"Diversity Oriented Synthesis of a Vinblastine-Templated Library of 7-Aryl Octahydroazonino[5,4-*b*]indoles via a Three-Component Reaction"

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Supporting Information

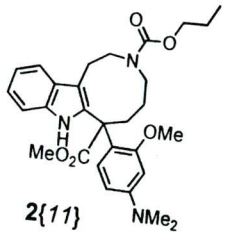
General Methods. All reagents and solvents were purchased and used without further purification. Reactions were performed into two-drum round bottom vials in 24-well plates. All reactions were monitored by reverse phase HPLC on a Shimadzu LC system. Routine LC/MS was run in an integrated LC/MS system with a Shimadzu LC and a Micromass DMZ MS instrument. Solvent was removed from reaction vials utilizing a Savant or Genevac evaporation system. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian Mercury spectrometer. Low-resolution mass spectra were recorded in ES^{+} mode.

Purification Conditions. The crude products were dissolved in 500 μL of DMSO and then purified by reverse phase prep-HPLC with mass triggered fraction collection. An Xterra Prep MS-C18 column (19 × 50 mm) was utilized with water and acetonitrile as gradients (80 mL/min) and NH_3 (10 mM) as modifier. Samples were collected in 24-vial bar-coded purification blocks followed by solvent evaporation. The dried samples were then weighed using a balance controlled by an automation system to calculate the recovery, and then diluted in DMSO to a 30 mM concentration. An aliquot of 20 μL was pulled from each vial and then diluted into 500 μL of DMSO for characterization. The samples were analyzed by a 2.5-minute reverse-phase HPLC/UV_{214nm}/ELSD/MS method to confirm the MS of the products and to determine their purity. The samples were finally reformatted in a 96-well plate for biological screening.

1B5
STANDARD 1H OBSERVE

Archive directory: /export/home/auto/vnmrsys/data
Sample directory: auto_16Nov2005

Pulse Sequence: s2pul



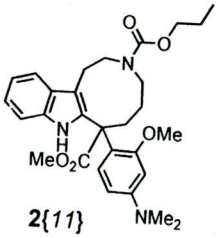
2{11}

VIN-1B5-C13
13C OBSERVE

pad=2 run with findz0 before acquisition

expl s2pul

SAMPLE		SPECIAL	
date	Oct 17 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_17.10.05/VIN-1B5~		pw90	13.500
	-C1301.fid	alfa	20.000
ACQUISITION		FLAGS	
sw	18832.4	il	n
at	1.815	in	n
np	68362	dp	y
fb	10400	hs	nn
bs	64	PROCESSING	
d1	2.000	lb	1.00
nt	5000	fn	not used
ct	5000	DISPLAY	
TRANSMITTER		sp	-37.7
tn	C13	wp	16960.8
sfrq	75.390	rfl	6946.8
tof	740.3	rfp	5804.4
tpwr	58	rp	-78.4
pw	6.750	lp	-301.2
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	3907
dmm	w	th	50
dpwr	42	ai	no ph
dmf	6744		



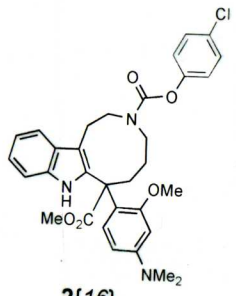
2{*11*}

1B6
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1B602

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #20
File: 1B601
Mercury-300BB "horror"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885555 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



2{*16*}

3857-1D1
2{16}

~ DMSO

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

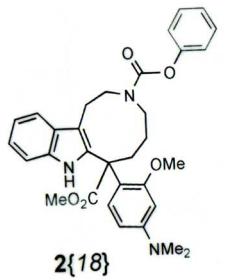
29.39 5.14 57.33 5.71 1.31 0.43 0.67

1C1
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1C102

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #21
File: 1C101
Mercury-300BB "horror"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885529 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



2{18}

3857-1D3

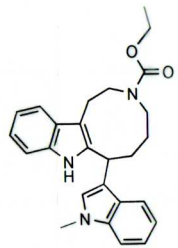
2{18}

vin-2B4-c13
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_20.10.05
File : vin-2B4-c1302

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #4
File: vin-2B4-c1301
Mercury-300BB "horror"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885540 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



3{5}

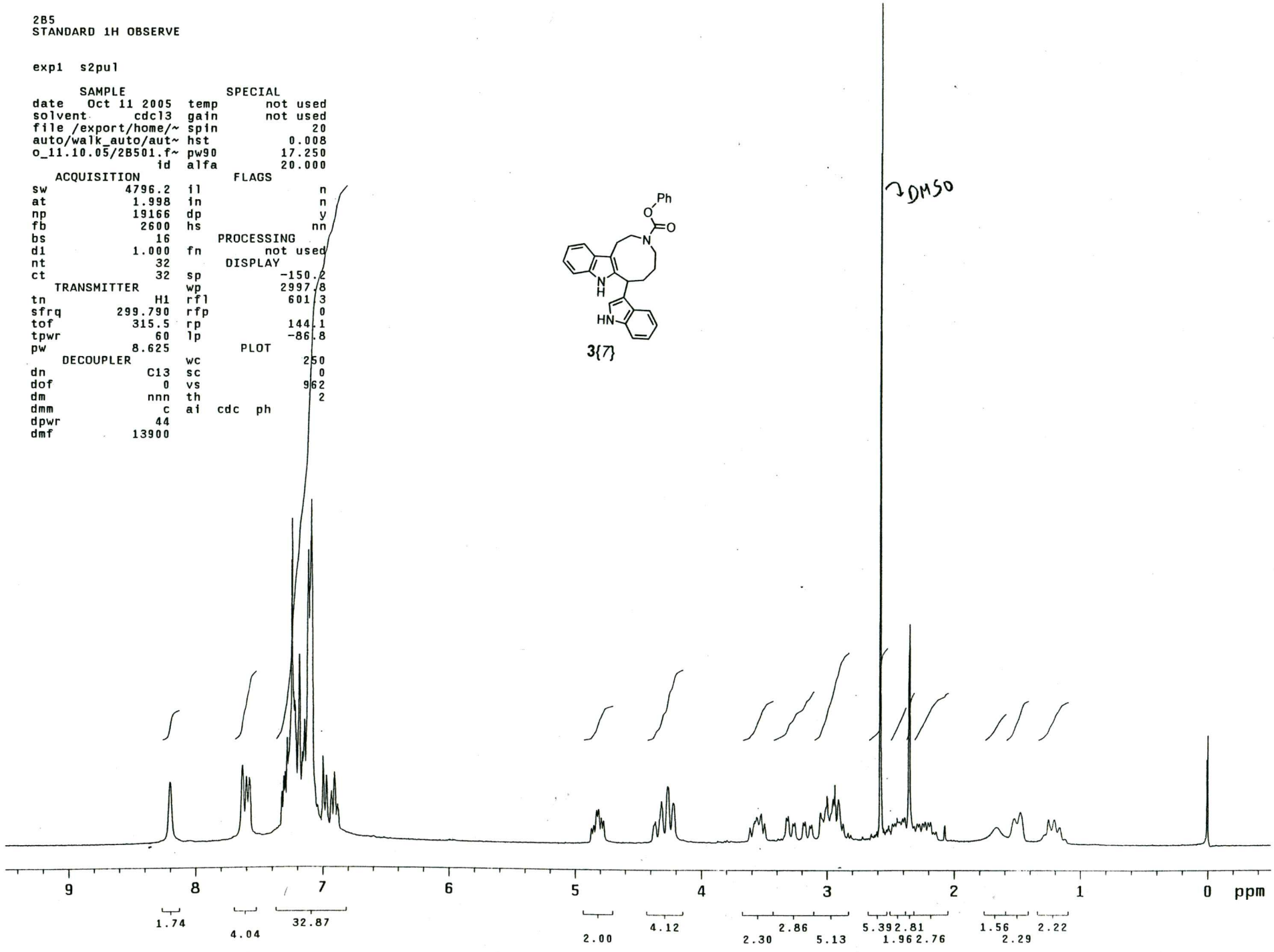
3854-1A 5

3{5}

DMSO

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

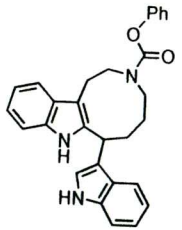
0.09 34.46 2.32 47.43 14.13 1.57


2B5
STANDARD 1H OBSERVE
exp1 s2pul
SAMPLE
date Oct 11 2005
solvent cdcl3
file /export/home/~
auto/walk_auto/aut~
o_11.10.05/2B501.f~
id
ACQUISITION
sw 4796.2
at 1.998
np 19166
fb 2600
bs 16
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 299.790
tof 315.5
tpwr 60
pw 8.625
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 13900
SPECIAL
temp not used
gain not used
spin 20
hst 0.008
pw90 17.250
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn not used
DISPLAY
sp -150.2
wp 2997.8
rfl 601.3
rfp 0
rp 144.1
lp -86.8
PLOT
wc 250
sc 0
vs 962
th 2
ai cdc ph
Ph
O
O
N
N
H
HN
3{7}
DMSO
9
8
7
6
5
4
3
2
1
0
ppm
1.74
4.04
32.87
2.00
4.12
2.30
2.86
5.13
5.39
2.81
1.96
2.76
1.56
2.29
2.22

vin-2B5-c13

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 23 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_20.10.05/vin-1B5~		pw90	13.500
-c1301.fid		alfa	20.000
ACQUISITION		**FLAGS**	
sw	18832.4	il	n
at	1.815	in	n
np	68362	dp	y
fb	10400	hs	nn
bs	64	**PROCESSING**	
d1	2.000	lb	1.00
nt	5000	fn	not used
ct	5000	**DISPLAY**	
TRANSMITTER		sp	-37.9
tn	C13	wp	16960.8
sfrq	75.390	rfl	1124.2
tof	740.3	rfp	0
tpwr	58	rp	-97.0
pw	6.750	lp	-264.3
DECOUPLER		**PLOT**	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	3123
dmm	w	th	10
dpwr	42	ai	no ph
dmf	6744		

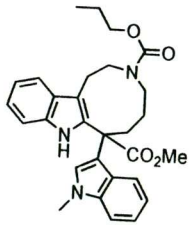


3{7}

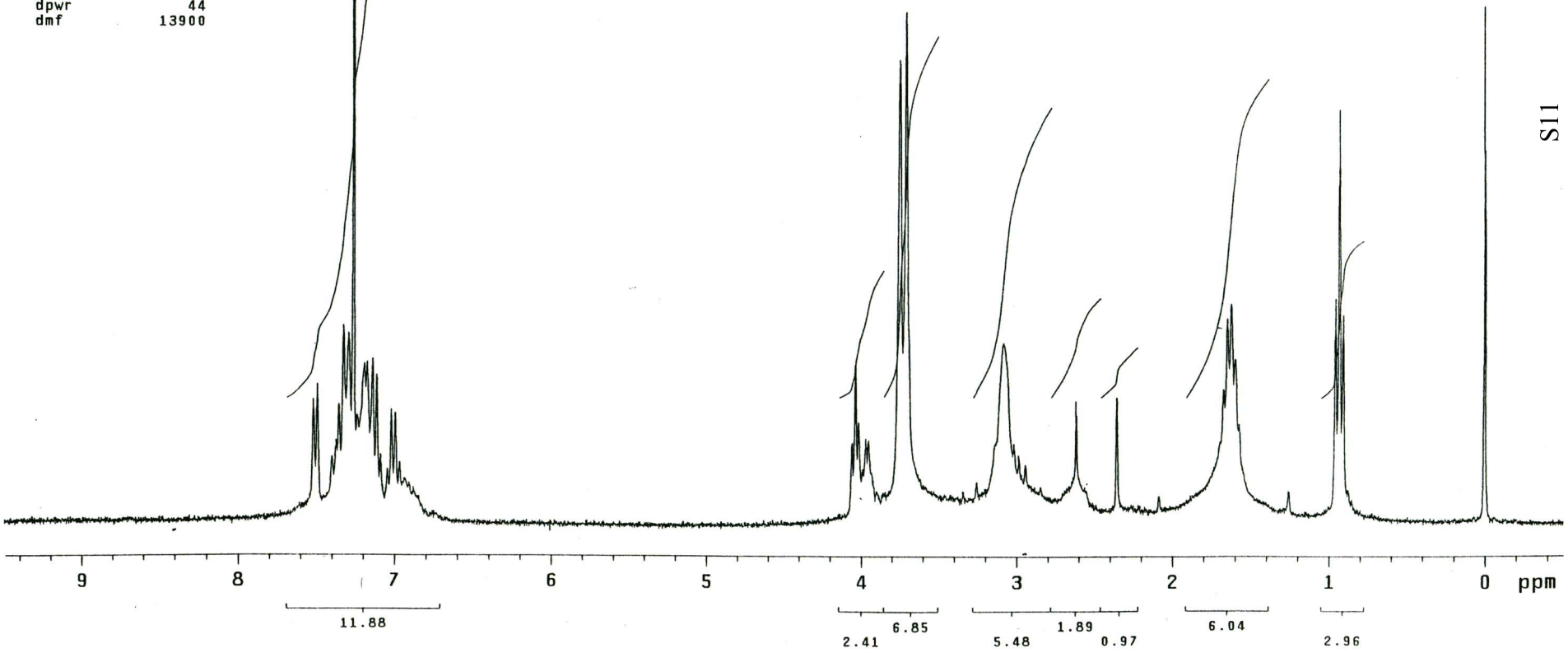
2B6
STANDARD 1H OBSERVE

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 11 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_11.10.05/2B601.f~		pw90	17.250
	id	alfa	20.000
ACQUISITION		FLAGS	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	PROCESSING	
d1	1.000	fn	not used
nt	32	DISPLAY	
ct	32	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	596.6
sfrq	299.790	rfp	0
tof	315.5	rp	131.3
tpwr	60	lp	-53.9
pw	8.625	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	1148
dm	nnn	th	10
dmm	c	ai cdc ph	
dpwr	44		
dmf	13900		



