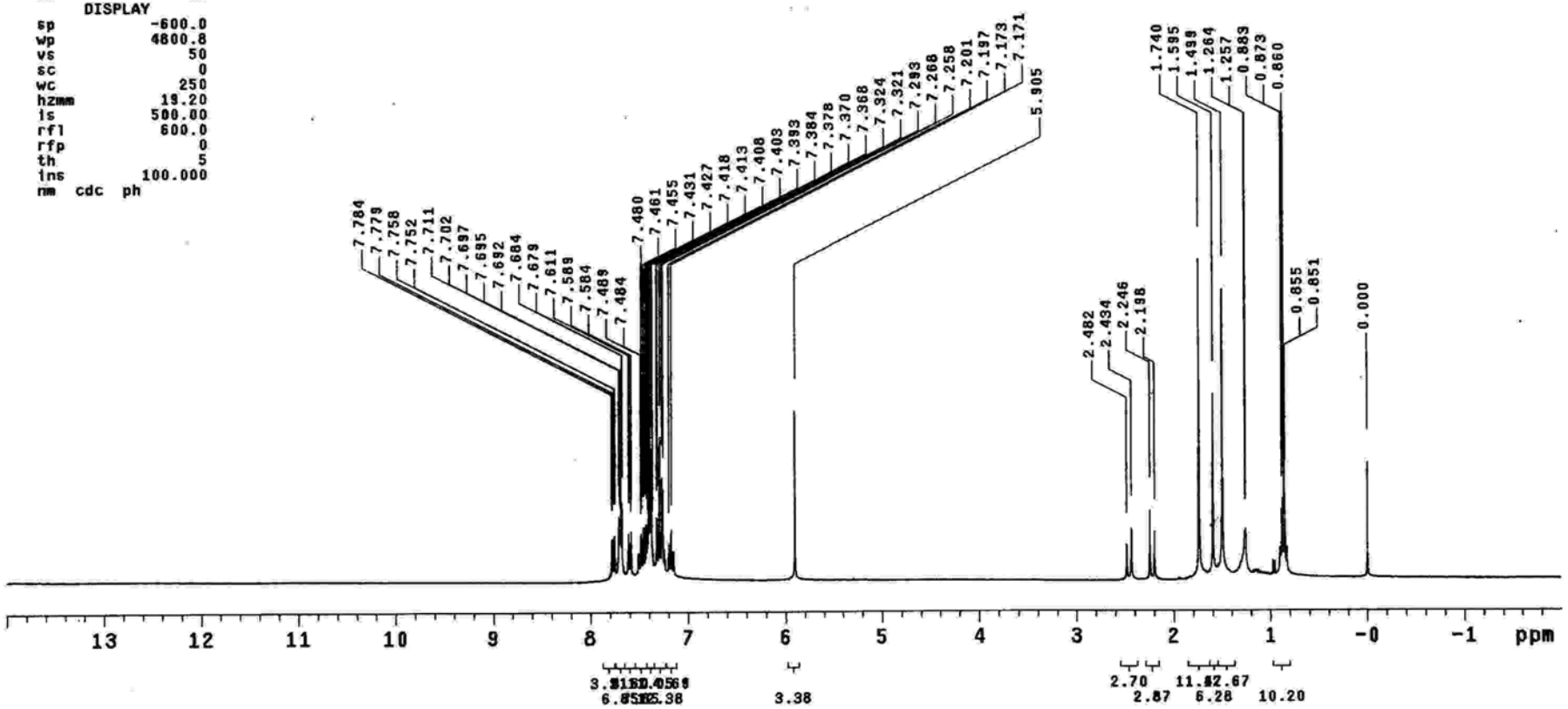
exp6 std1h

SAMPLE		DEC. & VT	
date	Jan 29 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-600.0		
wp	4800.8		
vs	50		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	600.0		
rfp	0		
th	5		
ins	100.000		

nm cdc ph



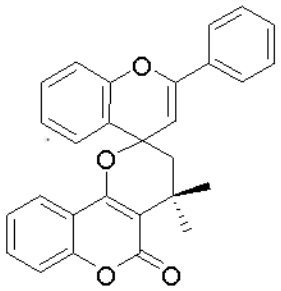
2a



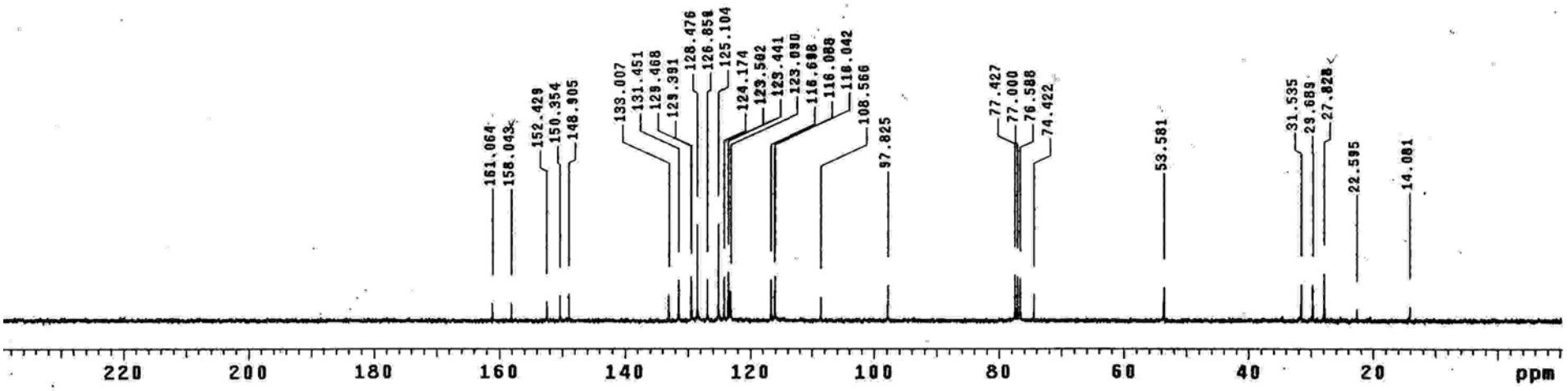
dyyjr152C

exp2 std13c

SAMPLE		DEC. & VT	
date	Nov 6 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	6708
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	**PROCESSING**	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	256	math	f
ct	176		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-778.2		
wp	18859.0		
vs	17		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6587.9		
rfp	5809.7		
th	2		
ins	100.000		
nm no ph			



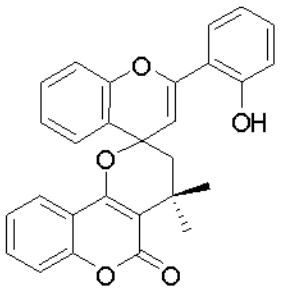
2a



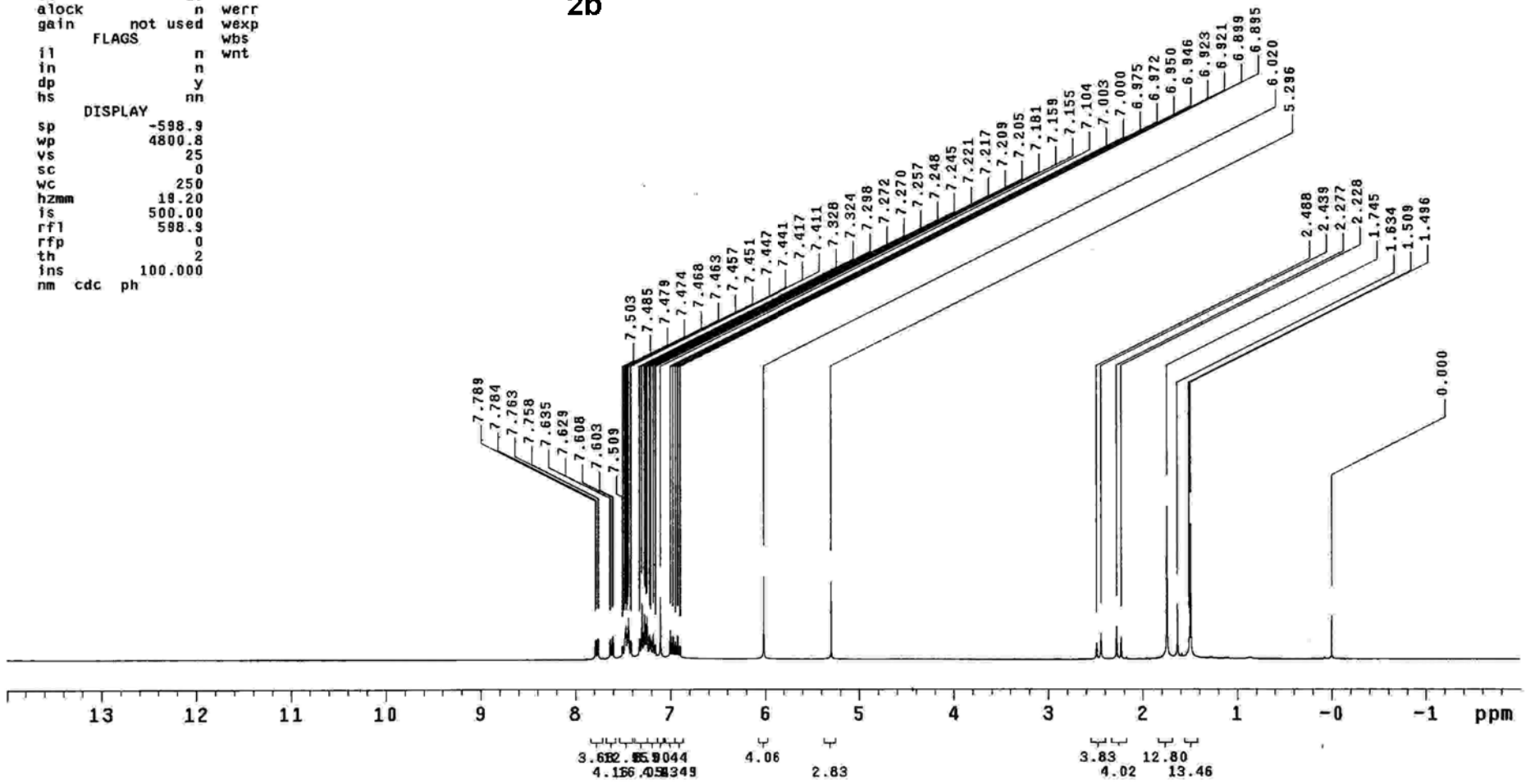
dyyjr105

exp1 std1h

SAMPLE		DEC. & VT	
date	Mar 6 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	**PROCESSING**	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-598.9		
wp	4800.8		
vs	25		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	598.9		
rfp	0		
th	2		
ins	100.000		
nm	cdc ph		



2b

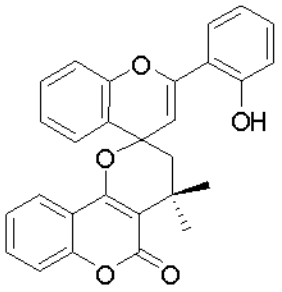


13C OBSERVE

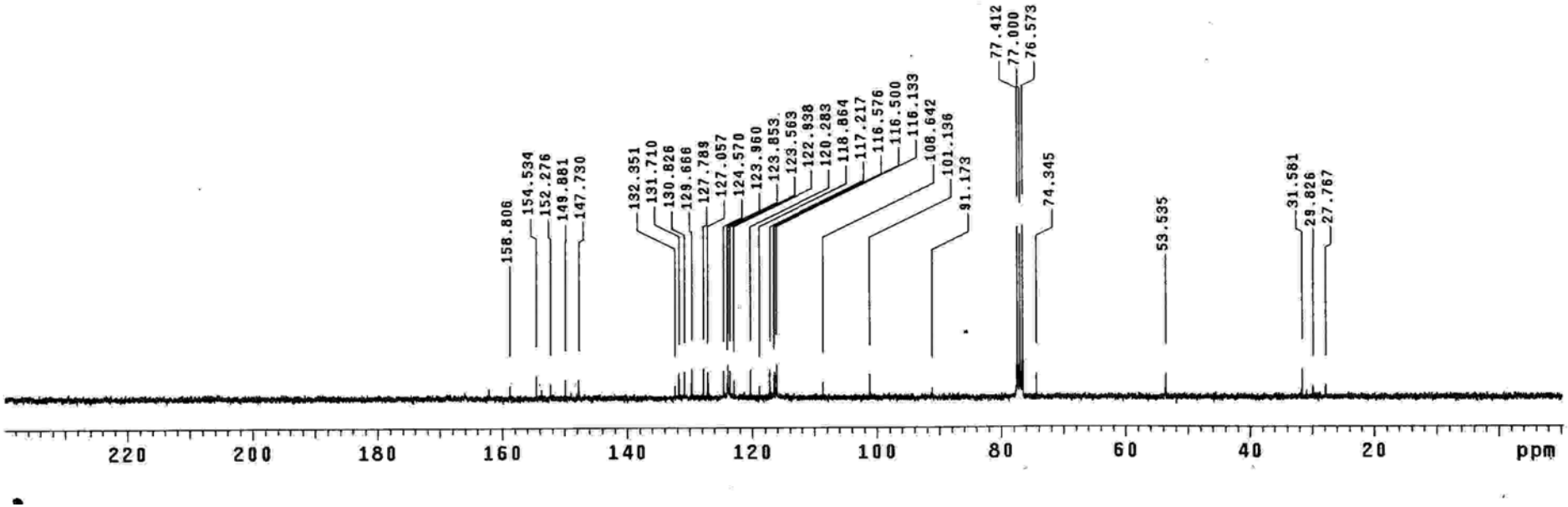
exp1 std13c

SAMPLE		DEC. & VT	
date	Oct 15 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	6708
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	1024	math	f
ct	736		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-773.6		
wp	18859.0		
vs	29		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6583.3		
rfp	5809.7		
th	2		
ins	100.000		

nm no ph



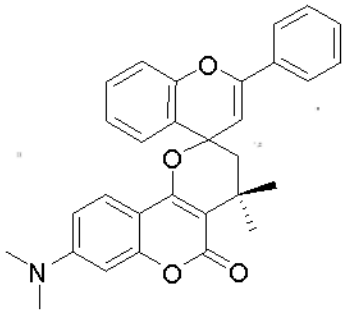
2b



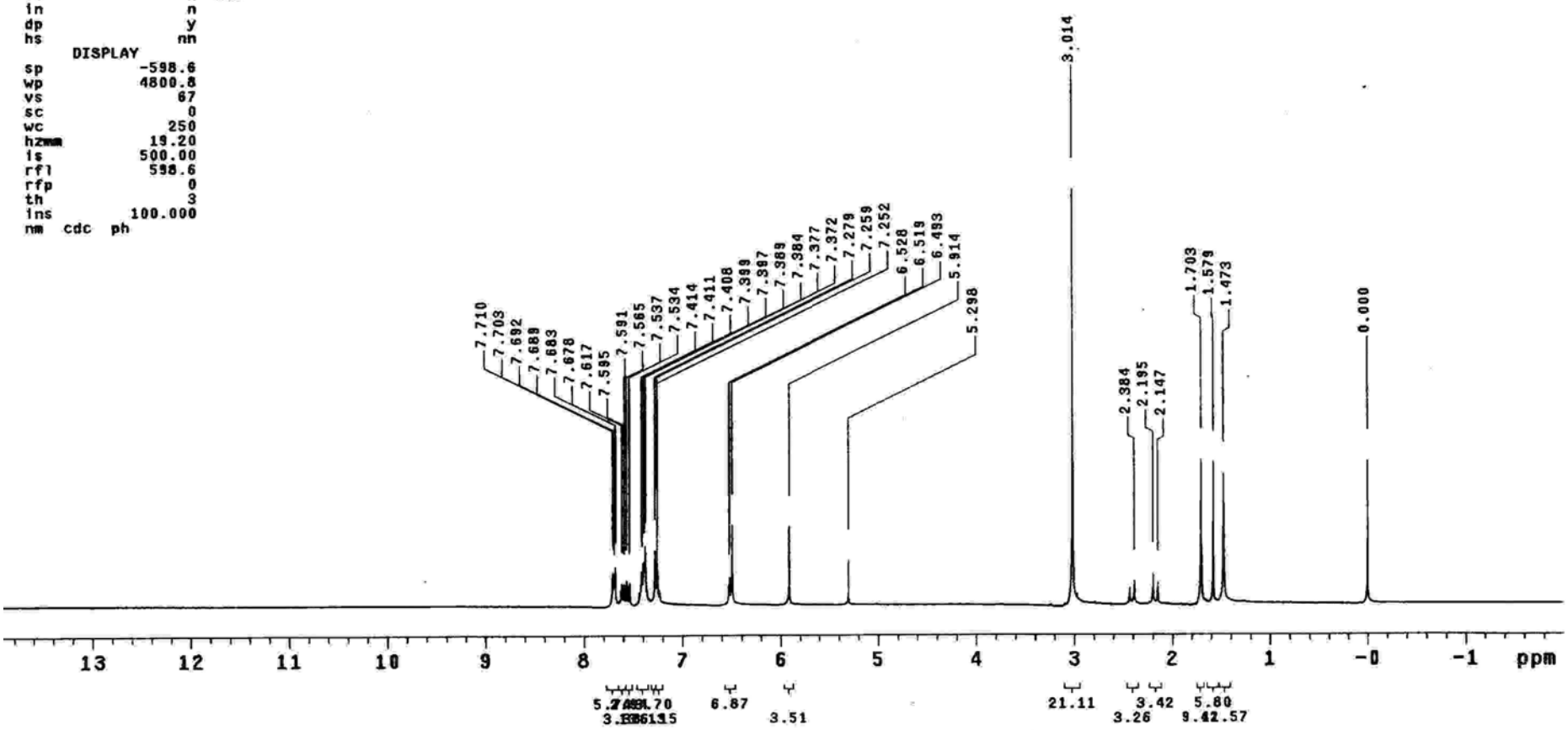
dyyjr016

exp1 stdlh

SAMPLE		DEC. & VT	
date	Feb 5 2007	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-598.6		
wp	4800.8		
vs	67		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	598.6		
rfp	0		
th	3		
ins	100.000		
nm cdc ph			



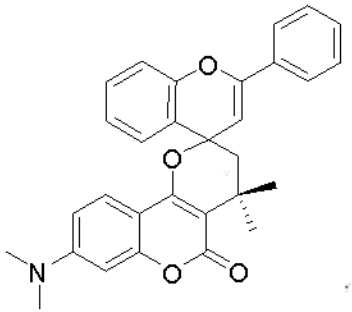
2c



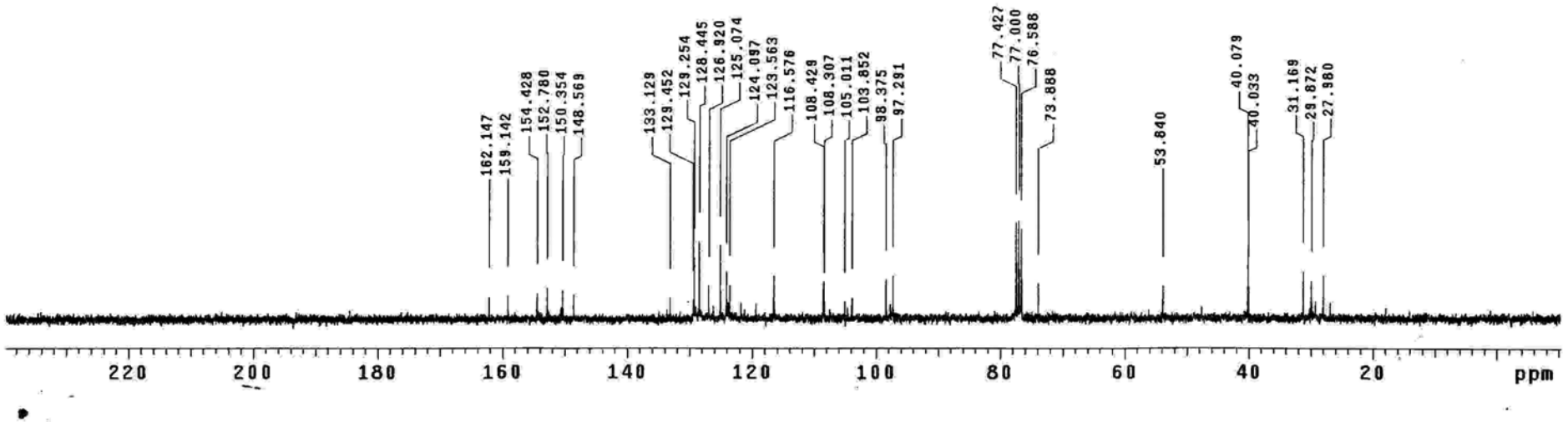
dyyjt035C

exp3 std13c

SAMPLE		DEC. & VT	
date	Jul 18 2007	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-777.0		
wp	18859.0		
vs	17		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6586.8		
rfp	5809.7		
th	3		
ins	100.000		
nm no ph			



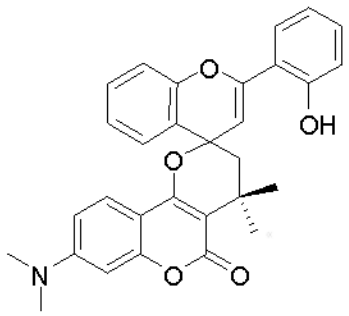
2c



dyyjr111

exp1 std1h

SAMPLE		DEC. & VT	
date	Mar 27 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-597.5		
wp	4800.8		
vs	69		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	597.5		
rfp	0		
th	2		
ins	100.000		
nm cdc ph			