3{*17*}



1B2
STANDARD 1H OBSERVE

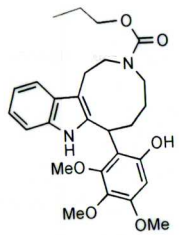
Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1B202

Pulse Sequence: s2pul

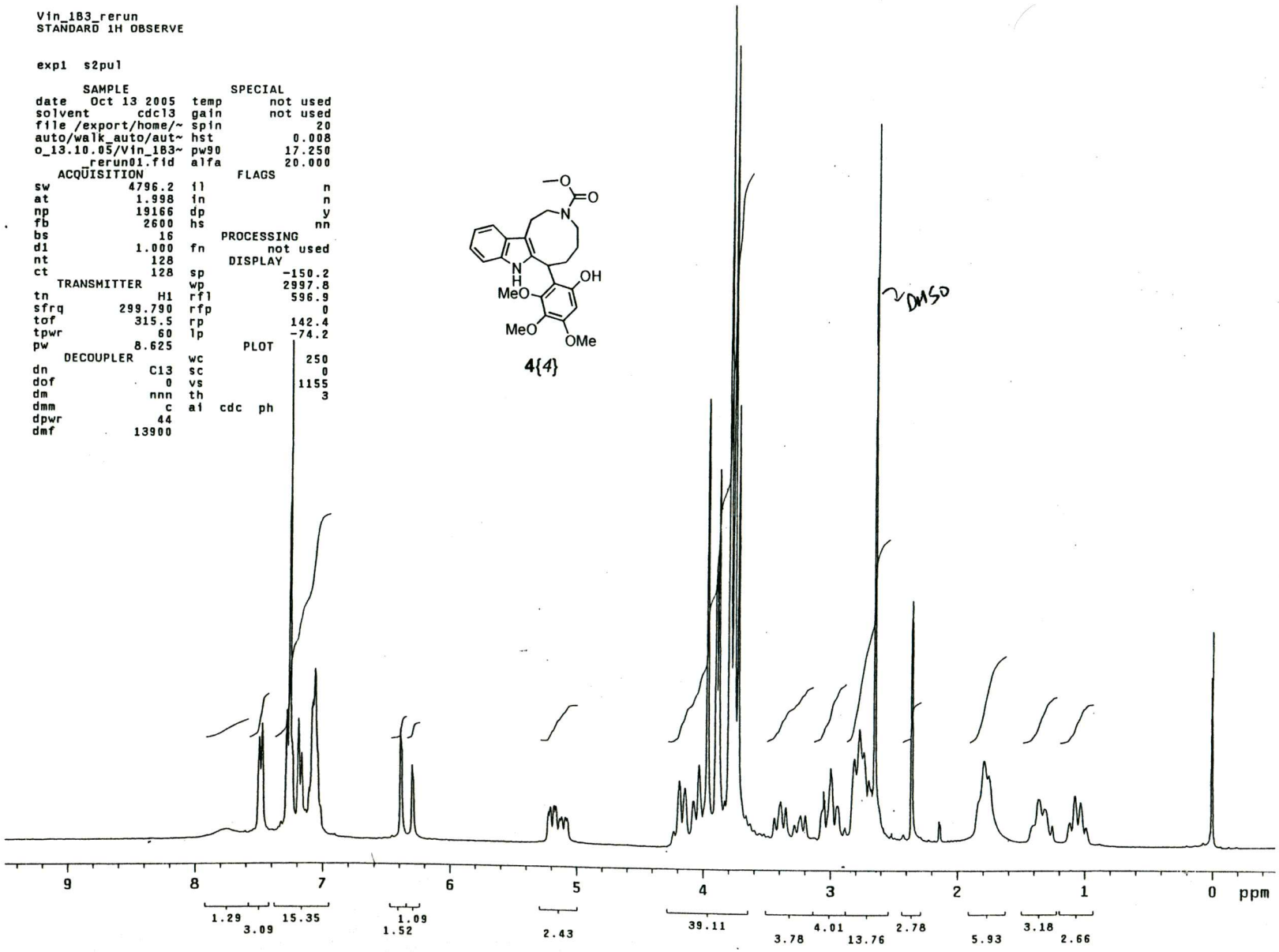
Solvent: cdcl3
Ambient temperature
Sample #16
File: 1B201
Mercury-300BB "horror"

3855-1A1
4{1}

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885479 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



4{1}

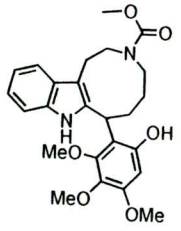

Vin_1B3_rerun
STANDARD 1H OBSERVE
exp1 s2pul
SAMPLE
date Oct 13 2005
solvent cdcl3
file /export/home/~
auto/walk_auto/aut~
o_13.10.05/Vin_1B3~
_rerun01.fid
ACQUISITION
sw 4796.2
at 1.998
np 19166
fb 2600
bs 16
d1 1.000
nt 128
ct 128
TRANSMITTER
tn H1
sfrq 299.790
tof 315.5
tpwr 60
pw 8.625
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 13900
SPECIAL
temp not used
gain not used
spin 20
hst 0.008
pw90 17.250
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn not used
DISPLAY
sp -150.2
wp 2997.8
rfl 596.9
rfp 0
rp 142.4
lp -74.2
PLOT
wc 250
sc 0
vs 1155
th 3
ai cdc ph
4{4}
DMSO
9
8
7
6
5
4
3
2
1
0 ppm
1.29
3.09
15.35
1.09
1.52
2.43
39.11
3.78
4.01
13.76
2.78
5.93
3.18
2.66

VIN-1B3-C13
13C OBSERVE

pad=2 run with findz0 before acquisition

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 17 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
	auto/walk_auto/aut~	hst	0.008
	o_17.10.05/VIN-1B3~	pw90	13.500
	-C1301.fid	alfa	20.000
ACQUISITION		FLAGS	
sw	18832.4	il	n
at	1.815	in	n
np	68362	dp	y
fb	10400	hs	nn
bs	64	PROCESSING	
d1	2.000	lb	1.00
nt	5000	fn	not used
ct	5000	DISPLAY	
TRANSMITTER		sp	-37.9
tn	C13	wp	16960.8
sfrq	75.390	rfl	6945.8
tof	740.3	rfp	5804.4
tpwr	58	rp	-98.4
pw	6.750	lp	-251.5
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	3059
dmm	w	th	5
dpwr	42	ai no ph	
dmf	6744		



4{*4*}

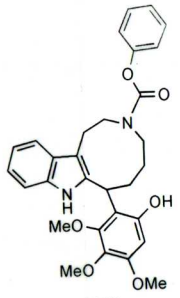
1B4
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1B402

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #18
File: 1B401
Mercury-300BB "horror"

3855-1B3
4{8}

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885408 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



4{8}

→DHSO

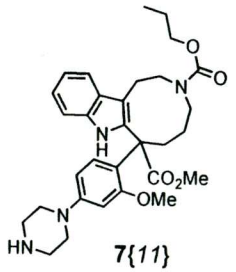
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 ppm

2.29 29.23 2.26 2.27 6.03 45.29 0.54 11.05 1.05

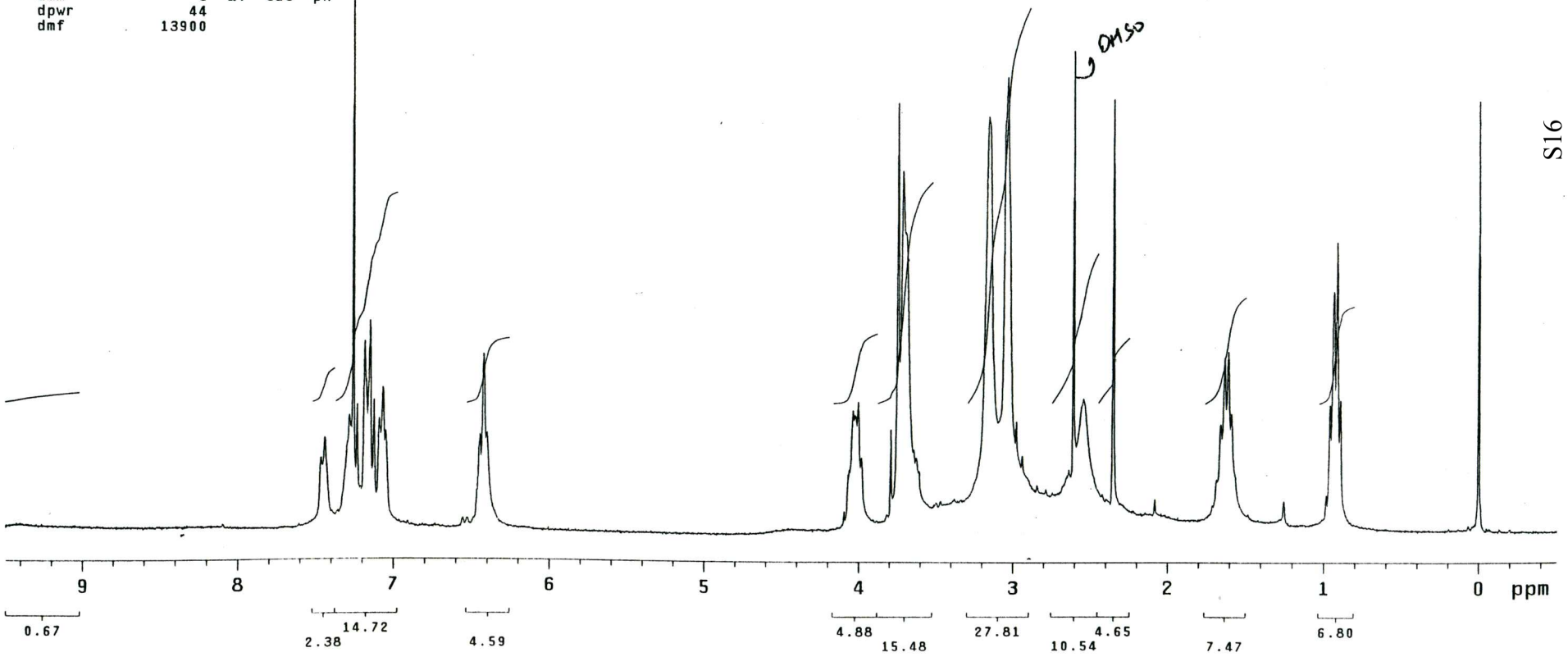
2A5
STANDARD 1H OBSERVE

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 11 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_11.10.05/2A501.f~		pw90	17.250
	id	alfa	20.000
ACQUISITION		**FLAGS**	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	**PROCESSING**	
d1	1.000	fn	not used
nt	32	**DISPLAY**	
ct	32	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	597.5
sfrq	299.790	rfp	0
tof	315.5	rp	139.3
tpwr	60	lp	-65.9
pw	8.625	**PLOT**	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	1791
dm	nnn	th	16
dmm	c	ai cdc ph	
dpwr	44		
dmf	13900		



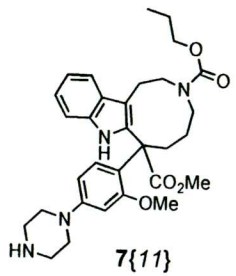
7{11}



vin-2A5-c13

exp1 std13c

SAMPLE		DEC. & VT	
date	Oct 24 2005	dfrq	400.120
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	37
mkaselj/vin-2A5-C1~	3	dof	0
		dm	yyy
ACQUISITION		dmm	w
sfrq	100.619	dmf	9700
tn	C13	PROCESSING	
at	1.199	lb	1.00
np	59968	wtfile	
sw	25000.0	proc	ft
fb	13800	fn	not used
bs	16		
ss	4	werr	
tpwr	58	wexp	
pw	11.7	wbs	
d1	2.000	wnt	
tof	0		
nt	100000		
ct	16304		
alock	y		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-642.6		
wp	22637.2		
vs	134		
sc	0		
wc	250		
hzmm	90.55		
is	500.00		
rfl	3005.4		
rfp	0		
th	20		
ins	100.000		
nm no ph			

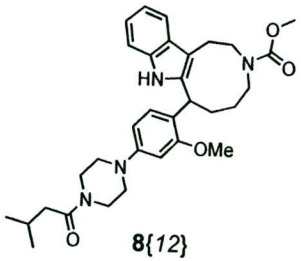


7{11}

1A1_rerun
STANDARD 1H OBSERVE

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 12 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_12.10.05/1A1_rer~		pw90	17.250
	un01.fid	alfa	20.000
ACQUISITION		FLAGS	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	PROCESSING	
d1	1.000	fn	not used
nt	32	DISPLAY	
ct	32	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	594.3
sfrq	299.790	rfp	0
tof	315.5	rp	139.6
tpwr	60	lp	-57.0
pw	8.625	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	1167
dm	nnn	th	2
dmm	c	ai cdc ph	
dpwr	44		
dmf	13900		