2d

7.641 7.636 7.615 7.610 7.565 7.535 7.450 7.442 7.436 7.425 7.420 7.416 7.410 7.398 7.392 7.316 7.312 7.288 7.266 7.259 7.242 7.236 7.226 7.223 7.199 7.196 7.130 6.992 6.989 6.964 6.961 6.938 6.934 6.912 6.888 6.532 6.524 6.502 6.494 6.469 6.461 5.984 3.006 2.436 2.388 2.222 2.174 1.705 1.622 1.471 0.883 0.863 0.000

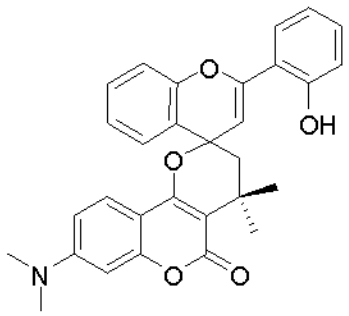
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

2.89 3.01 1.85 3.68 6.32 2.94 18.34 3.00 3.01 6.88 3.32 3.74

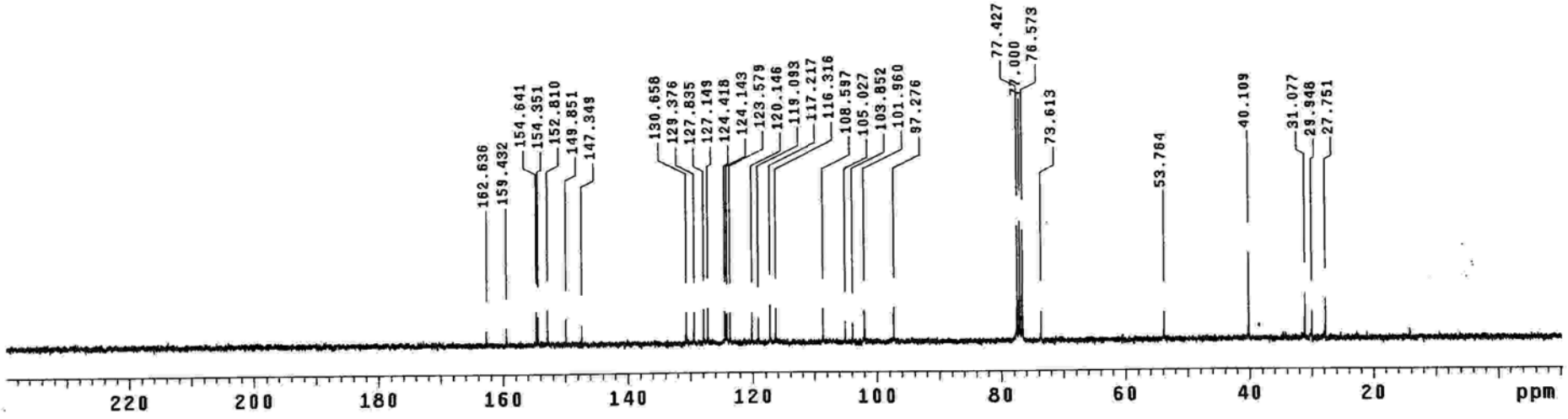
dyyjr150C

exp6 std13c

SAMPLE		DEC. & VT	
date	Oct 17 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	6708
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	512	math	f
ct	400		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-774.7		
wp	18859.0		
vs	20		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6584.5		
rfp	5809.7		
th	2		
ins	100.000		
nm no ph			



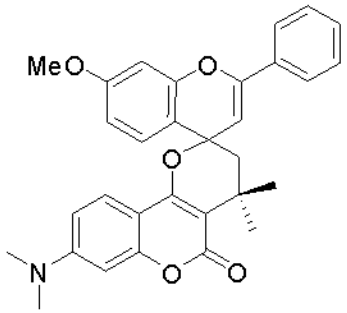
2d



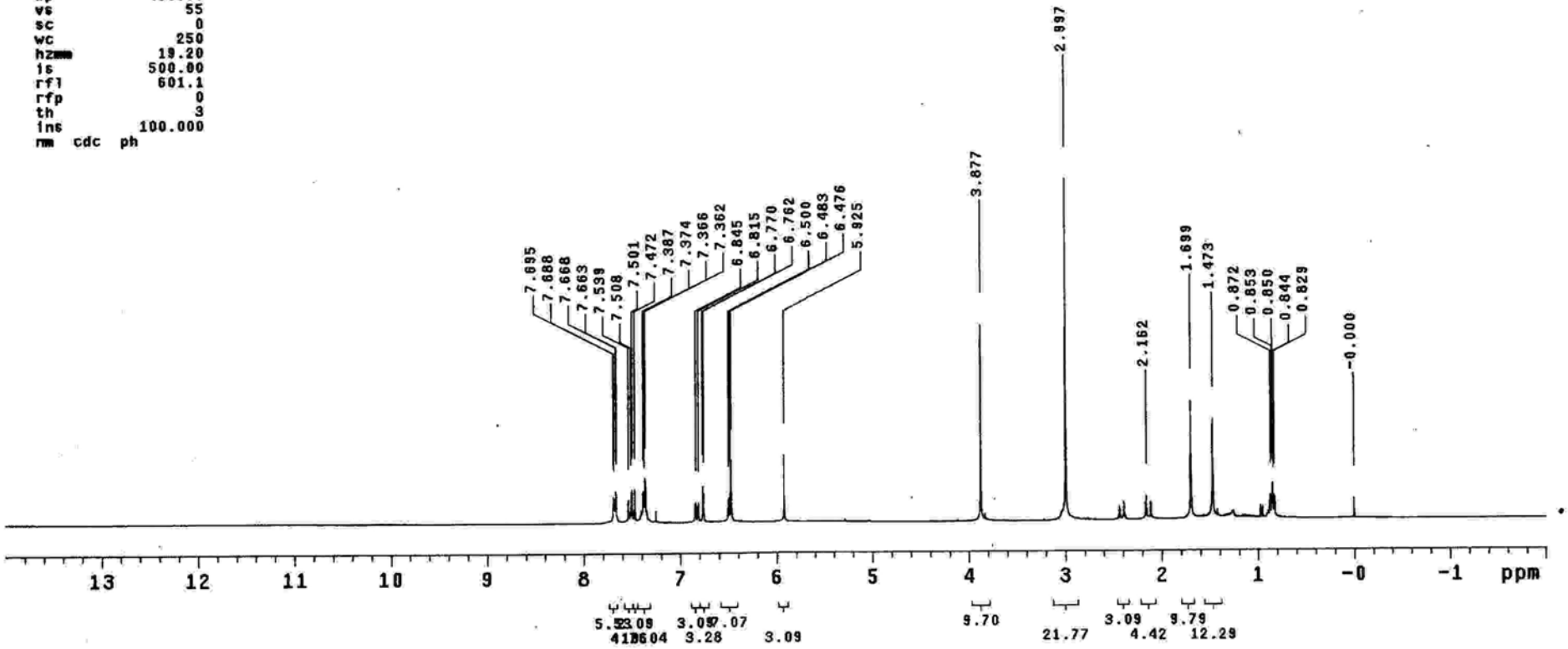
dyyjr091

exp4 std1h

SAMPLE		DEC. & VT	
date	Jan 14 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-601.1		
wp	4800.8		
vs	55		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	601.1		
rfp	0		
th	3		
ins	100.000		
nm cdc ph			



2e

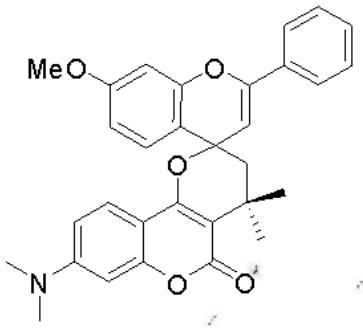


dyyjt036C

exp5 std13c

SAMPLE	
date	Jul 18 2007
solvent	CDCl3
file	exp
ACQUISITION	
sfrq	75.460
tn	C13
at	0.869
np	32768
sw	18858.0
fb	10400
bs	16
tpwr	55
pw	4.8
d1	2.000
tof	1220.8
nt	128
ct	128
alock	n
gain	not used
FLAGS	
il	n
in	n
dp	y
hs	nn
DISPLAY	
sp	-778.2
wp	18859.0
vs	18
sc	0
wc	250
hzmm	75.44
is	500.00
rfl	6587.9
rfp	5809.7
th	2
ins	100.000
nm no ph	

DEC. & VT	
dfrq	300.065
dn	H1
dpwr	40
dof	0
dm	yyy
dmm	w
dmf	7704
dseq	
dres	1.0
homo	n
PROCESSING	
lb	1.00
wtfile	
proc	ft
fn	not used
math	f
werr	
wexp	
wbs	
wnt	



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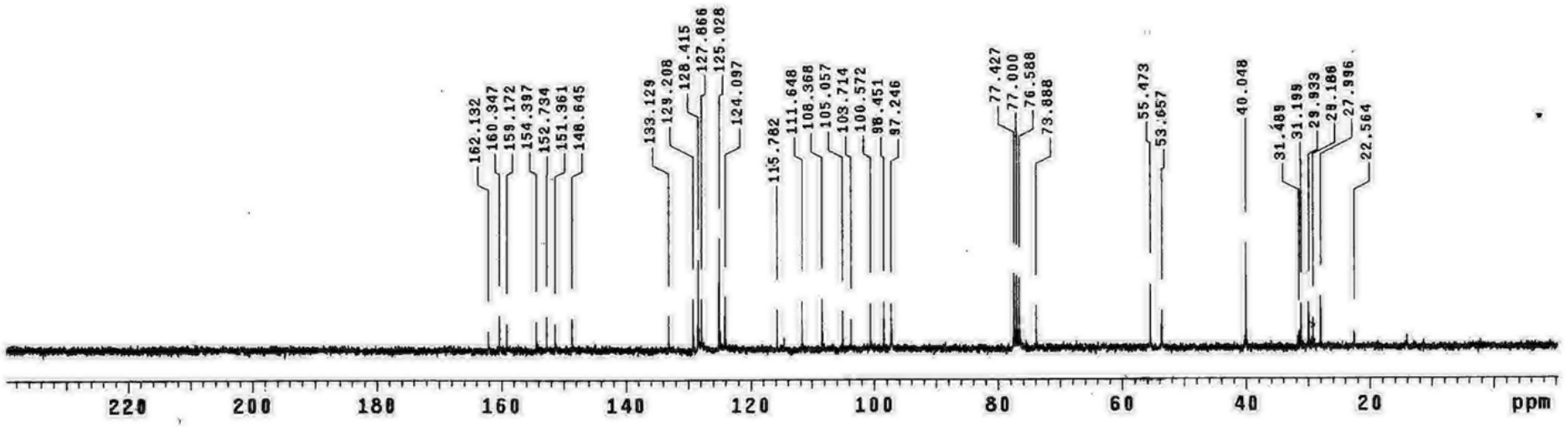
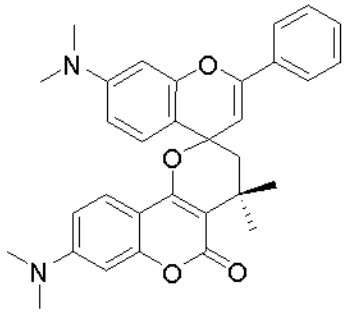


dyyjr112

expl stdlh

SAMPLE		DEC. & VT	
date	Apr 7 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
dl	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-599.7		
wp	4800.8		
vs	61		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	599.7		
rfp	0		
th	2		
ins	100.000		
nm cdc ph			



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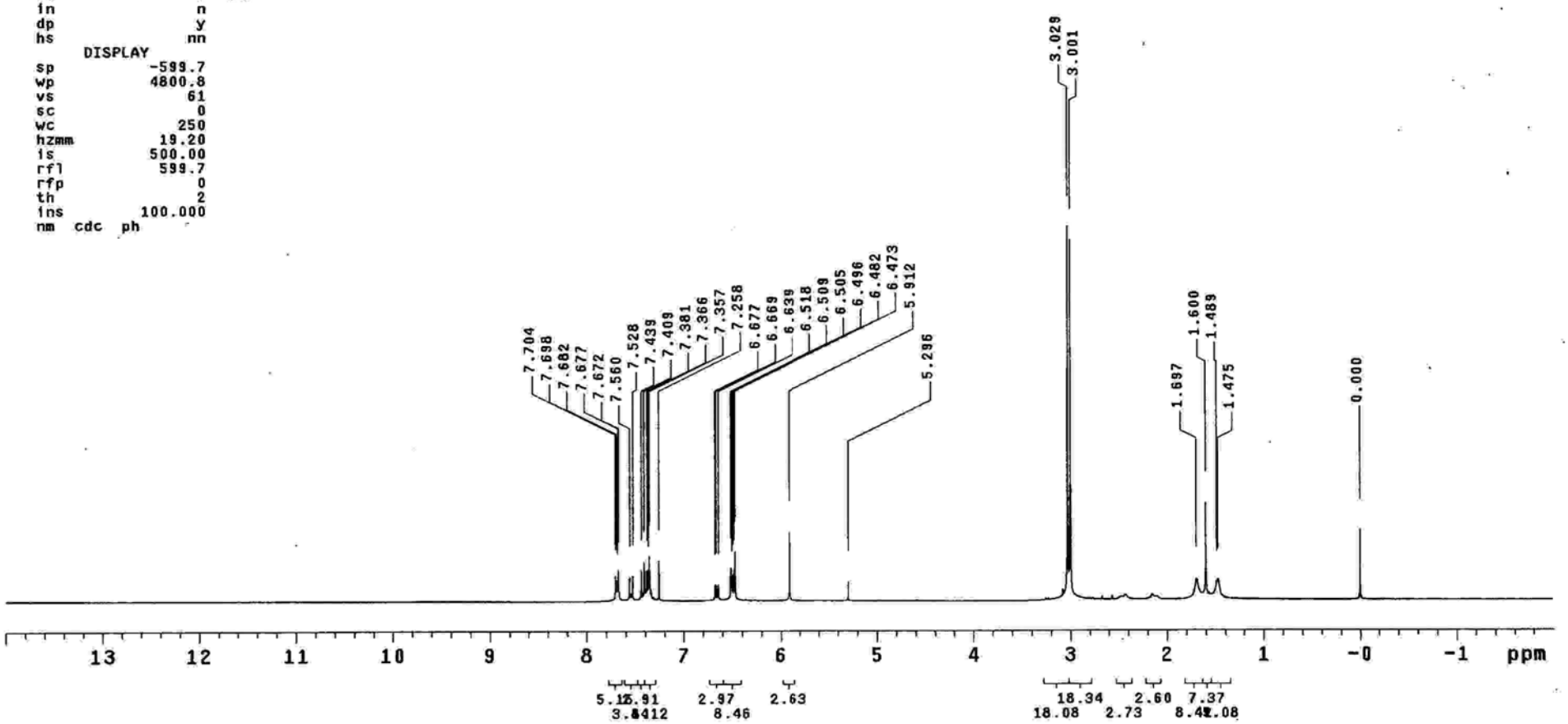
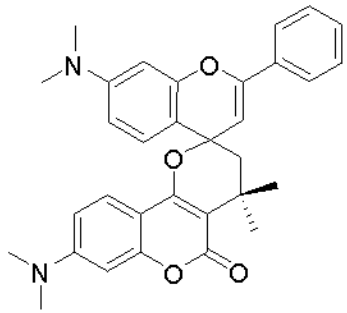


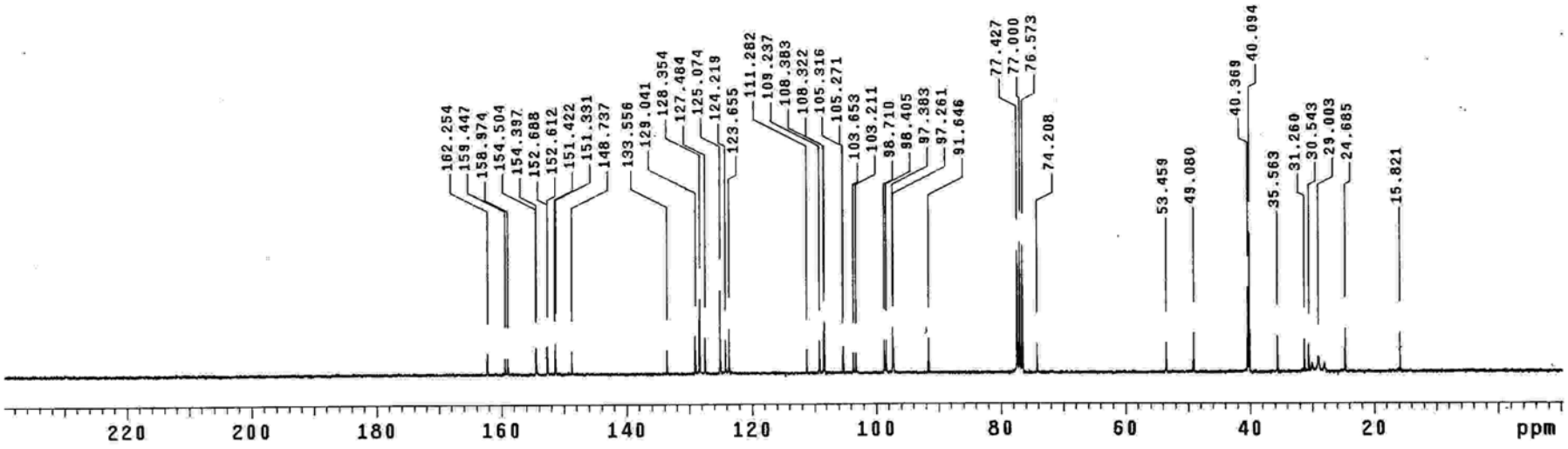
DYYJR148

exp5 std13c

SAMPLE		DEC. & VT	
date	Oct 2 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	6708
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	3072	math	f
ct	3072		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-777.0		
wp	18859.0		
vs	22		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6586.8		
rfp	5809.7		
th	2		
ins	100.000		
nm no ph			



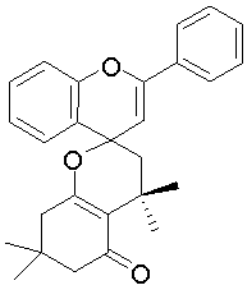
2f



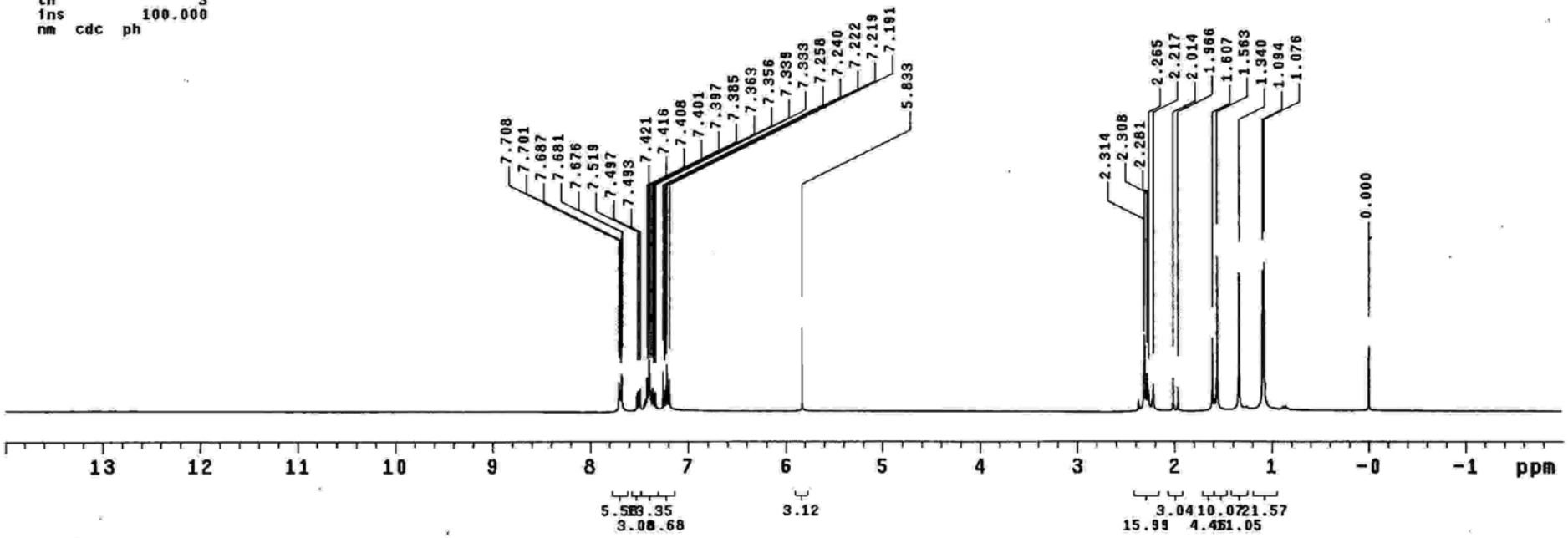
dyyjr110

exp2 std1h

SAMPLE		DEC. & VT	
date	Mar 21 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	**PROCESSING**	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-598.9		
wp	4800.8		
vs	25		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	598.9		
rfp	0		
th	3		
ins	100.000		
nm cdc ph			