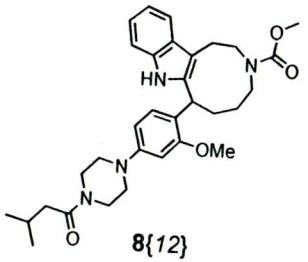
8{12}

VIN-1A1-C13
13C OBSERVE

pad=2 run with findz0 before acquisition

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 13 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
	auto/walk_auto/aut~	hst	0.008
	o_13.10.05/VIN-1A1~	pw90	13.500
	-C1301.fid	alfa	20.000
ACQUISITION		FLAGS	
sw	18832.4	il	n
at	1.815	in	n
np	68362	dp	y
fb	10400	hs	nn
bs	64	PROCESSING	
d1	2.000	lb	1.00
nt	5000	fn	not used
ct	5000	DISPLAY	
TRANSMITTER		sp	-37.9
tn	C13	wp	16960.8
sfrq	75.390	rfl	6946.7
tof	740.3	rfp	5804.4
tpwr	58	rp	-93.9
pw	6.750	lp	-269.0
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	3049
dmm	w	th	11
dpwr	42	ai no ph	
dmf	6744		



8{12}

1A2
STANDARD 1H OBSERVE

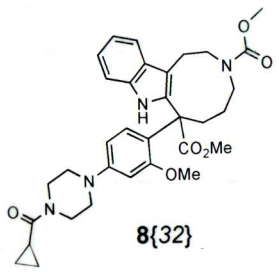
Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1A202

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
Sample #10
File: 1A201
Mercury-300BB "horror"

3839-2AS
8{32}

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885464 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



8{32}

DMSO

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

17.62 4.53 60.89 7.44 8.68 0.84

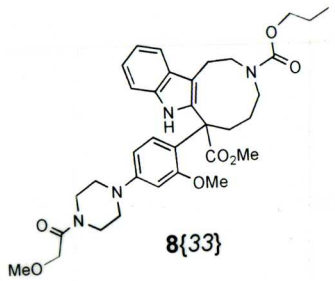
1A3
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1A302

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #11
File: 1A301
Mercury-300BB "horror"

3839-282
8{33}

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885493 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



8{33}

DMSO

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

0.17 14.56 3.96 54.50 8.88 9.33 0.98 6.35 1.26

1A4
STANDARD 1H OBSERVE

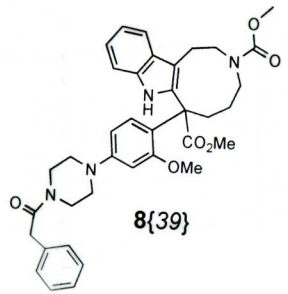
Automation directory: /export/home/auto/walk_auto/auto_12.10.05
File : 1A402

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
Sample #12
File: 1A401
Mercury-300BB "horror"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885508 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec

3839-2C4
8{39}

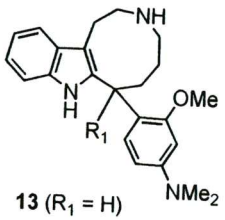


8{*39*}

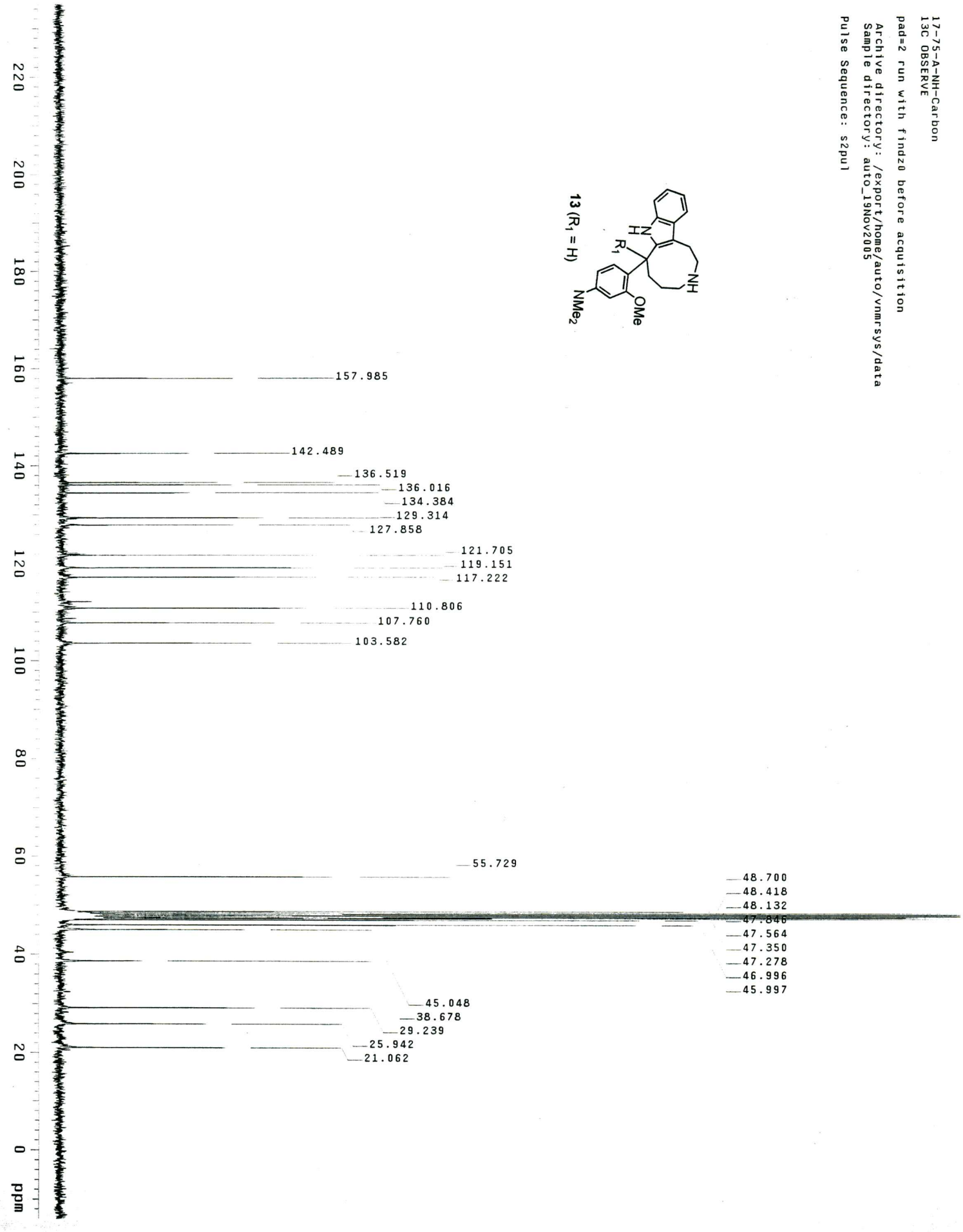
17-75-A-NH-Proton

Archive directory: /export/home/auto/vnmrsys/data
Sample directory: auto_18Nov2005

Pulse Sequence: s2pul



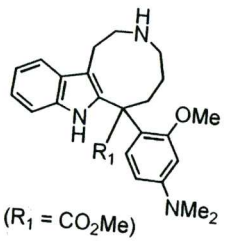
13 (R_1 = H)


17-75-A-NH-Carbon
13C OBSERVE
pad=2 run with findz0 before acquisition
Archive directory: /export/home/auto/vnmrsys/data
Sample directory: auto_19Nov2005
Pulse Sequence: s2pul
13 (R_1 = H)
NMe2
OMe
NH
157.985
142.489
136.519
136.016
134.384
129.314
127.858
121.705
119.151
117.222
110.806
107.760
103.582
55.729
48.700
48.418
48.132
47.846
47.564
47.350
47.278
46.996
45.997
45.048
38.678
29.239
25.942
21.062
ppm

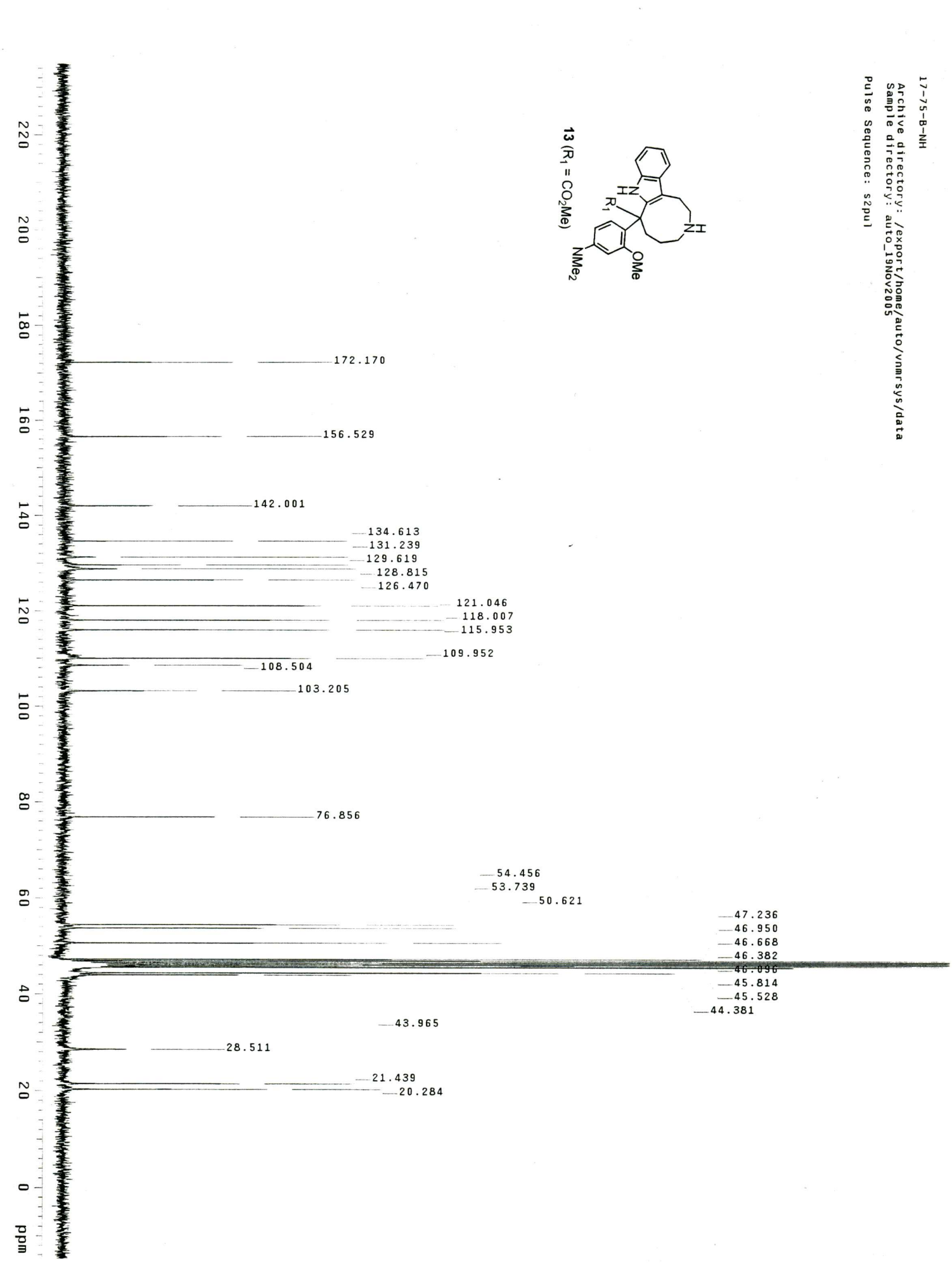
17-75-B-NH-Proton

Archive directory: /export/home/auto/vnmrsys/data
Sample directory: auto_18Nov2005

Pulse Sequence: s2pul



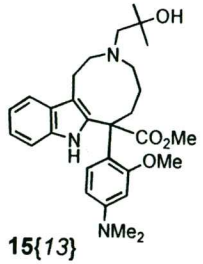
13 (R_1 = CO_2Me)


17-75-B-NH
Archive directory: /export/home/auto/vnmrsys/data
Sample directory: auto_19Nov2005
Pulse Sequence: s2pul
13 (R_1 = CO_2Me)
NMe2
OMe
172.170
156.529
142.001
134.613
131.239
129.619
128.815
126.470
121.046
118.007
115.953
109.952
108.504
103.205
76.856
54.456
53.739
50.621
47.236
46.950
46.668
46.382
46.096
45.814
45.528
44.381
43.965
28.511
21.439
20.284
ppm

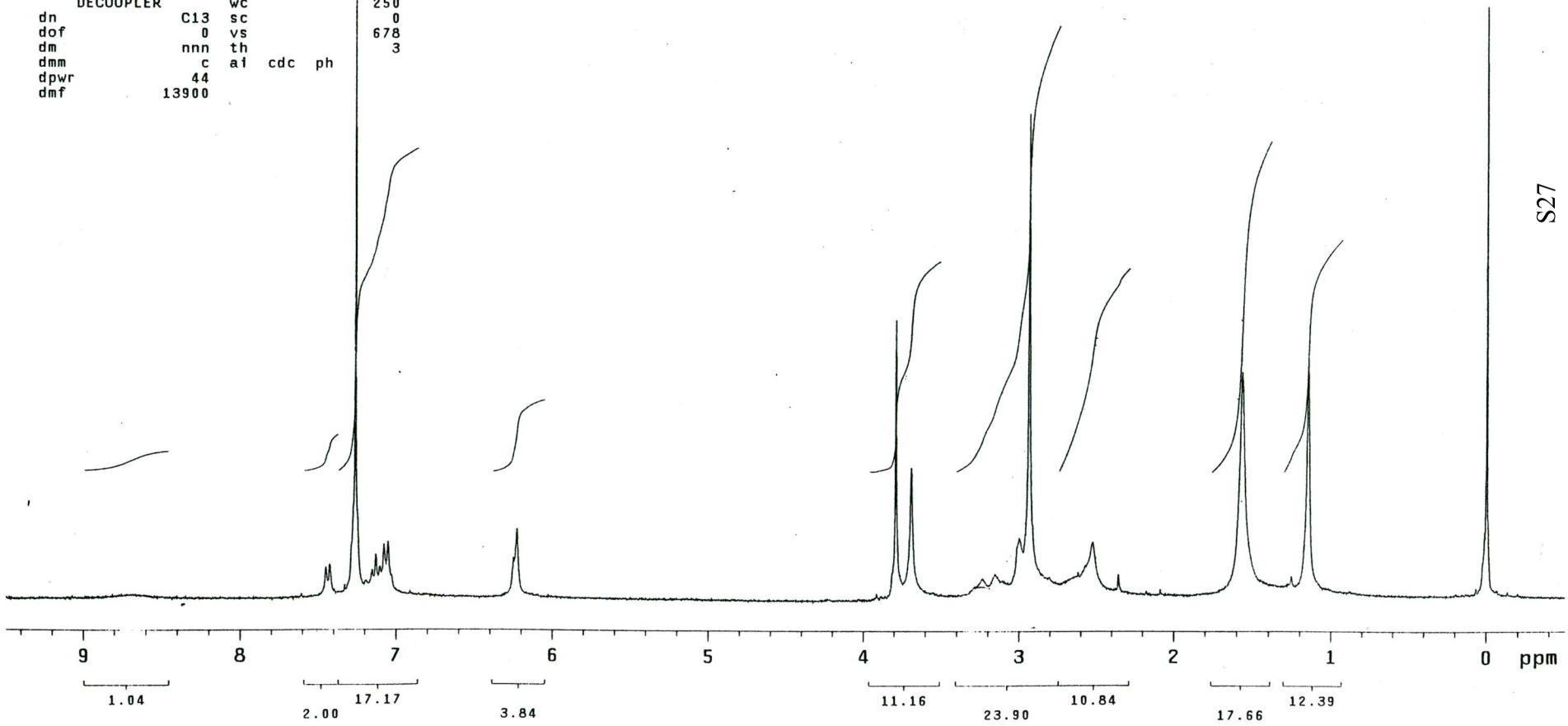
Vin 1A6 re-run
STANDARD 1H OBSERVE

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 13 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_13.10.05/Vin02.f~		pw90	17.250
	id	alfa	20.000
ACQUISITION		**FLAGS**	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	**PROCESSING**	
d1	1.000	fn	not used
nt	128	**DISPLAY**	
ct	128	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	590.8
sfrq	299.790	rfp	0
tof	315.5	rp	126.0
tpwr	60	lp	-61.7
pw	8.625	**PLOT**	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	678
dm	nnn	th	3
dmm	c	ai cdc ph	
dpwr	44		
dmf	13900		



15{*13*}



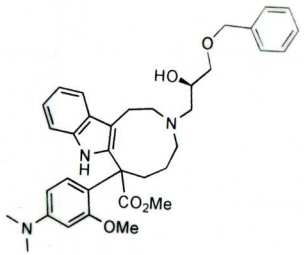
Vin 1B1 re-run
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_13.10.05
File : Vin04

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #15
File: Vin03
Mercury-300BB "horror"

3912-104
15{23}

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
128 repetitions
OBSERVE H1, 299.7885508 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 38 sec

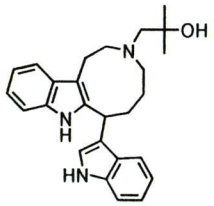


15{*23*}

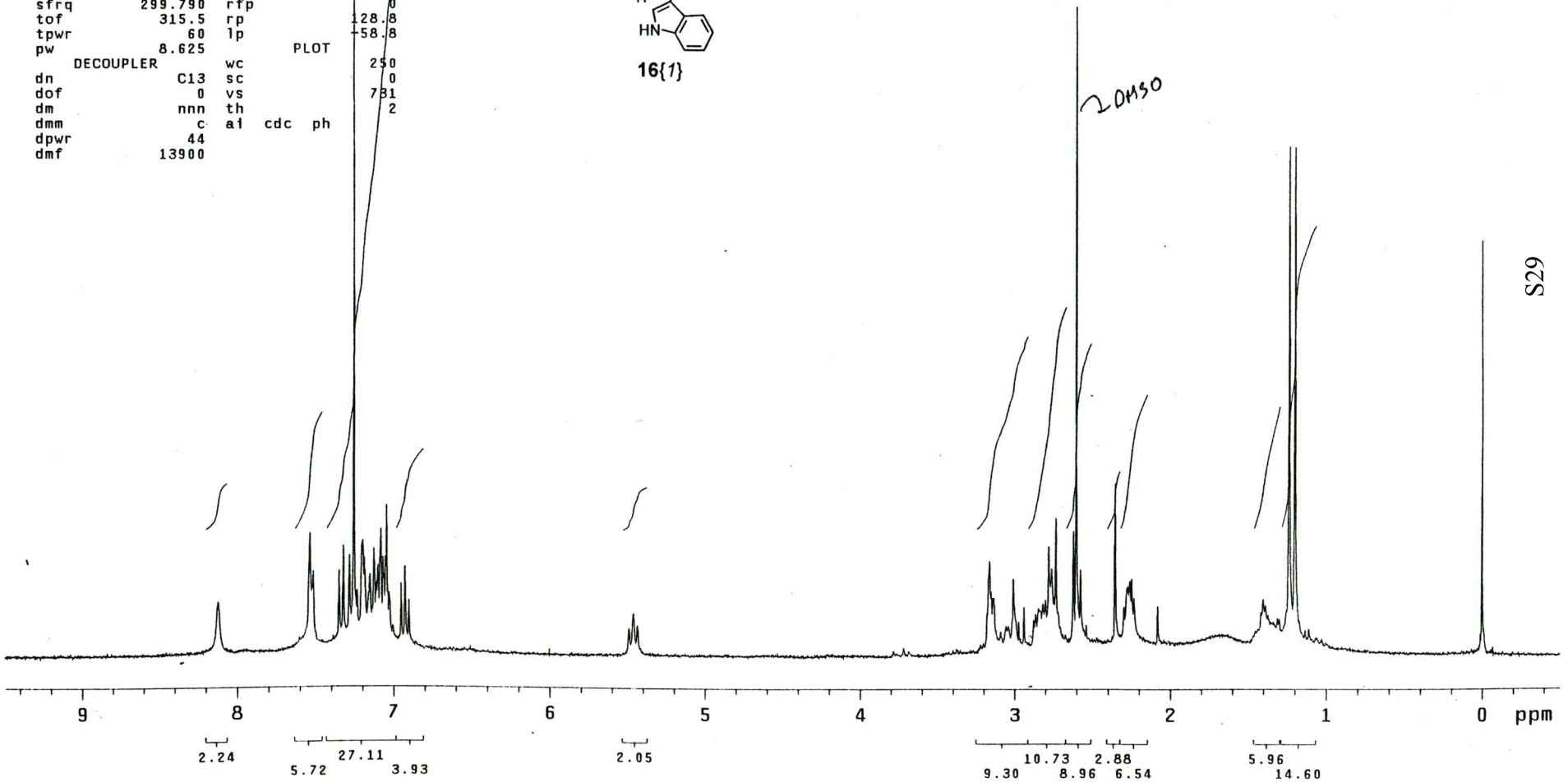
1C5
STANDARD 1H OBSERVE

expl s2pul

SAMPLE		SPECIAL	
date	Oct 12 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
auto/walk_auto/aut~		hst	0.008
o_12.10.05/1C501.f~		pw90	17.250
	id	alfa	20.000
ACQUISITION		**FLAGS**	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	**PROCESSING**	
d1	1.000	fn	not used
nt	32	**DISPLAY**	
ct	32	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	597.8
sfrq	299.790	rfp	0
tof	315.5	rp	128.8
tpwr	60	lp	-58.8
pw	8.625	**PLOT**	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	731
dm	nnn	th	2
dmm	c	ai	cdc ph
dpwr	44		
dmf	13900		



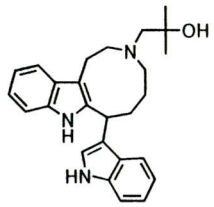
16{*1*}



Vin-1C5-C13

exp1 std13c

SAMPLE		DEC. & VT	
date	Oct 18 2005	dfrq	400.120
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	37
mkaselj/vin-1c5-c1~	3	dof	0
		dm	yyy
ACQUISITION		dmm	w
sfrq	100.619	dmf	9700
tn	C13	PROCESSING	
at	1.199	lb	1.00
np	59968	wtfile	
sw	25000.0	proc	ft
fb	13800	fn	not used
bs	16		
ss	4	werr	
tpwr	58	wexp	
pw	11.7	wbs	
d1	2.000	wnt	
tof	0		
nt	100000		
ct	16896		
alock	y		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-642.7		
wp	22637.2		
vs	151		
sc	0		
wc	250		
hzmm	90.55		
is	500.00		
rfl	3005.5		
rfp	0		
th	20		
ins	100.000		
nm no ph			

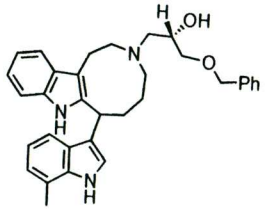


16{*1*}

1D1
STANDARD 1H OBSERVE

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 12 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
	auto/walk_auto/aut~	hst	0.008
	o_12.10.05/1D101.f~	pw90	17.250
	id	alfa	20.000
ACQUISITION		**FLAGS**	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	**PROCESSING**	
d1	1.000	fn	not used
nt	32	**DISPLAY**	
ct	32	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	597.8
sfrq	299.790	rfp	0
tof	315.5	rp	145.5
tpwr	60	lp	-81.9
pw	8.625	**PLOT**	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	1338
dm	nnn	th	6
dmm	c	ai cdc ph	
dpwr	44		
dmf	13900		

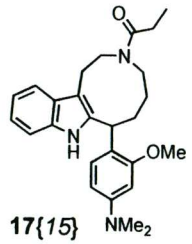


16{*12*}

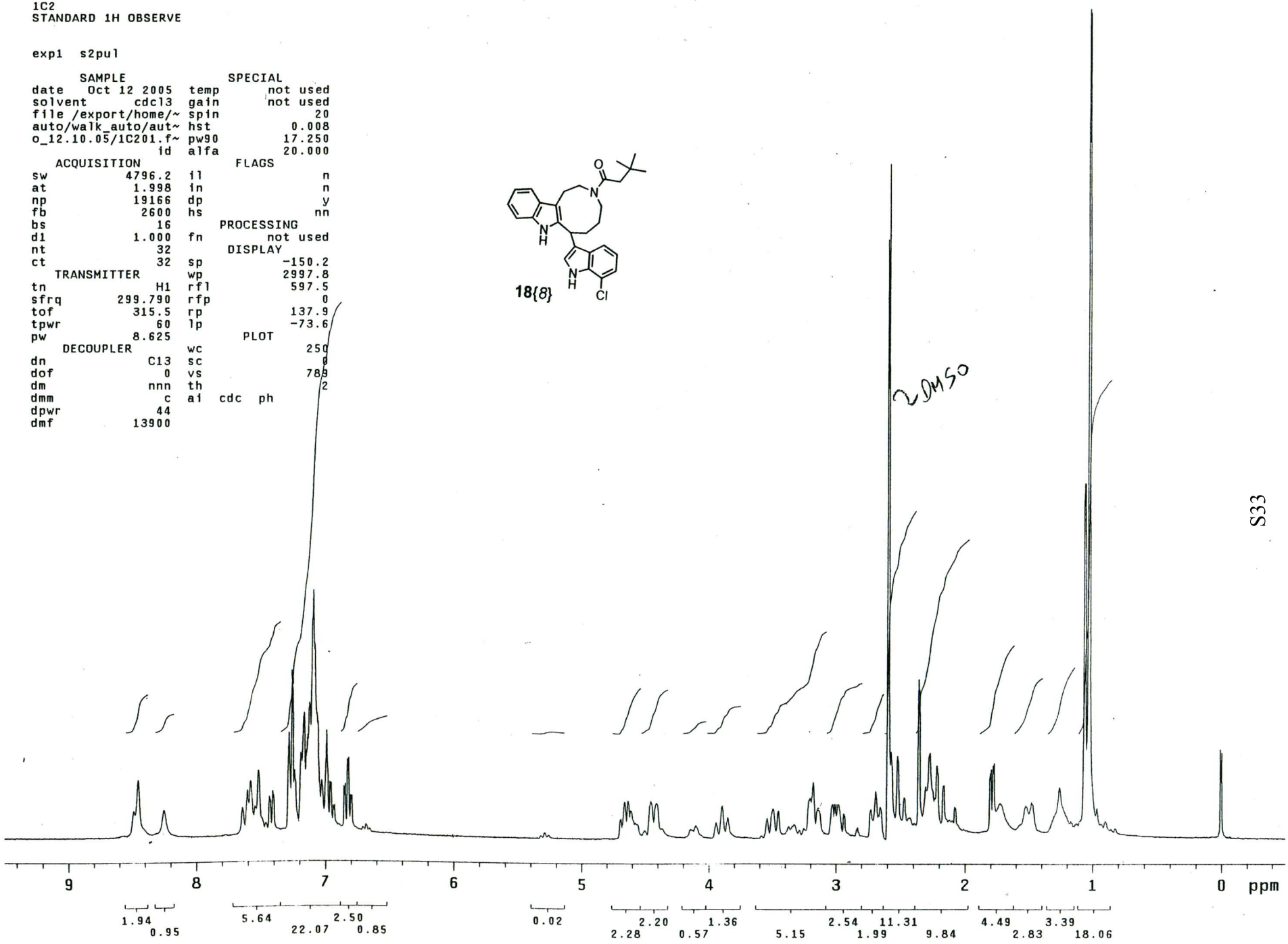
1D3
STANDARD 1H OBSERVE

Archive directory: /export/home/auto/vnmrsys/data
Sample directory: auto_16Nov2005