2g

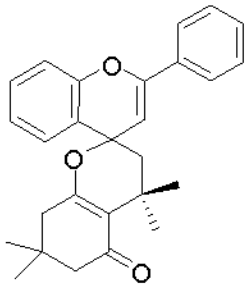


dyyjr154C

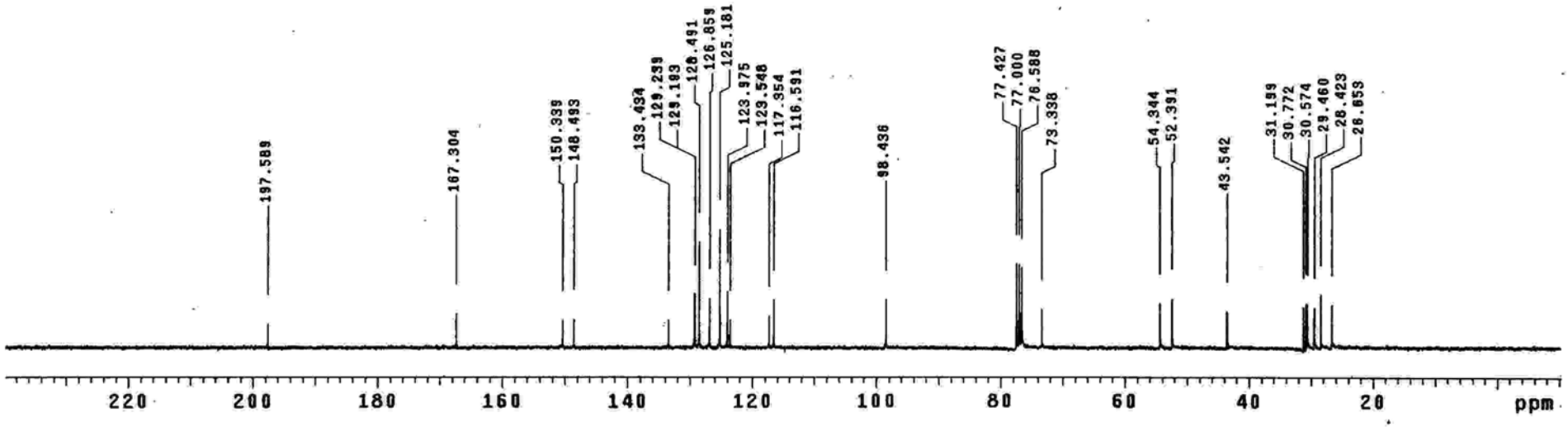
exp4 std13c

SAMPLE		DEC. & VT	
date	Nov 10 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	6708
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	1024	math	f
ct	656		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-774.7		
wp	18859.0		
vs	20		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6584.5		
rfp	5809.7		
th	2		
ins	100.000		

nm no ph



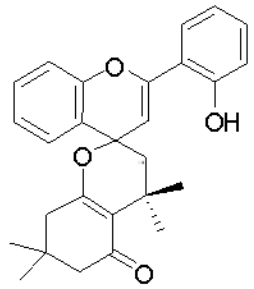
2g



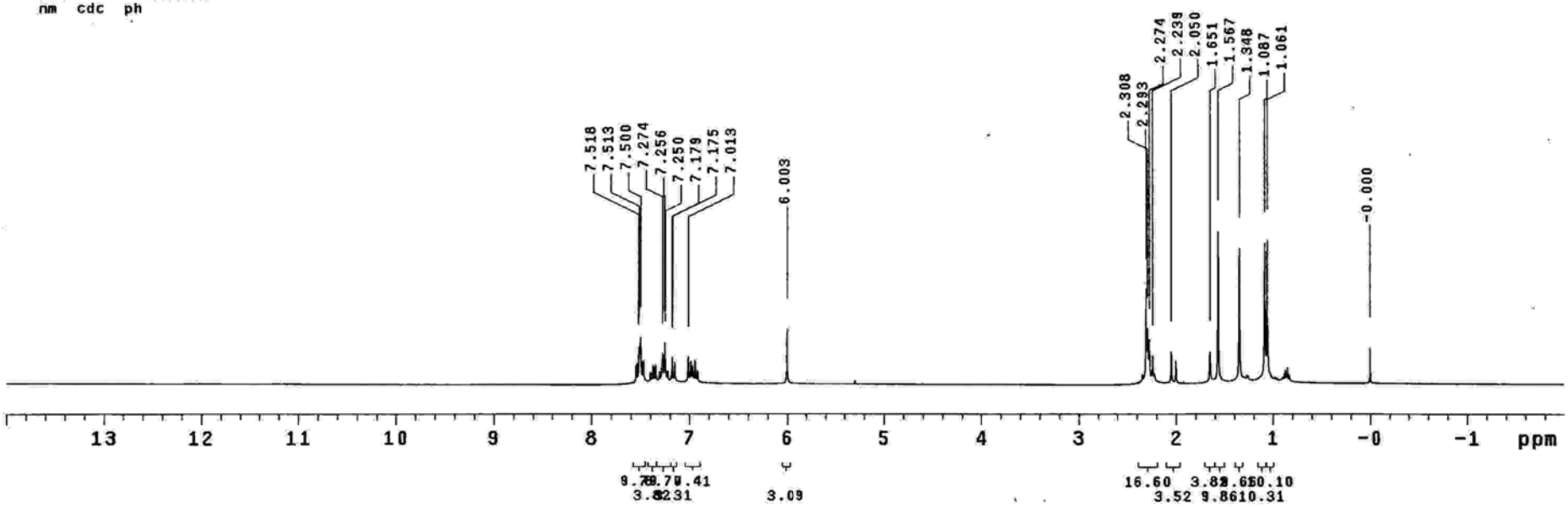
dyyjr118

exp2 std1h

SAMPLE		DEC. & VT	
date	Apr 25 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	**PROCESSING**	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-599.5		
wp	4800.8		
vs	25		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	599.5		
rfp	0		
th	4		
ins	100.000		
nm cdc ph			



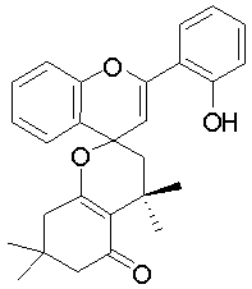
2h



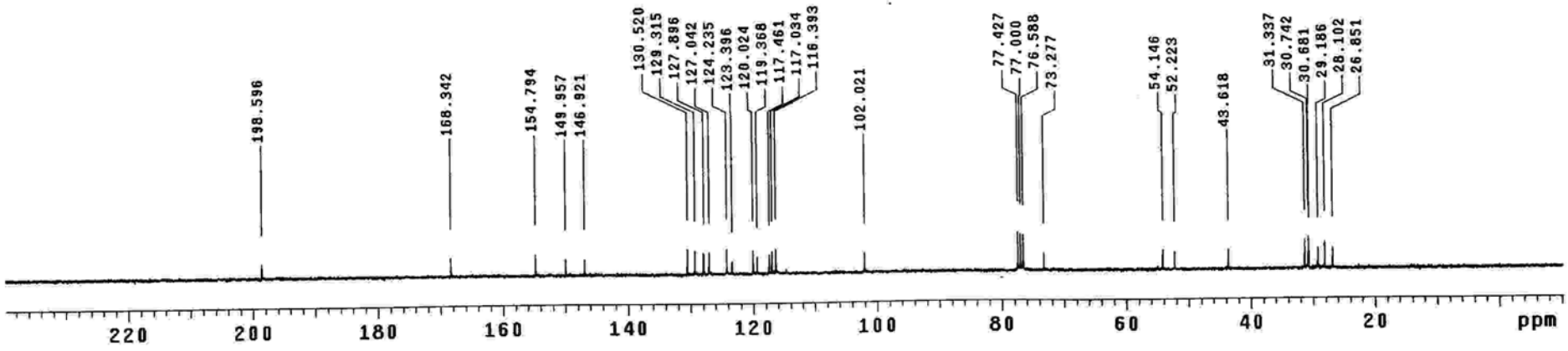
dyyjr147C

exp5 std13c

SAMPLE		DEC. & VT	
date	Sep 25 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	6708
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	**PROCESSING**	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	256	math	f
ct	256		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-773.6		
wp	18859.0		
vs	6		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	6583.3		
rfp	5809.7		
th	2		
ins	100.000		
nm no ph			



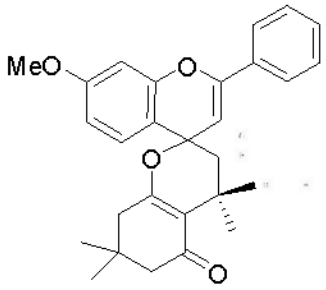
2h



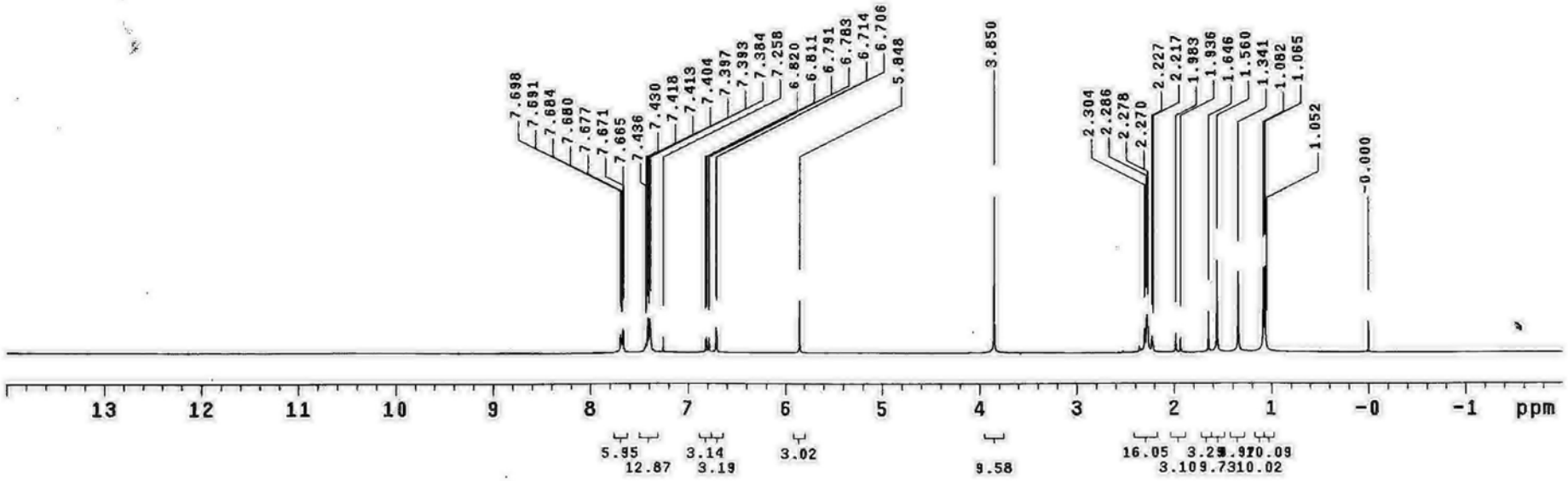
dyyjr109

exp4 std1h

SAMPLE		DEC. & VT	
date	Mar 19 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	300.066	dm	nnn
tn	H1	dmm	c
at	3.413	dmf	200
np	32768	dseq	
sw	4800.8	dres	1.0
fb	2600	homo	n
bs	4	PROCESSING	
tpwr	55	lb	0.10
pw	6.2	wtfile	
d1	0	proc	ft
tof	723.5	fn	65536
nt	16	math	f
ct	16		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-599.1		
wp	4800.8		
vs	25		
sc	0		
wc	250		
hzmm	19.20		
is	500.00		
rfl	599.1		
rfp	0		
th	1		
ins	100.000		
nm cdc ph			



2i

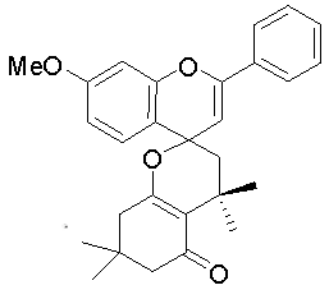


dyyjr114C

exp5 std13c

SAMPLE		DEC. & VT	
date	Apr 11 2008	dfrq	300.065
solvent	CDCl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	75.460	dm	yyy
tn	C13	dmm	w
at	0.869	dmf	7704
np	32768	dseq	
sw	18859.0	dres	1.0
fb	10400	homo	n
bs	16	PROCESSING	
tpwr	55	lb	1.00
pw	4.8	wtfile	
d1	2.000	proc	ft
tof	1220.8	fn	not used
nt	128	math	f
ct	128		
alock	n	werr	
gain	not used	wexp	
FLAGS		wbs	
il	n	wnt	
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-780.5		
wp	18859.0		
vs	17		
sc	0		
wc	250		
hzmm	75.44		
is	500.00		
rfl	8590.2		
rfp	5809.7		
th	3		
ins	100.000		

nm no ph



2i

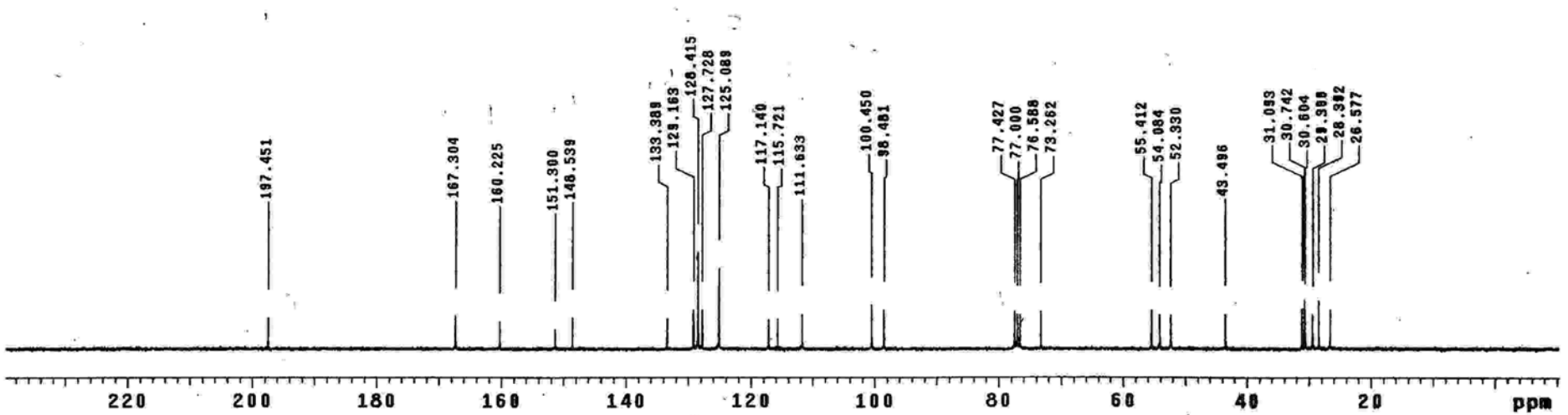
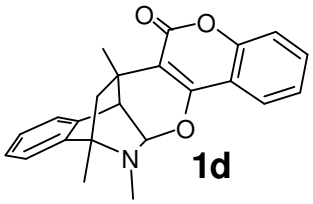


Table 1. Crystal data and structure refinement for ch060m.



1d

Identification code	ch060m	
Empirical formula	C23 H21 N O3	
Formula weight	359.41	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.2085(9) Å	α= 77.0530(10)°.
	b = 9.6607(10) Å	β= 80.455(2)°.
	c = 11.2222(13) Å	γ = 71.635(2)°.
Volume	918.49(17) $Å^3$	
Z	2	
Density (calculated)	1.300 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	380	
Crystal size	0.47 x 0.33 x 0.30 mm^3	
Theta range for data collection	1.87 to 26.02°.	
Index ranges	-9<=h<=11, -11<=k<=11, -13<=l<=12	
Reflections collected	5252	
Independent reflections	3569 [R(int) = 0.0210]	
Completeness to theta = 26.02°	98.7 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9747 and 0.9607	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3569 / 0 / 244	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1328	
R indices (all data)	R1 = 0.0696, wR2 = 0.1484	
Largest diff. peak and hole	0.220 and -0.260 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for ch060m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6033(1)	6346(1)	9552(1)	48(1)
O(2)	8883(2)	8805(2)	9682(1)	61(1)
O(3)	10423(2)	8034(2)	8106(2)	75(1)
N	5799(2)	6436(2)	7457(1)	45(1)
C(1)	7041(2)	7098(2)	9545(1)	41(1)
C(2)	6587(2)	8070(2)	10434(2)	44(1)
C(3)	5259(2)	8221(2)	11258(2)	52(1)
C(4)	4945(2)	9133(2)	12101(2)	62(1)
C(5)	5955(3)	9932(2)	12129(2)	66(1)
C(6)	7263(2)	9822(2)	11327(2)	63(1)
C(7)	7571(2)	8888(2)	10483(2)	50(1)
C(8)	9299(2)	7916(2)	8806(2)	53(1)
C(9)	8382(2)	6945(2)	8797(2)	42(1)
C(10)	8886(2)	5861(2)	7909(1)	43(1)
C(11)	8342(2)	6663(2)	6624(2)	48(1)
C(12)	6990(2)	6202(2)	6370(2)	46(1)
C(13)	7594(2)	4559(2)	6346(2)	47(1)
C(14)	7652(2)	3846(2)	5390(2)	58(1)
C(15)	8336(2)	2327(3)	5516(2)	67(1)
C(16)	8930(2)	1522(2)	6586(2)	66(1)
C(17)	8854(2)	2216(2)	7561(2)	58(1)
C(18)	8197(2)	3729(2)	7439(2)	45(1)
C(19)	8026(2)	4665(2)	8389(1)	43(1)
C(20)	6333(2)	5484(2)	8579(2)	44(1)
C(21)	10621(2)	5073(2)	7831(2)	56(1)
C(22)	6354(2)	7163(2)	5191(2)	65(1)
C(23)	4271(2)	6394(3)	7295(2)	65(1)

Table 3. Bond lengths [Å] and angles [°] for ch060m.

O(1)-C(1)	1.3448(18)
O(1)-C(20)	1.4580(18)
O(2)-C(7)	1.373(2)
O(2)-C(8)	1.377(2)
O(3)-C(8)	1.211(2)
N-C(20)	1.440(2)
N-C(23)	1.462(2)
N-C(12)	1.505(2)
C(1)-C(9)	1.360(2)
C(1)-C(2)	1.444(2)
C(2)-C(7)	1.391(2)
C(2)-C(3)	1.395(2)
C(3)-C(4)	1.370(2)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.390(3)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.369(3)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.387(3)
C(6)-H(6A)	0.9300
C(8)-C(9)	1.449(2)
C(9)-C(10)	1.522(2)
C(10)-C(21)	1.535(2)
C(10)-C(19)	1.552(2)
C(10)-C(11)	1.557(2)
C(11)-C(12)	1.534(2)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.512(3)
C(12)-C(22)	1.524(2)
C(13)-C(14)	1.385(2)
C(13)-C(18)	1.400(2)
C(14)-C(15)	1.388(3)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.371(3)
C(15)-H(15A)	0.9300

C(16)-C(17)	1.387(3)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.379(3)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.505(2)
C(19)-C(20)	1.514(2)
C(19)-H(19A)	0.9800
C(20)-H(20A)	0.9800
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600

C(1)-O(1)-C(20)	116.20(12)
C(7)-O(2)-C(8)	122.49(13)
C(20)-N-C(23)	111.24(14)
C(20)-N-C(12)	112.35(13)
C(23)-N-C(12)	115.70(14)
O(1)-C(1)-C(9)	123.81(15)
O(1)-C(1)-C(2)	113.68(14)
C(9)-C(1)-C(2)	122.49(14)
C(7)-C(2)-C(3)	118.00(17)
C(7)-C(2)-C(1)	117.14(16)
C(3)-C(2)-C(1)	124.85(15)
C(4)-C(3)-C(2)	120.90(17)
C(4)-C(3)-H(3A)	119.5
C(2)-C(3)-H(3A)	119.5
C(3)-C(4)-C(5)	119.7(2)
C(3)-C(4)-H(4A)	120.2
C(5)-C(4)-H(4A)	120.2
C(6)-C(5)-C(4)	121.04(19)
C(6)-C(5)-H(5A)	119.5
C(4)-C(5)-H(5A)	119.5

C(5)-C(6)-C(7)	118.67(18)
C(5)-C(6)-H(6A)	120.7
C(7)-C(6)-H(6A)	120.7
O(2)-C(7)-C(6)	117.60(16)
O(2)-C(7)-C(2)	120.70(16)
C(6)-C(7)-C(2)	121.70(18)
O(3)-C(8)-O(2)	115.31(16)
O(3)-C(8)-C(9)	126.19(18)
O(2)-C(8)-C(9)	118.50(15)
C(1)-C(9)-C(8)	118.16(16)
C(1)-C(9)-C(10)	122.04(14)
C(8)-C(9)-C(10)	119.70(14)
C(9)-C(10)-C(21)	112.86(13)
C(9)-C(10)-C(19)	107.28(12)
C(21)-C(10)-C(19)	108.10(14)
C(9)-C(10)-C(11)	109.96(13)
C(21)-C(10)-C(11)	112.09(14)
C(19)-C(10)-C(11)	106.19(12)
C(12)-C(11)-C(10)	111.39(13)
C(12)-C(11)-H(11A)	109.3
C(10)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11B)	109.3
C(10)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
N-C(12)-C(13)	108.78(13)
N-C(12)-C(22)	110.82(15)
C(13)-C(12)-C(22)	114.68(15)
N-C(12)-C(11)	106.25(13)
C(13)-C(12)-C(11)	106.30(14)
C(22)-C(12)-C(11)	109.59(15)
C(14)-C(13)-C(18)	119.43(18)
C(14)-C(13)-C(12)	128.08(17)
C(18)-C(13)-C(12)	112.46(15)
C(13)-C(14)-C(15)	119.71(19)
C(13)-C(14)-H(14A)	120.1
C(15)-C(14)-H(14A)	120.1
C(16)-C(15)-C(14)	120.55(19)
C(16)-C(15)-H(15A)	119.7