Pulse Sequence: s2pul



17{*15*}


1C2
STANDARD 1H OBSERVE
exp1 s2pul
SAMPLE
date Oct 12 2005
solvent cdcl3
file /export/home/~
auto/walk_auto/aut~
o_12.10.05/1C201.f~
id
ACQUISITION
sw 4796.2
at 1.998
np 19166
fb 2600
bs 16
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 299.790
tof 315.5
tpwr 60
pw 8.625
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 44
dmf 13900
SPECIAL
temp not used
gain not used
spin 20
hst 0.008
pw90 17.250
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn not used
DISPLAY
sp -150.2
wp 2997.8
rfl 597.5
rfp 0
rp 137.9
lp -73.6
PLOT
wc 250
sc 0
vs 789
th 2
ai cdc ph
18{8}
DMSO
9
8
7
6
5
4
3
2
1
0
ppm
1.94
0.95
5.64
22.07
2.50
0.85
0.02
2.28
2.20
0.57
1.36
5.15
2.54
1.99
11.31
9.84
4.49
2.83
3.39
18.06

2B1
STANDARD 1H OBSERVE

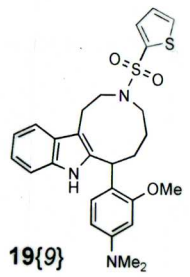
Automation directory: /export/home/auto/walk_auto/auto_11.10.05
File : 2B102

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
Sample #14
File: 2B101
Mercury-300BB "horror"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885473 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec

3931-1B3
19593



19{9}

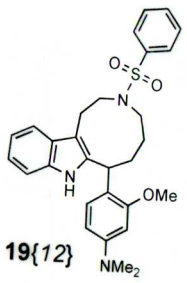
2B2
STANDARD 1H OBSERVE

Automation directory: /export/home/auto/walk_auto/auto_11.10.05
File : 2B202

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
Sample #15
File: 2B201
Mercury-300BB "horror"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4796.2 Hz
32 repetitions
OBSERVE H1, 299.7885529 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



19{*12*}

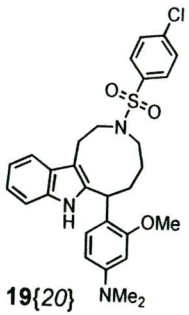
3931-1B6

19{12}

2B3
STANDARD 1H OBSERVE

exp1 s2pul

SAMPLE		SPECIAL	
date	Oct 11 2005	temp	not used
solvent	cdcl3	gain	not used
file	/export/home/~	spin	20
	auto/walk_auto/aut~	hst	0.008
	o_11.10.05/2B301.f~	pw90	17.250
	id	alfa	20.000
ACQUISITION		FLAGS	
sw	4796.2	il	n
at	1.998	in	n
np	19166	dp	y
fb	2600	hs	nn
bs	16	PROCESSING	
d1	1.000	fn	not used
nt	32	DISPLAY	
ct	32	sp	-150.2
TRANSMITTER		wp	2997.8
tn	H1	rfl	599.6
sfrq	299.790	rfp	0
tof	315.5	rp	143.5
tpwr	60	lp	-77.8
pw	8.625	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	635
dm	nnn	th	6
dmm	c	ai cdc ph	
dpwr	44		
dmf	13900		



19{*20*}

Tables describing the synthesis layout of chemsets 2-4, 7-10, 15-20[a]

Table 1. Array layout of chemset **2**

Table 2. Array layout of chemset **3**

Table 3. Array layout of chemset **4**

Table 4. Array layout of chemset **7**

Table 5. Array layout of chemset **8**

Table 6. Array layout of chemset **9**

Table 7. Array layout of chemset **10**

Table 8. Array layout of chemset **15**

Table 9. Array layout of chemset **16**

Table 10. Array layout of chemset **17**

Table 11. Array layout of chemset **18**

Table 12. Array layout of chemset **19**

Table 13. Array layout of chemset **20**

[a]Numbers in parentheses represent the isolated yield (% yield or μmol quantity), the % purity by UV_{214nm} and ELSD (evaporative light scattering detector), respectively, of each individual compound prepared on 100 μmol scale and recovered after mass-triggered high throughput reverse phase HPLC purification.

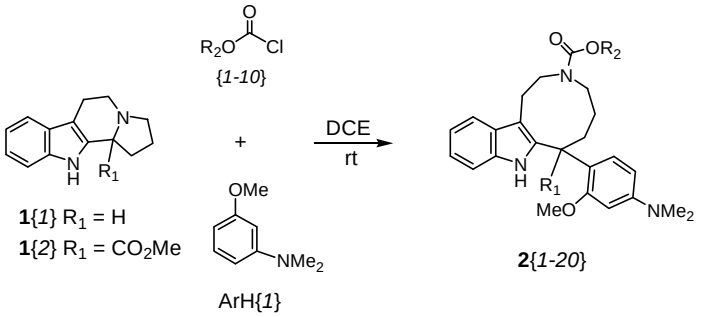
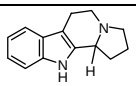
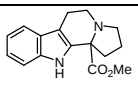
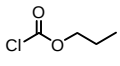
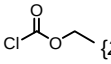
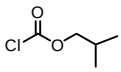
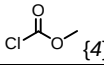
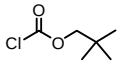
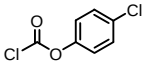
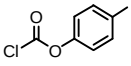
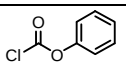
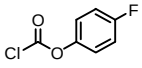
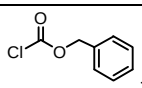


Table 1. Array layout of chemset **2**{*1-20*}

Library Scaffolds		 **1**{*1*}	 **1**{*2*}
Chloroformates {*1-10*}	**ArH**{*1*}	**Product**	**Product**
 {*1*}		**2**{*1*} (47.5, 89, 100)	**2**{*11*} (27.6, 100, 100)
 {*2*}		**2**{*2*} (49.5, 90, 100)	**2**{*12*} Not isolated
 {*3*}		**2**{*3*} (59.9, 90, 100)	**2**{*13*} (42.0, 100, 100)
 {*4*}		**2**{*4*} (52.4, 89, 100)	**2**{*14*} (30.9, 96, 100)
 {*5*}		**2**{*5*} (58.9, 90, 100)	**2**{*15*} (41.3, 100, 100)
 {*6*}		**2**{*6*} (53, 89, 100)	**2**{*16*} (63, 100, 100)
 {*7*}		**2**{*7*} (55.3, 90, 100)	**2**{*17*} (61.2, 100, 100)
 {*8*}		**2**{*8*} (26.3, 74, 100)	**2**{*18*} (64.3, 100, 100)
 {*9*}		**2**{*9*} (57.5, 88, 100)	**2**{*19*} (65, 100, 100)
 {*10*}		**2**{*10*} (13.9, 60, 100)	**2**{*20*} (25.1, 100, 100)

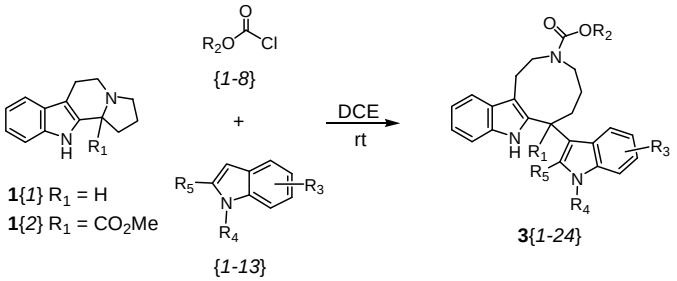
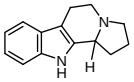
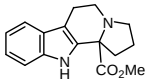
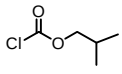
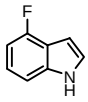
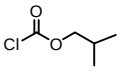
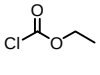
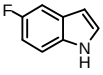
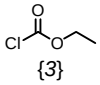
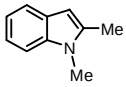
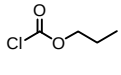
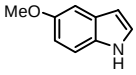
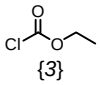
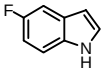
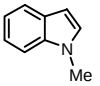
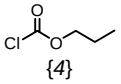
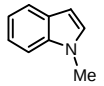
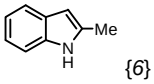
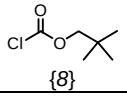
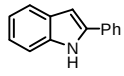
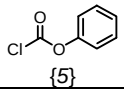
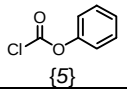
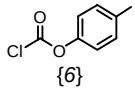
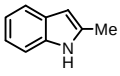
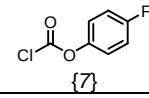
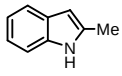
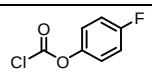
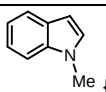
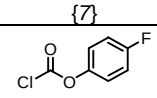
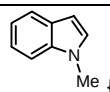
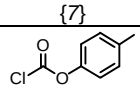


Table 2. Array layout of chemset **3**{*1-24*}

Library Scaffolds		 **1**{*1*}	**Library Scaffolds**		 **1**{*2*}
Chloroformates {*1-8*}	**Indoles**{*1-13*}	**Product**	**Chloroformates** {*1-8*}	**Indoles**{*1-13*}	**Product**
 {*1*}	 {*1*}	**3**{*1*} (42.7, 95, 100)	 {*2*}	 {*9*}	**3**{*13*} Not isolated
 {*2*}	 {*2*}	**3**{*2*} Not isolated	 {*1*}	 {*1*}	**3**{*14*} (12.8, 96, 100)
 {*3*}	 {*3*}	**3**{*3*} (28.7, 100, 100)	 {*3*}	 {*10*}	**3**{*15*} (27.2, 100, 100)
 {*4*}	 {*4*}	**3**{*4*} (29.7, 94, 100)	 {*3*}	 {*3*}	**3**{*16*} (11.6, 100, 100)
 {*3*}	 {*5*}	**3**{*5*} (60.6, 100, 100)	 {*4*}	 {*5*}	**3**{*17*} (16.7, 100, 100)
 {*3*}	 {*6*}	**3**{*6*} (46.1, 93, 100)	 {*8*}	 {*11*}	**3**{*18*} (29.0, 100, 100)
 {*5*}	 {*1*}	**3**{*7*} (41.9, 100, 100)	 {*5*}	 {*1*}	**3**{*19*} Not isolated
 {*6*}	 {*6*}	**3**{*8*} Not isolated	 {*7*}	 {*6*}	**3**{*20*} Not isolated
 {*7*}	 {*5*}	**3**{*9*} (60.5, 100, 100)	 {*7*}	 {*5*}	**3**{*21*} (27.4, 100, 100)
 {*6*}	{*3*}	**3**{*10*} (63.8, 100, 100)	{*6*}	{*3*}	**3**{*22*} Not isolated
{*7*}	{*7*}	**3**{*11*} (58.7, 100, 100)	{*5*}	{*12*}	**3**{*23*} (14.6, 85, 100)
{*5*}	{*8*}	**3**{*12*} (46, 85, 100)	{*7*}	{*13*}	**3**{*24*} Not isolated

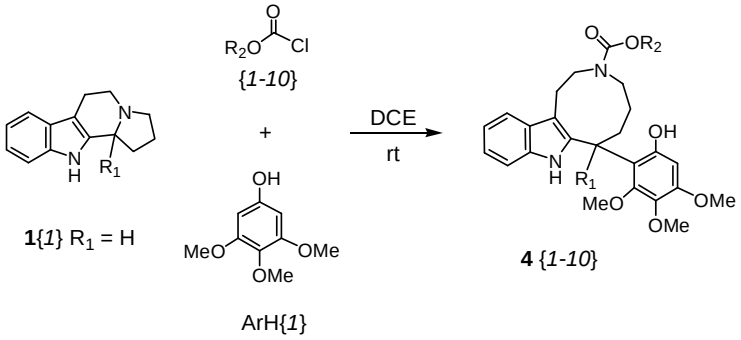
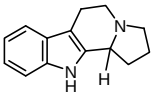
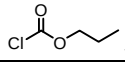
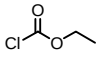
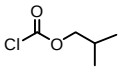
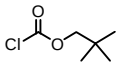
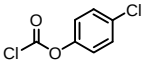
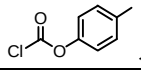
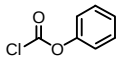
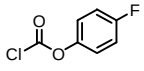
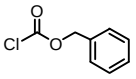


Table 3. Array layout of chemset **4**{*1-10*}

Library Scaffolds		 **1**{*1*}
Chloroformates {*1-10*}	**ArH**{*1*}	**Product**
 {*1*}	3,4,5-trimethoxyphenol	**4**{*1*} (28.0, 100, 100)
 {*2*}	3,4,5-trimethoxyphenol	**4**{*2*} (33.8, 96, 100)
 {*3*}	3,4,5-trimethoxyphenol	**4**{*3*} Not isolated
 {*4*}	3,4,5-trimethoxyphenol	**4**{*4*} (43.7, 100, 100)
 {*5*}	3,4,5-trimethoxyphenol	**4**{*5*} (10.2, 71, 76)
 {*6*}	3,4,5-trimethoxyphenol	**4**{*6*} Not isolated
 {*7*}	3,4,5-trimethoxyphenol	**4**{*7*} (25.1, 100, 100)
 {*8*}	3,4,5-trimethoxyphenol	**4**{*8*} (43.4, 100, 100)
 {*9*}	3,4,5-trimethoxyphenol	**4**{*9*} (47.3, 100, 100)
 {*10*}	3,4,5-trimethoxyphenol	**4**{*10*} Not isolated