C(14)-C(15)-H(15A)	119.7
C(15)-C(16)-C(17)	120.4(2)
C(15)-C(16)-H(16A)	119.8
C(17)-C(16)-H(16A)	119.8
C(18)-C(17)-C(16)	119.53(19)
C(18)-C(17)-H(17A)	120.2
C(16)-C(17)-H(17A)	120.2
C(17)-C(18)-C(13)	120.38(16)
C(17)-C(18)-C(19)	126.84(16)
C(13)-C(18)-C(19)	112.78(15)
C(18)-C(19)-C(20)	106.77(12)
C(18)-C(19)-C(10)	110.94(13)
C(20)-C(19)-C(10)	106.80(13)
C(18)-C(19)-H(19A)	110.7
C(20)-C(19)-H(19A)	110.7
C(10)-C(19)-H(19A)	110.7
N-C(20)-O(1)	110.18(14)
N-C(20)-C(19)	110.94(13)
O(1)-C(20)-C(19)	110.86(12)
N-C(20)-H(20A)	108.3
O(1)-C(20)-H(20A)	108.3
C(19)-C(20)-H(20A)	108.3
C(10)-C(21)-H(21A)	109.5
C(10)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(10)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(12)-C(22)-H(22A)	109.5
C(12)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(12)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N-C(23)-H(23A)	109.5
N-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N-C(23)-H(23C)	109.5

H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

Symmetry transformations used to generate equivalent atoms:

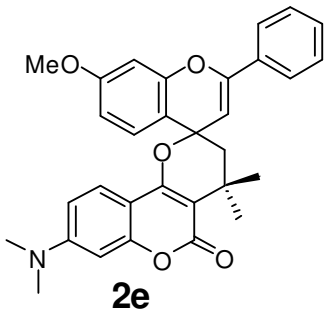
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ch060m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	47(1)	66(1)	42(1)	-18(1)	6(1)	-33(1)
O(2)	55(1)	66(1)	76(1)	-19(1)	-7(1)	-33(1)
O(3)	54(1)	83(1)	96(1)	-19(1)	11(1)	-42(1)
N	35(1)	60(1)	45(1)	-12(1)	-6(1)	-17(1)
C(1)	42(1)	46(1)	37(1)	-1(1)	-9(1)	-20(1)
C(2)	46(1)	45(1)	42(1)	-2(1)	-12(1)	-15(1)
C(3)	54(1)	55(1)	49(1)	-10(1)	-6(1)	-18(1)
C(4)	68(1)	65(1)	54(1)	-19(1)	-4(1)	-15(1)
C(5)	77(2)	60(1)	67(1)	-24(1)	-16(1)	-13(1)
C(6)	68(1)	56(1)	76(1)	-17(1)	-23(1)	-22(1)
C(7)	49(1)	49(1)	55(1)	-5(1)	-17(1)	-17(1)
C(8)	44(1)	58(1)	59(1)	-4(1)	-9(1)	-22(1)
C(9)	38(1)	50(1)	41(1)	-1(1)	-9(1)	-18(1)
C(10)	35(1)	56(1)	38(1)	-2(1)	-5(1)	-19(1)
C(11)	46(1)	61(1)	38(1)	1(1)	-4(1)	-22(1)
C(12)	42(1)	60(1)	37(1)	-7(1)	-7(1)	-17(1)
C(13)	39(1)	65(1)	39(1)	-12(1)	-1(1)	-18(1)
C(14)	53(1)	79(1)	47(1)	-21(1)	-1(1)	-23(1)
C(15)	65(1)	84(2)	63(1)	-34(1)	4(1)	-26(1)
C(16)	64(1)	61(1)	76(2)	-25(1)	2(1)	-18(1)
C(17)	56(1)	57(1)	59(1)	-9(1)	-5(1)	-17(1)
C(18)	40(1)	57(1)	42(1)	-10(1)	-1(1)	-18(1)
C(19)	44(1)	51(1)	34(1)	-1(1)	-7(1)	-18(1)
C(20)	45(1)	57(1)	40(1)	-14(1)	1(1)	-27(1)
C(21)	40(1)	72(1)	56(1)	-10(1)	-5(1)	-16(1)
C(22)	67(1)	77(1)	48(1)	-1(1)	-20(1)	-16(1)
C(23)	40(1)	87(1)	74(1)	-23(1)	-11(1)	-20(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ch060m.

	x	y	z	U(eq)
H(3A)	4577	7696	11235	62
H(4A)	4062	9218	12652	74
H(5A)	5738	10551	12702	80
H(6A)	7931	10363	11347	76
H(11A)	8030	7728	6587	58
H(11B)	9190	6425	5993	58
H(14A)	7234	4383	4667	69
H(15A)	8391	1850	4868	81
H(16A)	9387	504	6660	80
H(17A)	9243	1666	8291	69
H(19A)	8393	4044	9160	51
H(20A)	5758	4750	8827	53
H(21A)	10909	4596	8639	84
H(21B)	11175	5788	7489	84
H(21C)	10863	4344	7315	84
H(22A)	5511	6871	5032	97
H(22B)	7148	7039	4518	97
H(22C)	6003	8185	5279	97
H(23A)	3597	6554	8033	97
H(23B)	4343	5443	7124	97
H(23C)	3871	7157	6622	97

Table 1. Crystal data and structure refinement for jr016m.



2e

Identification code	jr016m	
Empirical formula	C31 H29 N O5	
Formula weight	495.55	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.6289(18) Å	α= 75.761(4)°.
	b = 12.161(2) Å	β= 89.878(4)°.
	c = 13.927(3) Å	γ = 70.641(4)°.
Volume	1485.7(5) $Å^3$	
Z	2	
Density (calculated)	1.108 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	524	
Crystal size	0.69 x 0.55 x 0.46 mm^3	
Theta range for data collection	2.25 to 26.12°.	
Index ranges	-11<=h<=11, -14<=k<=8, -17<=l<=16	
Reflections collected	8502	
Independent reflections	5777 [R(int) = 0.0244]	
Completeness to theta = 26.12°	97.8 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 1.000	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5777 / 0 / 346	
Goodness-of-fit on F^2	1.122	
Final R indices [I>2sigma(I)]	R1 = 0.0778, wR2 = 0.2280	
R indices (all data)	R1 = 0.1196, wR2 = 0.2627	
Largest diff. peak and hole	0.871 and -0.344 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for jr016m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N	2259(3)	3769(3)	4679(2)	75(1)
O(1)	5674(2)	2696(2)	914(1)	50(1)
O(2)	6518(2)	4151(2)	3117(1)	66(1)
O(3)	8519(3)	4386(2)	2500(2)	82(1)
O(4)	7573(2)	-224(2)	6(2)	65(1)
O(5)	4118(3)	1319(2)	-2856(2)	97(1)
C(1)	6006(3)	3220(2)	1586(2)	45(1)
C(2)	4991(3)	3350(2)	2341(2)	48(1)
C(3)	3717(3)	3035(2)	2390(2)	55(1)
C(4)	2827(3)	3159(3)	3148(2)	60(1)
C(5)	3159(4)	3625(3)	3922(2)	58(1)
C(6)	4414(4)	3948(3)	3879(2)	61(1)
C(7)	5293(3)	3814(2)	3103(2)	53(1)
C(8)	7489(4)	4061(3)	2382(2)	59(1)
C(9)	7208(3)	3596(2)	1568(2)	49(1)
C(10)	8195(3)	3587(2)	727(2)	53(1)
C(11)	7588(3)	3136(2)	-70(2)	54(1)
C(12)	6898(3)	2178(2)	320(2)	49(1)
C(13)	7904(3)	1035(2)	979(2)	52(1)
C(14)	8208(3)	-54(2)	808(2)	52(1)
C(15)	6514(3)	765(3)	-617(2)	53(1)
C(16)	6153(3)	1909(2)	-500(2)	50(1)
C(17)	5093(3)	2826(3)	-1195(2)	62(1)
C(18)	4422(4)	2596(3)	-1962(2)	67(1)
C(19)	4835(4)	1439(3)	-2061(2)	66(1)
C(20)	5867(4)	514(3)	-1394(2)	67(1)
C(21)	1119(5)	3266(5)	4825(3)	108(1)
C(22)	2643(7)	4243(7)	5456(4)	98(2)
C(23)	8119(4)	4890(3)	224(2)	67(1)
C(24)	9832(3)	2823(3)	1076(3)	70(1)
C(25)	9240(3)	-1187(2)	1431(2)	55(1)
C(26)	8984(4)	-2266(3)	1539(2)	66(1)

C(27)	9923(5)	-3323(3)	2148(3)	80(1)
C(28)	11134(5)	-3304(3)	2659(3)	90(1)
C(29)	11434(4)	-2253(3)	2560(3)	83(1)
C(30)	10478(4)	-1193(3)	1940(2)	68(1)
C(31)	4454(6)	126(4)	-2977(3)	116(2)

Table 3. Bond lengths [Å] and angles [°] for jr016m.