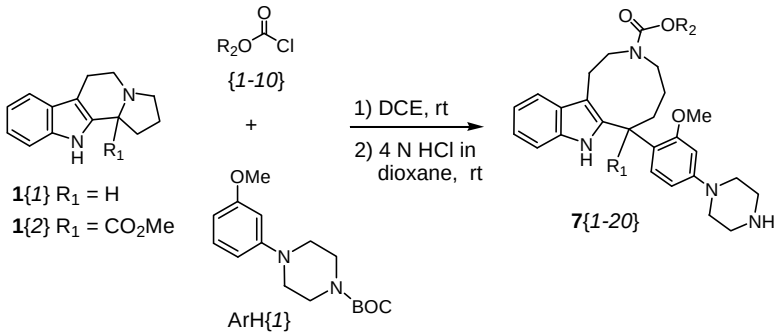
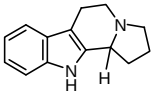
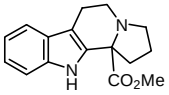
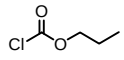
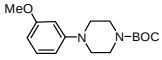
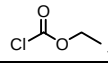
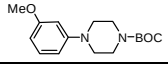
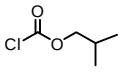
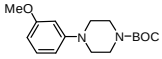
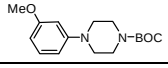
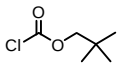
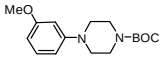
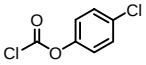
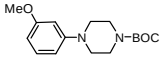
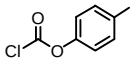
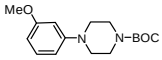
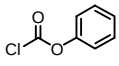
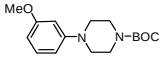
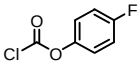
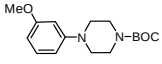
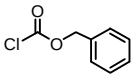
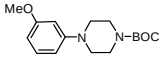


Table 4. Array layout of chemset **7**{*1-20*}

Library Scaffolds		 **1**{*1*}	 **1**{*2*}
Chloroformates {*1-10*}	**ArH**{*1*}	**Product**	**Product**
 {*1*}		**7**{*1*} (27.2, 96, 100)	**7**{*11*} (28.8, 100, 100)
 {*2*}		**7**{*2*} (26.1, 100, 100)	**7**{*12*} (32.3, 100, 100)
 {*3*}		**7**{*3*} (28.1, 93, 100)	**7**{*13*} (30.5, 94, 100)
 {*4*}		**7**{*4*} (28.8, 96, 100)	**7**{*14*} (34.2, 97, 100)
 {*5*}		**7**{*5*} (23.1, 88, 94)	**7**{*15*} (27.7, 77, 88)
 {*6*}		**7**{*6*} (18.0, 82, 92)	**7**{*16*} (32.3, 73, 87)
 {*7*}		**7**{*7*} (24.5, 82, 90)	**7**{*17*} (33.5, 69, 81)
 {*8*}		**7**{*8*} Not isolated	**7**{*18*} (33.4, 79, 93)
 {*9*}		**7**{*9*} (25.2, 81, 92)	**7**{*19*} (37.2, 78, 91)
 {*10*}		**7**{*10*} (25.6, 83, 97)	**7**{*20*} (29.1, 91, 100)

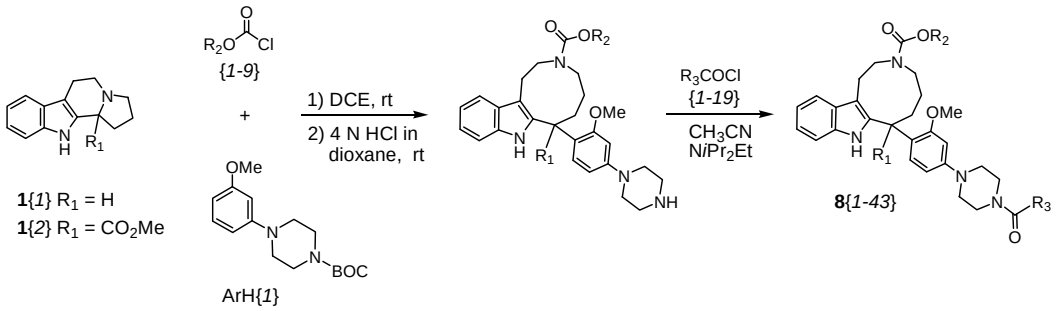
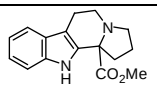
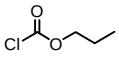
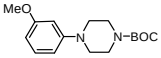
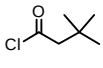
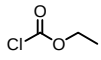
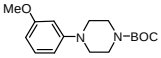
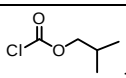
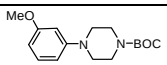
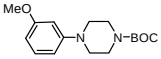
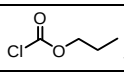
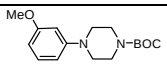
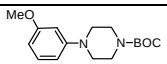
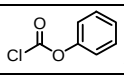
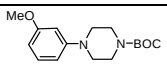
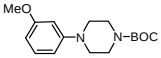
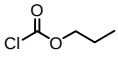
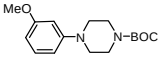
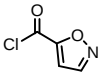
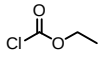
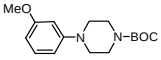
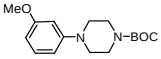
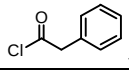
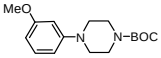
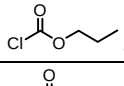
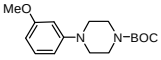


Table 5. Array layout of chemset **8**{*1-43*}

Library Scaffolds			**1**{*1*}	**Library Scaffolds**			**1**{*1*}
Chloroformates {*1-9*}	**ArH**{*1*}	**Acid Chlorides** {*1-19*}	**Product**	**Chloroformates** {*1-9*}	**ArH**{*1*}	**Acid Chlorides** {*1-19*}	**Product**
{*1*}	{*1*}	{*1*}	**8**{*1*} (22.2, 81, 95)	{*3*}	{*11*}	**8**{*15*} Not isolated
{*2*}	{*2*}	{*2*}	**8**{*2*} (30.7, 100, 100)	{*6*}	{*11*}	**8**{*16*} Not isolated
{*2*}	{*3*}	{*7*}	**8**{*3*} (33.2, 78, 100)	{*12*}	**8**{*17*} Not isolated
{*3*}	{*4*}	{*5*}	**8**{*4*} (6.0, 100, 100)	{*13*}	**8**{*18*} (26.9, 100, 100)
{*4*}	{*5*}	{*2*}	**8**{*5*} (18.8, 100, 93)	{*6*}	**8**{*19*} (9.0, 66, 78)
{*5*}	{*6*}	{*2*}	**8**{*6*} (20.1, 100, 100)	{*14*}	**8**{*20*} (15.8, 100, 100)
{*1*}	{*3*}	{*3*}	**8**{*7*} (52.9, 84, 100)	{*12*}	**8**{*21*} (14.9, 100, 69)
{*2*}	{*7*}	{*4*}	**8**{*8*} (27.1, 80, 92)	{*15*}	**8**{*22*} (25.7, 100, 100)
{*3*}	{*8*}	{*8*}	**8**{*9*} (22.3, 100, 100)	{*7*}	**8**{*23*} (34.2, 88, 97)
{*6*}	{*9*}	{*5*}	**8**{*10*} (6.0, 100, 100)	{*7*}	**8**{*24*} (39.1, 85, 100)
{*7*}	{*7*}	{*5*}	**8**{*11*} Not isolated	{*11*}	**8**{*25*} Not isolated
{*5*}	{*10*}	{*5*}	**8**{*12*} (31.4, 100, 100)	{*3*}	**8**{*26*} (40.3, 95, 100)
{*1*}	{*4*}	{*9*}	**8**{*13*} (18.9, 72, 79)	{*7*}	**8**{*27*} (28.9, 78, 86)
{*2*}	{*11*}	{*9*}	**8**{*14*} Not isolated	{*16*}	**8**{*28*} (22.7, 100, 100)

Table 5 (contd)

Library Scaffolds			 **1**{*2*}
Chloroformates {*1-9*}	**ArH**{*1*}	**Acid Chlorides** {*1-19*}	**Product**
 {*1*}		 {*8*}	**8**{*29*} (16.4, 100, 100)
 {*2*}		 {*17*}	**8**{*30*} (3.9, 49, 81)
 {*3*}		 {*7*}	**8**{*31*} (3.3, 44, 83)
 {*5*}		 {*17*}	**8**{*32*} (36.8, 100, 100)
 {*1*}		 {*7*}	**8**{*33*} (26.8, 100, 100)
 {*2*}		 {*18*}	**8**{*34*} (3.7, 38, 40)
 {*4*}		 {*3*}	**8**{*35*} (36.1, 80, 93)
 {*5*}		 {*7*}	**8**{*36*} (47.9, 58, 86)
 {*1*}		 {*11*}	**8**{*37*} Not isolated
 {*2*}		 {*7*}	**8**{*38*} (3.0, 32, 38)
 {*5*}		 {*6*}	**8**{*39*} (24.5, 100, 100)
 {*5*}		 {*3*}	**8**{*40*} (52.0, 55, 81)
 {*1*}		 {*19*}	**8**{*41*} (3.4, 44, 71)
{*2*}		{*3*}	**8**{*42*} (3.7, 61, 87)
{*5*}		{*9*}	**8**{*43*} (20.8, 100, 100)

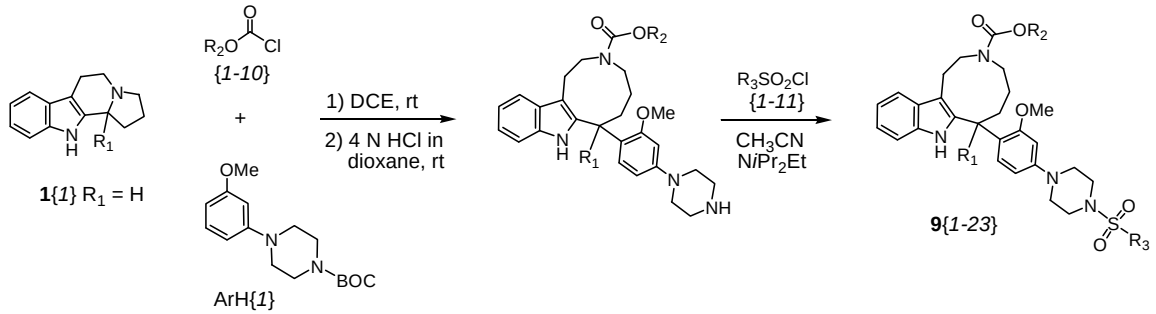


Table 6. Array layout of chemset **9**{*1-23*}

Library Scaffolds			**1**{*1*}	**Library Scaffolds**			**1**{*1*}
Chloroformates {*1-10*}	**ArH**{*1*}	**Sulfonyl Chlorides** {*1-11*}	**Product**	**Chloroformates** {*1-10*}	**ArH**{*1*}	**Sulfonyl Chlorides** {*1-11*}	**Product**
{*1*}		{*1*}	**9**{*1*} Not isolated	{*9*}		{*1*}	**9**{*13*} (7.7, 69, 86)
{*2*}		{*2*}	**9**{*2*} (5.9, 100, 100)	{*9*}		{*2*}	**9**{*14*} (4.5, 95, 100)
{*3*}		{*3*}	**9**{*3*} (13.8, 97, 100)	{*6*}		{*8*}	**9**{*15*} (5.5, 100, 100)
{*2*}		{*4*}	**9**{*4*} (17.3, 100, 100)	{*3*}		{*7*}	**9**{*16*} (11.6, 90, 100)
{*3*}		{*5*}	**9**{*5*} (13.7, 100, 100)	{*8*}		{*8*}	**9**{*17*} (9.3, 100, 100)
{*4*}		{*6*}	**9**{*6*} (5.2, 100, 100)	{*3*}		{*1*}	**9**{*18*} (7.5, 68, 91)
{*5*}		{*3*}	**9**{*7*} (5.3, 80, 100)	{*10*}		{*3*}	**9**{*19*} (5.9, 100, 100)
{*6*}		{*2*}	**9**{*8*} (3.9, 77, 100)	{*4*}		{*9*}	**9**{*20*} (9.7, 94, 100)
{*7*}		{*1*}	**9**{*9*} (6.2, 65, 87)	{*2*}		{*10*}	**9**{*21*} (13.3, 100, 100)
{*8*}		{*2*}	**9**{*10*} (4.8, 74, 86)	{*2*}		{*11*}	**9**{*22*} (4.7, 28, 12)
{*5*}		{*5*}	**9**{*11*} (11.6, 88, 100)	{*3*}		{*4*}	**9**{*23*} (17.3, 91, 100)
{*8*}		{*7*}	**9**{*12*} (5.4, 80, 95)				

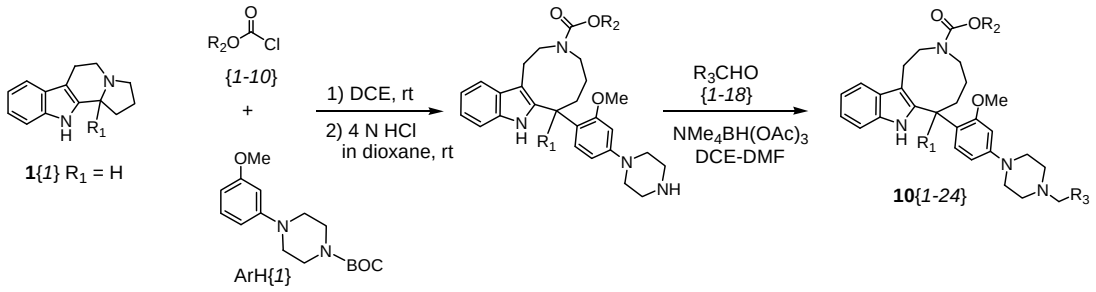
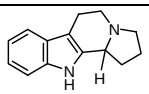
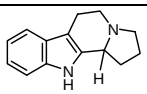
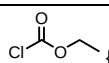
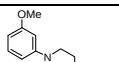
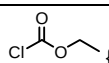
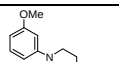
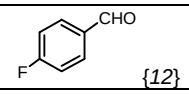
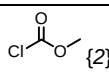
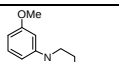
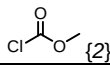
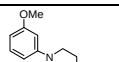
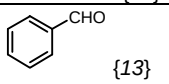
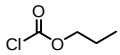
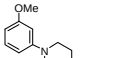
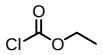
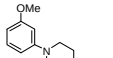
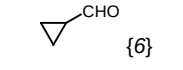
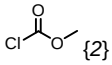
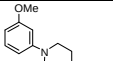
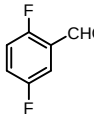
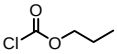
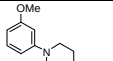
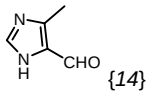
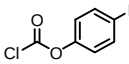
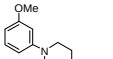
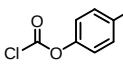
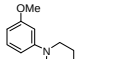
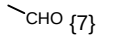
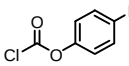
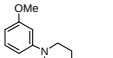
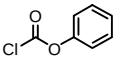
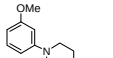
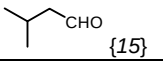
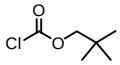


Table 7. Array layout of chemset **10**{*1-24*}

Library Scaffolds			 **1**{*1*}	**Library Scaffolds**			 **1**{*1*}
Chloroformates {*1-10*}	**ArH**{*1*}	**Aldehydes** {*1-18*}	**Product**	**Chloroformates** {*1-10*}	**ArH**{*1*}	**Aldehydes** {*1-18*}	**Product**
 {*1*}		 {*1*}	**10**{*1*} (9.1, 100, 100)	 {*1*}		 {*12*}	**10**{*13*} (8.9, 100, 100)
 {*2*}		 {*2*}	**10**{*2*} (12.8, 100, 100)	 {*2*}		 {*13*}	**10**{*14*} (7.1, 96, 100)
 {*3*}		 {*3*}	**10**{*3*} (8.4, 100, 100)	 {*1*}		 {*6*}	**10**{*15*} (7.4, 92, 100)
 {*2*}		 {*4*}	**10**{*4*} (5.9, 74, 100)	 {*3*}		 {*14*}	**10**{*16*} (12.4, 100, 100)
 {*4*}		 {*5*}	**10**{*5*} Not isolated	 {*8*}		 {*7*}	**10**{*17*} (12.2, 100, 100)
 {*4*}		 {*6*}	**10**{*6*} (9.2, 100, 100)	 {*9*}		 {*15*}	**10**{*18*} (8.9, 94, 100)
 {*5*}		{*7*}	**10**{*7*} (6.1, 100, 100)	{*6*}		{*11*}	**10**{*19*} (6.4, 100, 100)
{*1*}		{*8*}	**10**{*8*} (6.6, 95, 100)	{*1*}		{*16*}	**10**{*20*} Not isolated
{*6*}		{*9*}	**10**{*9*} (8.0, 96, 100)	{*6*}		{*17*}	**10**{*21*} Not isolated
{*2*}		{*10*}	**10**{*10*} (7.7, 100, 100)	{*9*}		{*18*}	**10**{*22*} Not isolated
{*7*}		{*9*}	**10**{*11*} (7.8, 100, 100)	{*9*}		{*1*}	**10**{*23*} (9.4, 92, 100)
{*7*}		{*11*}	**10**{*12*} (9.6, 100, 100)	{*10*}		{*7*}	**10**{*24*} (10.4, 96, 100)

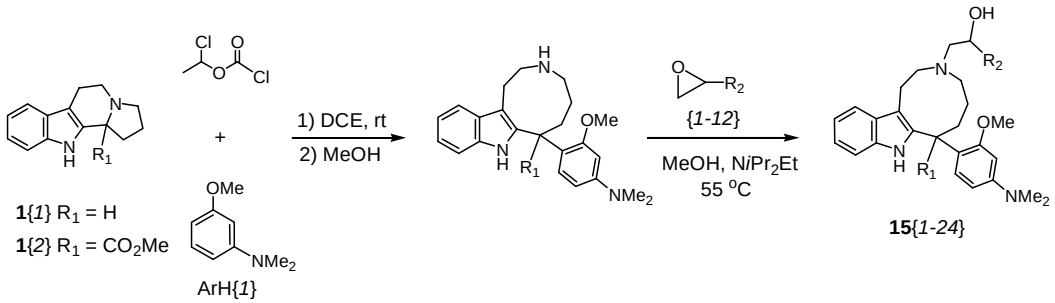
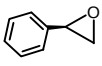
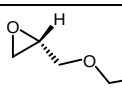
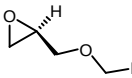


Table 8. Array layout of chemset **15**{*1-24*}

Library Scaffolds		**1**{*1*}	**1**{*2*}
ArH{*1*}	**Epoxides**{*1-12*}	**Product**	**Product**
	 {*1*}	**15**{*1*} (31.7, 85, 100)	**15**{*13*} (27.1, 100, 100)
	 {*2*}	**15**{*2*} (48.7, 88, 100)	**15**{*14*} (33.9, 100, 100)
	 {*3*}	**15**{*3*} Not isolated	**15**{*15*} (5.8, 79, 100)
	 {*4*}	**15**{*4*} (52.7, 90, 100)	**15**{*16*} Not isolated
	 {*5*}	**15**{*5*} (35.4, 94, 100)	**15**{*17*} (41.3, 100, 100)
	 {*6*}	**15**{*6*} (24.0, 100, 100)	**15**{*18*} (21.1, 56, 83)
	 {*7*}	**15**{*7*} (24.8, 100, 100)	**15**{*19*} (30.3, 76, 100)
	 {*8*}	**15**{*8*} Not isolated	**15**{*20*} (25.7, 100, 100)
	 {*9*}	**15**{*9*} (31.7, 100, 100)	**15**{*21*} (28.9, 100, 100)
	 {*10*}	**15**{*10*} (45.2, 100, 100)	**15**{*22*} (56.5, 88, 100)
	 {*11*}	**15**{*11*} (42.7, 92, 100)	**15**{*23*} (46.3, 100, 100)
	 {*12*}	**15**{*12*} (27.6, 85, 100)	**15**{*24*} (44.4, 75, 100)

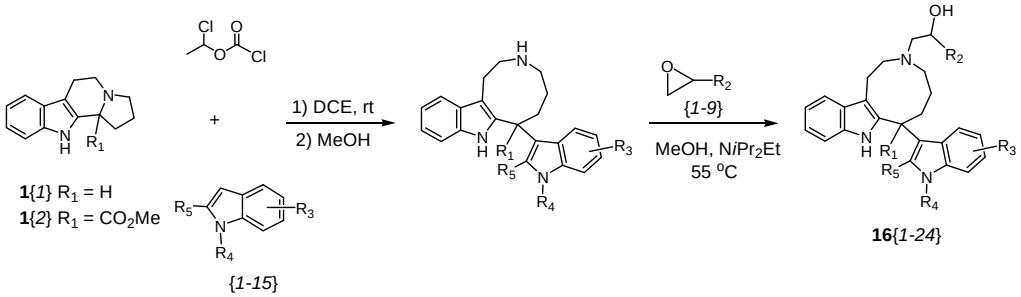
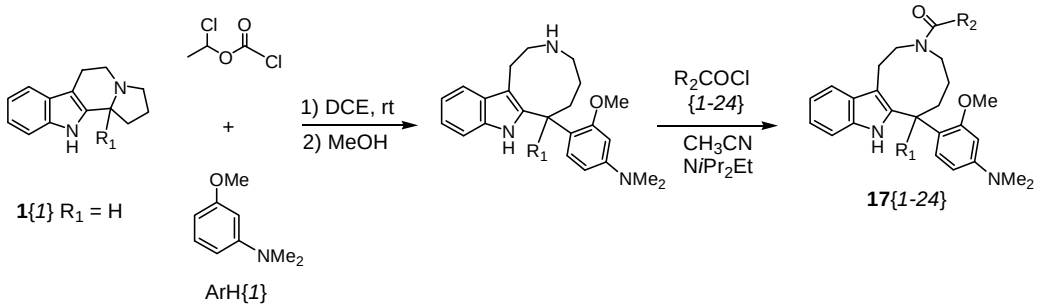


Table 9. Array layout of chemset **16**{*1-24*}

Library Scaffolds		**1**{*1*}	**Library Scaffolds**		**1**{*2*}
Indoles{*1-15*}	**Epoxides**{*1-9*}	**Product**	**Indoles**{*1-15*}	**Epoxides**{*1-9*}	**Product**
{*1*}	{*1*}	**16**{*1*} (15.6, 97, 100)	{*12*}	{*1*}	**16**{*13*} (8.4, 65, 89)
{*2*}	{*2*}	**16**{*2*} (41.9, 76, 94)	{*1*}	{*4*}	**16**{*14*} (11.7, 26, 16)
{*3*}	{*3*}	**16**{*3*} (44.6, 50, 100)	{*7*}	{*6*}	**16**{*15*} (10.5, 73, 93)
{*4*}	{*4*}	**16**{*4*} (21.7, 72, 88)	{*3*}	{*4*}	**16**{*16*} Not isolated
{*5*}	{*1*}	**16**{*5*} (24.9, 91, 100)	{*5*}	{*1*}	**16**{*17*} (3.0, 69, 97)
{*6*}	{*4*}	**16**{*6*} (38.9, 61, 79)	{*8*}	{*3*}	**16**{*18*} (16.3, 67, 100)
{*1*}	{*5*}	**16**{*7*} (12.5, 97, 100)	{*1*}	{*8*}	**16**{*19*} (8.8, 93, 100)
{*7*}	{*1*}	**16**{*8*} (29.7, 86, 100)	{*6*}	{*9*}	**16**{*20*} (13.2, 67, 100)
{*8*}	{*6*}	**16**{*9*} (32.1, 100, 100)	{*13*}	{*3*}	**16**{*21*} (27.0, 50, 100)
{*9*}	{*3*}	**16**{*10*} (36.0, 95, 100)	{*11*}	{*7*}	**16**{*22*} (8.9, 33, 45)
{*10*}	{*7*}	**16**{*11*} (26.3, 94, 100)	{*14*}	{*1*}	**16**{*23*} Not isolated
{*11*}	{*8*}	**16**{*12*} (29.6, 97, 100)	{*15*}	{*4*}	**16**{*24*} (14.2, 71, 96)

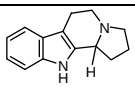
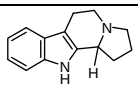
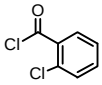
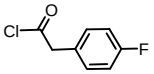
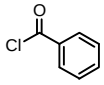
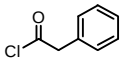
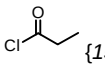
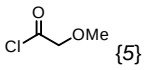
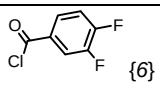
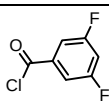
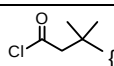
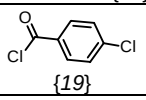
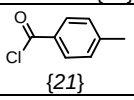
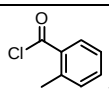
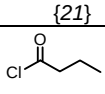
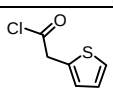
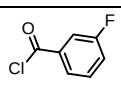
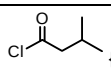
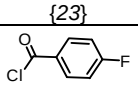