N-C(5)	1.370(4)
N-C(21)	1.416(5)
N-C(22)	1.445(5)
O(1)-C(1)	1.347(3)
O(1)-C(12)	1.493(3)
O(2)-C(7)	1.373(3)
O(2)-C(8)	1.384(4)
O(3)-C(8)	1.209(4)
O(4)-C(14)	1.365(3)
O(4)-C(15)	1.384(3)
O(5)-C(19)	1.368(4)
O(5)-C(31)	1.432(4)
C(1)-C(9)	1.376(4)
C(1)-C(2)	1.436(4)
C(2)-C(7)	1.391(4)
C(2)-C(3)	1.398(4)
C(3)-C(4)	1.363(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.418(4)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.386(4)
C(6)-C(7)	1.378(4)
C(6)-H(6A)	0.9300
C(8)-C(9)	1.448(4)
C(9)-C(10)	1.507(4)
C(10)-C(23)	1.544(4)
C(10)-C(11)	1.545(4)
C(10)-C(24)	1.547(4)
C(11)-C(12)	1.514(4)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.482(4)
C(12)-C(16)	1.506(4)
C(13)-C(14)	1.341(4)
C(13)-H(13A)	0.9300
C(14)-C(25)	1.465(4)

C(15)-C(16)	1.369(4)
C(15)-C(20)	1.395(4)
C(16)-C(17)	1.393(4)
C(17)-C(18)	1.380(4)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.372(4)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.365(4)
C(20)-H(20A)	0.9300
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	1.02(4)
C(22)-H(22B)	0.88(6)
C(22)-H(22C)	0.88(5)
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(30)	1.385(4)
C(25)-C(26)	1.386(4)
C(26)-C(27)	1.374(5)
C(26)-H(26A)	0.9300
C(27)-C(28)	1.377(6)
C(27)-H(27A)	0.9300
C(28)-C(29)	1.376(6)
C(28)-H(28A)	0.9300
C(29)-C(30)	1.387(4)
C(29)-H(29A)	0.9300
C(30)-H(30A)	0.9300
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600

C(5)-N-C(21)	121.6(3)
C(5)-N-C(22)	119.4(3)

C(21)-N-C(22)	117.9(3)
C(1)-O(1)-C(12)	116.2(2)
C(7)-O(2)-C(8)	122.4(2)
C(14)-O(4)-C(15)	118.0(2)
C(19)-O(5)-C(31)	117.1(3)
O(1)-C(1)-C(9)	123.9(2)
O(1)-C(1)-C(2)	113.9(2)
C(9)-C(1)-C(2)	122.2(2)
C(7)-C(2)-C(3)	116.3(2)
C(7)-C(2)-C(1)	118.1(3)
C(3)-C(2)-C(1)	125.7(2)
C(4)-C(3)-C(2)	122.1(3)
C(4)-C(3)-H(3A)	118.9
C(2)-C(3)-H(3A)	118.9
C(3)-C(4)-C(5)	120.8(3)
C(3)-C(4)-H(4A)	119.6
C(5)-C(4)-H(4A)	119.6
N-C(5)-C(6)	121.1(3)
N-C(5)-C(4)	121.2(3)
C(6)-C(5)-C(4)	117.6(3)
C(7)-C(6)-C(5)	120.3(3)
C(7)-C(6)-H(6A)	119.9
C(5)-C(6)-H(6A)	119.9
O(2)-C(7)-C(6)	116.7(2)
O(2)-C(7)-C(2)	120.4(2)
C(6)-C(7)-C(2)	122.9(3)
O(3)-C(8)-O(2)	114.6(3)
O(3)-C(8)-C(9)	126.3(3)
O(2)-C(8)-C(9)	119.1(3)
C(1)-C(9)-C(8)	117.7(3)
C(1)-C(9)-C(10)	123.0(2)
C(8)-C(9)-C(10)	119.2(2)
C(9)-C(10)-C(23)	109.5(2)
C(9)-C(10)-C(11)	108.5(2)
C(23)-C(10)-C(11)	106.6(2)
C(9)-C(10)-C(24)	112.8(2)
C(23)-C(10)-C(24)	107.8(3)
C(11)-C(10)-C(24)	111.4(2)

C(12)-C(11)-C(10)	115.8(2)
C(12)-C(11)-H(11A)	108.3
C(10)-C(11)-H(11A)	108.3
C(12)-C(11)-H(11B)	108.3
C(10)-C(11)-H(11B)	108.3
H(11A)-C(11)-H(11B)	107.4
C(13)-C(12)-O(1)	107.2(2)
C(13)-C(12)-C(16)	109.7(2)
O(1)-C(12)-C(16)	104.6(2)
C(13)-C(12)-C(11)	115.2(2)
O(1)-C(12)-C(11)	107.0(2)
C(16)-C(12)-C(11)	112.5(2)
C(14)-C(13)-C(12)	124.6(3)
C(14)-C(13)-H(13A)	117.7
C(12)-C(13)-H(13A)	117.7
C(13)-C(14)-O(4)	122.6(3)
C(13)-C(14)-C(25)	125.4(3)
O(4)-C(14)-C(25)	112.0(2)
C(16)-C(15)-O(4)	122.9(2)
C(16)-C(15)-C(20)	122.3(3)
O(4)-C(15)-C(20)	114.8(3)
C(15)-C(16)-C(17)	116.9(3)
C(15)-C(16)-C(12)	121.9(2)
C(17)-C(16)-C(12)	121.2(2)
C(18)-C(17)-C(16)	121.9(3)
C(18)-C(17)-H(17A)	119.1
C(16)-C(17)-H(17A)	119.1
C(19)-C(18)-C(17)	119.3(3)
C(19)-C(18)-H(18A)	120.3
C(17)-C(18)-H(18A)	120.3
C(20)-C(19)-O(5)	125.0(3)
C(20)-C(19)-C(18)	120.7(3)
O(5)-C(19)-C(18)	114.3(3)
C(19)-C(20)-C(15)	119.0(3)
C(19)-C(20)-H(20A)	120.5
C(15)-C(20)-H(20A)	120.5
N-C(21)-H(21A)	109.5
N-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
N-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N-C(22)-H(22A)	105(2)
N-C(22)-H(22B)	107(4)
H(22A)-C(22)-H(22B)	98(4)
N-C(22)-H(22C)	105(3)
H(22A)-C(22)-H(22C)	106(4)
H(22B)-C(22)-H(22C)	134(5)
C(10)-C(23)-H(23A)	109.5
C(10)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(10)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(10)-C(24)-H(24A)	109.5
C(10)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(10)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(30)-C(25)-C(26)	118.8(3)
C(30)-C(25)-C(14)	120.3(3)
C(26)-C(25)-C(14)	120.9(3)
C(27)-C(26)-C(25)	121.0(3)
C(27)-C(26)-H(26A)	119.5
C(25)-C(26)-H(26A)	119.5
C(26)-C(27)-C(28)	119.2(3)
C(26)-C(27)-H(27A)	120.4
C(28)-C(27)-H(27A)	120.4
C(29)-C(28)-C(27)	121.4(3)
C(29)-C(28)-H(28A)	119.3
C(27)-C(28)-H(28A)	119.3
C(28)-C(29)-C(30)	118.7(4)
C(28)-C(29)-H(29A)	120.6
C(30)-C(29)-H(29A)	120.6
C(25)-C(30)-C(29)	120.9(3)

C(25)-C(30)-H(30A)	119.6
C(29)-C(30)-H(30A)	119.6
O(5)-C(31)-H(31A)	109.5
O(5)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
O(5)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jr016m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N	85(2)	94(2)	55(2)	-32(1)	25(1)	-35(2)
O(1)	51(1)	56(1)	56(1)	-31(1)	11(1)	-23(1)
O(2)	77(1)	80(1)	63(1)	-39(1)	10(1)	-42(1)
O(3)	88(2)	103(2)	91(2)	-49(1)	13(1)	-62(2)
O(4)	76(1)	53(1)	72(1)	-31(1)	0(1)	-20(1)
O(5)	118(2)	102(2)	86(2)	-46(1)	-12(2)	-42(2)
C(1)	53(2)	40(1)	48(1)	-18(1)	3(1)	-18(1)
C(2)	56(2)	43(1)	50(1)	-18(1)	7(1)	-19(1)
C(3)	63(2)	57(2)	55(2)	-26(1)	8(1)	-27(1)
C(4)	65(2)	65(2)	61(2)	-25(1)	14(1)	-28(2)
C(5)	69(2)	54(2)	51(2)	-16(1)	11(1)	-20(1)
C(6)	78(2)	61(2)	48(2)	-24(1)	5(1)	-23(2)
C(7)	62(2)	50(2)	52(2)	-20(1)	2(1)	-22(1)
C(8)	66(2)	59(2)	65(2)	-27(1)	7(2)	-31(2)
C(9)	55(2)	45(1)	53(2)	-19(1)	3(1)	-22(1)
C(10)	52(2)	52(2)	63(2)	-21(1)	9(1)	-24(1)
C(11)	56(2)	57(2)	54(2)	-20(1)	11(1)	-22(1)
C(12)	49(2)	51(2)	53(2)	-25(1)	10(1)	-18(1)
C(13)	56(2)	52(2)	56(2)	-23(1)	3(1)	-20(1)
C(14)	54(2)	52(2)	57(2)	-21(1)	10(1)	-22(1)
C(15)	54(2)	58(2)	55(2)	-24(1)	9(1)	-23(1)
C(16)	49(2)	57(2)	51(2)	-26(1)	9(1)	-20(1)
C(17)	63(2)	63(2)	62(2)	-27(2)	4(2)	-16(2)
C(18)	72(2)	70(2)	60(2)	-24(2)	-5(2)	-19(2)
C(19)	70(2)	83(2)	60(2)	-33(2)	0(2)	-34(2)
C(20)	77(2)	67(2)	74(2)	-41(2)	10(2)	-31(2)
C(21)	110(3)	146(4)	93(3)	-55(3)	49(3)	-59(3)
C(22)	113(4)	130(5)	54(2)	-40(3)	21(3)	-31(3)
C(23)	78(2)	60(2)	74(2)	-19(2)	15(2)	-37(2)
C(24)	60(2)	76(2)	82(2)	-28(2)	7(2)	-27(2)
C(25)	57(2)	48(2)	64(2)	-20(1)	18(1)	-19(1)
C(26)	70(2)	60(2)	77(2)	-24(2)	23(2)	-28(2)
C(27)	97(3)	54(2)	91(3)	-16(2)	26(2)	-29(2)

C(28)	102(3)	56(2)	86(3)	-2(2)	16(2)	-7(2)
C(29)	77(2)	72(2)	88(2)	-16(2)	-4(2)	-12(2)
C(30)	65(2)	55(2)	80(2)	-17(2)	5(2)	-18(2)
C(31)	165(5)	108(3)	113(3)	-60(3)	2(3)	-72(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jr016m.

	x	y	z	U(eq)
H(3A)	3469	2730	1890	66
H(4A)	1991	2935	3156	73
H(6A)	4665	4256	4375	73
H(11A)	6854	3823	-517	64
H(11B)	8391	2816	-457	64
H(13A)	8357	1077	1552	63
H(17A)	4830	3615	-1141	74
H(18A)	3697	3219	-2406	81
H(20A)	6134	-272	-1457	80
H(21A)	975	2988	4257	162
H(21B)	219	3870	4908	162
H(21C)	1388	2600	5409	162
H(22A)	1830(40)	4260(30)	5930(30)	95(11)
H(22B)	3360(60)	3650(50)	5850(40)	150(20)
H(22C)	2520(60)	5000(50)	5160(40)	140(20)
H(23A)	8481	5210	696	101
H(23B)	7114	5382	-7	101
H(23C)	8716	4888	-329	101
H(24A)	9910	2006	1391	105
H(24B)	10193	3153	1540	105
H(24C)	10408	2836	512	105
H(26A)	8163	-2273	1194	80
H(27A)	9744	-4043	2215	96
H(28A)	11763	-4016	3080	108
H(29A)	12262	-2253	2903	100
H(30A)	10670	-477	1865	81
H(31A)	3889	156	-3556	174
H(31B)	4210	-374	-2401	174
H(31C)	5489	-206	-3055	174