1{*1*} R_1 = H

ArH{*1*}

17{*1-24*}

Table 10. Array layout of chemset **17**{*1-24*}

Library Scaffolds		 **1**{*1*}	**Library Scaffolds**		 **1**{*1*}
ArH{*1*}	**Acid Chlorides** {*1-24*}	**Product**	**ArH**{*1*}	**Acid Chlorides** {*1-24*}	**Product**
m-dimethylamino anisole	 {*1*}	**17**{*1*} (33.5, 0, 100)	*m*-dimethylamino anisole	 {*13*}	**17**{*13*} (30.5, 97, 100)
m-dimethylamino anisole	 {*2*}	**17**{*2*} (24.8, 74, 100)	*m*-dimethylamino anisole	 {*14*}	**17**{*14*} Not isolated
m-dimethylamino anisole	 {*3*}	**17**{*3*} (29.5, 67, 100)	*m*-dimethylamino anisole	 {*15*}	**17**{*15*} (37.6, 100, 100)
m-dimethylamino anisole	 {*4*}	**17**{*4*} (42.3, 89, 100)	*m*-dimethylamino anisole	 {*16*}	**17**{*16*} (47.4, 95, 100)
m-dimethylamino anisole	 {*5*}	**17**{*5*} (34.1, 100, 100)	*m*-dimethylamino anisole	 {*17*}	**17**{*17*} (36.6, 80, 100)
m-dimethylamino anisole	 {*6*}	**17**{*6*} (34.8, 97, 100)	*m*-dimethylamino anisole	 {*18*}	**17**{*18*} (16.9, 88, 100)
m-dimethylamino anisole	 {*7*}	**17**{*7*} (30.8, 100, 100)	*m*-dimethylamino anisole	 {*19*}	**17**{*19*} (29.9, 100, 100)
m-dimethylamino anisole	 {*8*}	**17**{*8*} (44.6, 94, 100)	*m*-dimethylamino anisole	 {*20*}	**17**{*20*} (38.8, 83, 100)
m-dimethylamino anisole	 {*9*}	**17**{*9*} (40.6, 83, 100)	*m*-dimethylamino anisole	 {*21*}	**17**{*21*} (40.1, 87, 100)
m-dimethylamino anisole	 {*10*}	**17**{*10*} (39.3, 85, 100)	*m*-dimethylamino anisole	 {*22*}	**17**{*22*} (45.1, 94, 100)
m-dimethylamino anisole	 {*11*}	**17**{*11*} (22.6, 65, 100)	*m*-dimethylamino anisole	 {*23*}	**17**{*23*} (17.3, 87, 100)
m-dimethylamino anisole	 {*12*}	**17**{*12*} (42.8, 87, 100)	*m*-dimethylamino anisole	 {*24*}	**17**{*24*} (35.9, 90, 100)

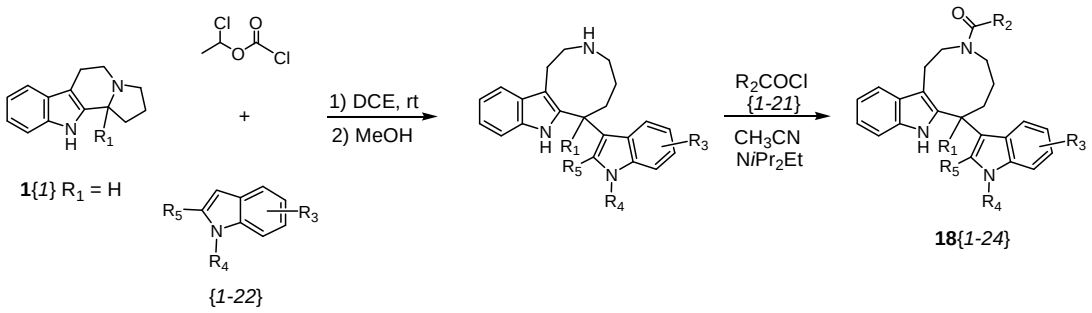
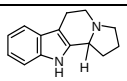
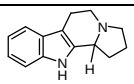
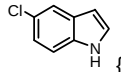
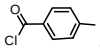
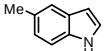
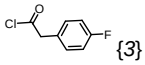
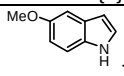
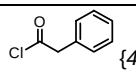
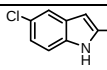
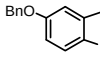
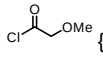
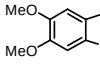
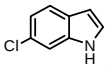
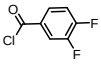
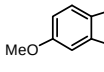
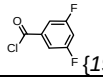
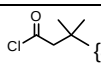
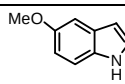
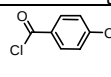
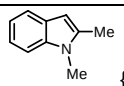
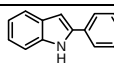
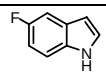


Table 11. Array layout of chemset **18**{*1-24*}

Library Scaffolds		 **1**{*1*}	**Library Scaffolds**		 **1**{*1*}
Indoles {*1-22*}	**Acid Chlorides** {*1-21*}	**Product**	**Indoles** {*1-22*}	**Acid Chlorides** {*1-21*}	**Product**
 {*1*}	 {*1*}	**18**{*1*} Not isolated	 {*12*}	 {*13*}	**18**{*13*} (38.6, 59, 100)
 {*2*}	 {*2*}	**18**{*2*} Not isolated	 {*13*}	 {*14*}	**18**{*14*} Not isolated
 {*3*}	 {*3*}	**18**{*3*} Not isolated	 {*14*}	 {*15*}	**18**{*15*} Not isolated
 {*4*}	 {*4*}	**18**{*4*} Not isolated	 {*15*}	 {*16*}	**18**{*16*} (25.3, 98, 100)
 {*5*}	 {*5*}	**18**{*5*} Not isolated	 {*16*}	 {*17*}	**18**{*17*} Not isolated
 {*6*}	 {*6*}	**18**{6} (18.5, 59, 60)	 {*17*}	 {*18*}	**18**{*18*} Not isolated
 {*7*}	 {*7*}	**18**{*7*} Not isolated	 {*18*}	 {*19*}	**18**{*19*} Not isolated
 {*8*}	 {*8*}	**18**{*8*} (46.9, 90, 100)	 {*19*}	 {*20*}	**18**{*20*} Not isolated
 {*9*}	 {*9*}	**18**{*9*} (36.2, 28, 100)	 {*20*}	 {*21*}	**18**{*21*} (13.5, 83, 100)
 {*10*}	{*10*}	**18**{*10*} (33.5, 77, 100)	{*21*}	{*16*}	**18**{*22*} (24.8, 89, 100)
{*10*}	{*11*}	**18**{*11*} (30.2, 67, 96)	{*22*}	{*6*}	**18**{*23*} Not isolated
{*11*}	{*12*}	**18**{*12*} Not isolated	{*1*}	{*18*}	**18**{*24*} Not isolated

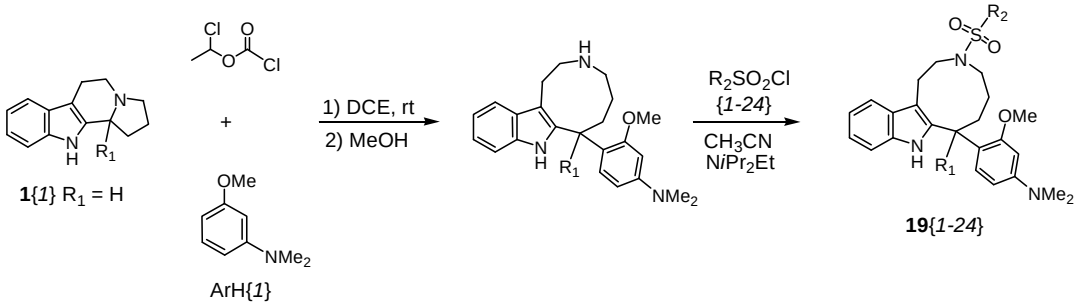
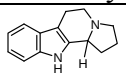
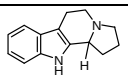
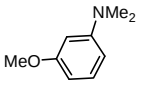
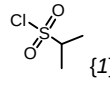
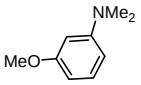
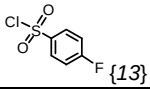
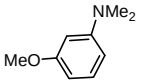
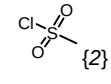
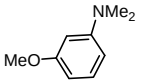
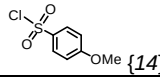
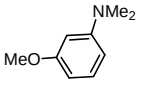
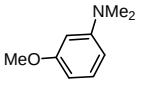
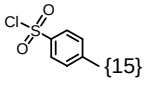
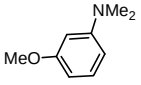
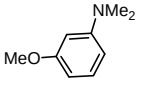
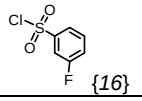
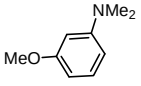
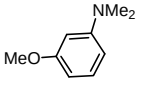
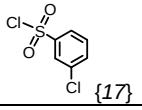
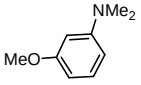
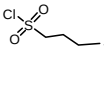
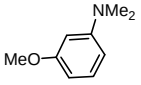
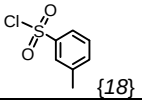
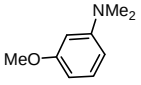
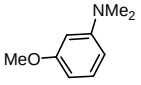
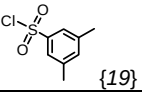
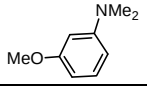
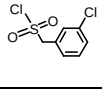
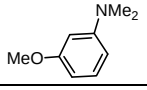
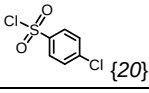
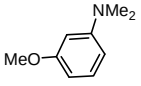
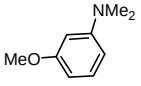
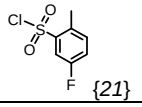
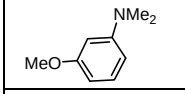


Table 12. Array layout of chemset **19**{*1-24*}

Library Scaffolds		 **1**{*1*}	**Library Scaffolds**		 **1**{*1*}
ArH{*1*}	**Sulfonyl Chlorides**{*1-24*}	**Product**	**ArH**{*1*}	**Sulfonyl Chlorides**{*1-24*}	**Product**
	 {*1*}	**19**{*1*} Not isolated		 {*13*}	**19**{*13*} (32.8, 100, 100)
	 {*2*}	**19**{*2*} (18.9, 100, 100)		 {*14*}	**19**{*14*} (30.7, 100, 100)
	 {*3*}	**19**{*3*} Not isolated		 {15}	**19**{*15*} (31.1, 100, 100)
	 {*4*}	**19**{*4*} (16.3, 68, 93)		 {*16*}	**19**{*16*} (30.7, 100, 100)
	 {*5*}	**19**{*5*} (10.1, 60, 88)		 {*17*}	**19**{*17*} (29.4, 100, 100)
	 {*6*}	**19**{*6*} Not isolated		 {*18*}	**19**{*18*} (30.3, 100, 100)
	 {*7*}	**19**{*7*} (10.0, 100, 100)		 {*19*}	**19**{*19*} (32.0, 100, 100)
	 {*8*}	**19**{*8*} (5.6, 100, 100)		 {*20*}	**19**{*20*} (30.3, 100, 100)
	 {*9*}	**19**{*9*} (33.8, 100, 100)		 {*21*}	**19**{*21*} (29.7, 100, 100)
	{*10*}	**19**{*10*} (29.3, 94, 100)		{*22*}	**19**{*22*} (27.3, 97, 100)
	{*11*}	**19**{*11*} (30.1, 97, 100)		{*23*}	**19**{*23*} (27.0, 100, 100)
	{*12*}	**19**{*12*} (29.6, 100, 100)		{*24*}	**19**{*24*} (29.9, 100, 100)

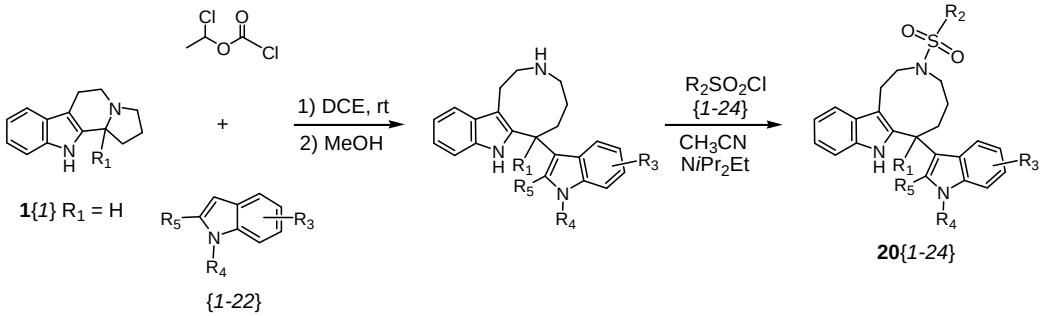


Table 13. Array layout of chemset **20**{*1-24*}

Library Scaffolds		**1**{*1*}	**Library Scaffolds**		**1**{*1*}
Indoles {*1-22*}	**Sulfonyl Chlorides**{*1-24*}	**Product**	**Indoles** {*1-22*}	**Sulfonyl Chlorides**{*1-24*}	**Product**
{*1*}	{*1*}	**20**{*1*} (4.2, 31, 25)	{*12*}	{*13*}	**20**{*13*} (12.5, 93, 100)
{*2*}	{*2*}	**20**{*2*} (15.0, 88, 100)	{*13*}	{*14*}	**20**{*14*} Not isolated
{*3*}	{*3*}	**20**{*3*} Not isolated	{*14*}	{*15*}	**20**{*15*} Not isolated
{*4*}	{*4*}	**20**{*4*} Not isolated	{*15*}	{*16*}	**20**{*16*} (5.4, 0, 100)
{*5*}	{*5*}	**20**{*5*} Not isolated	{*16*}	{*17*}	**20**{*17*} Not isolated
{*6*}	{*6*}	**20**{*6*} (5.2, 100, 100)	{*17*}	{*18*}	**20**{*18*} Not isolated
{*7*}	{*7*}	**20**{*7*} (6.5, 45, 98)	{*18*}	{*19*}	**20**{*19*} (8.7, 84, 100)
{*8*}	{*8*}	**20**{*8*} Not isolated	{*19*}	{*20*}	**20**{*20*} (7.3, 0, 100)
{*9*}	{*9*}	**20**{*9*} Not isolated	{*20*}	{*21*}	**20**{*21*} (20.1, 100, 100)
{*10*}	{*10*}	**20**{*10*} (22.1, 88, 100)	{*21*}	{*22*}	**20**{*22*} Not isolated
{*10*}	{*11*}	**20**{*11*} (112.6, 100, 100)	{*22*}	{*23*}	**20**{*23*} Not isolated
{*11*}	{*12*}	**20**{*12*} (15.0, 87, 100)	{*1*}	{*24*}	**20**{*24*} (17.6, 100, 100)