Spectral Data for:

**An Efficient Method for the Synthesis of Cyclopropanes via Pd(II/IV)
Catalysis**

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¹H and ¹³C NMR Data for all new compounds

Standard proton
Standard proton

File: 21LM98-F36-56H
exp2 Proton

Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Nov 7 2005 temp not used
solvent cdcl3 gain not used
file /home/lwelles- spin 20
/vnmr/s/data/Inov- hst 0.008
a.500/21LM98-F36-5- pw90 5.500
6H. fid alfa 6.600

ACQUISITION

FLAGS

PROCESSING

DISPLAY

TRANSMITTER

sw 5998.8 il
at 3.000 in
np 35992 dp
fb 3000 hs
bs 8
ss 2 lb
dl 0.500 fn
nt 16
ct 16 sp
tn H1 rfi
sfreq 499.907 rfp
toe 0.0 ip
tpwr 56 lp
pw 2.750
DECOUPLER WC
dn C13 sc
dof 1285.0 vs
dm nm th
dmm p ai cdc ph
dpwr 41
dnf 32258

INDEX	FREQUENCY	PPM	HEIGHT
1	3940.062	7.882	111.8
2	3938.780	7.879	135.0
3	3937.132	7.876	44.0
4	3933.654	7.869	45.6
5	3931.640	7.865	151.2
6	3930.359	7.862	128.7
7	3790.494	7.582	85.3
8	3783.172	7.568	64.1
9	3740.517	7.482	108.5
10	3738.869	7.479	45.4
11	3732.462	7.466	148.3
12	3731.180	7.464	46.6
13	3724.956	7.451	78.9
14	3619.325	7.240	96.0
15	2288.231	4.577	62.0
16	2283.472	4.568	63.8
17	2278.529	4.558	73.2
18	2273.952	4.549	72.8
19	2172.349	4.346	114.9
20	2162.829	4.326	97.3
21	1412.430	2.825	47.4
22	1404.375	2.809	49.3
23	1062.402	2.125	64.3
24	1057.642	2.116	69.7
25	1054.347	2.109	63.7
26	1049.587	2.100	64.7
27	721.711	1.444	73.5
28	716.585	1.433	129.0
29	711.642	1.424	72.8

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Standard carbon
Standard carbon

File: 2LW98-F36-56C
exp2 Carbon
Pulse Sequence: szpul

SAMPLE

SPECIAL

date Nov 7 2005 temp not used
solvent cdcl3 gain 50
file /home/lwlbbs~ spin 20
/vnmr/sys/data/lnov~ hst 0.008
a.500/2LW98-F36-5~ pw90 12.500
6C.fid alfa 10.000

ACQUISITION

FLAGS

sw 30165.9 11 n
at 1.300 1n n
np 78460 dp y
fb 17000 hs nn
bs 16
d1 0.100 1b 1.00
nt 5000 fn not used
ct 1328
PROCESSING
DISPLAY
-1883.9
sp
th C13 mp 30165.5
sfreq 125.714 rfi 1884.3
tof 1285.5 rfp 0
tpwr 59 ip -85.8
pw 6.250 1p -217.2

DECOUPLER

PLOT

dn H1 WC 250
dof 500.0 SC 0
dm YYY VS 6868
dmm w th 7
dpwr 31 ai cdc ph
dmf 12200

INDEX	FREQUENCY	PPM	HEIGHT
1	24148.587	192.111	9.2
2	21719.609	172.788	22.5
3	17041.628	135.573	25.7
4	16811.020	133.738	75.4
5	16243.936	129.227	151.2
6	16159.702	128.557	114.4
7	9716.949	77.302	61.9
8	9684.728	77.046	63.3
9	9652.968	76.793	60.6
10	8545.037	67.979	68.4
11	4503.644	35.828	28.6
12	3413.205	27.153	62.0
13	2419.887	19.251	73.7

220 200 180 160 140 120 100 80 60 40 20 0 ppm

Standard proton

exp2 Proton

SAMPLE		SPECIAL	
date	Oct 24 2005	temp	not used
solvent	cdcl3	gain	not used
file	/home/lwelbes~ spin		20
/vnmr/s/data/Inov~ hst			0.008
a.500/21LM82-f54-6~ pw90			5.500
	9H.fid	alfa	6.600

ACQUISITION		FLAGS	
sw	5998.8	il	n
at	3.000	in	nw
np	35992	dp	y
fb	3000	hs	nm
bs	8	PROCESSING	
ss	2	lb	0.20
d1	0.500	fn	not used
nt	16	DISPLAY	
ct	16	sp	-516.0
TRANSMITTER		wp	5998.6
tn	H1	rfl	4135.5
sfrq	499.907	rfp	3619.3
tof	0.0	rp	-12.7
tpwr	56	lp	-14.1
pw	2.750	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	1285.0	vs	21
dm	nm	th	50
dmm	p	ai	cdc
dpwr	41	ph	
dntf	32258

0.96
 1.00
 0.83
 2.73
 1.17
 0.94

Std Carbon

exp2 Carbon

SAMPLE

SPECIAL

date Mar 26 2006 temp not used
solvent cdcl3 gain 30
file /home/lwlbbs~ spin not used
/vnmr/sv/data/Inov~ hist 0.008
a.400/31M10C.fid pw90 16.700
ACQUISITION alfa 10.000

sw 24140.0

FLAGS

at 1.300 il n
np 62786 in n
fb 13000 dp y
bs 16 hs mn
ss 2 PROCESSING
d1 0.100 lb 1.00
nt 5000 fn not used
ct 2368 DISPLAY

TRANSMITTER
tn cl3 sp -1509.3
sfreq 100.582 wp 24139.3
tof 1028.5 rfi 1510.0
tpwr 58 ip 178.0
pw 8.350 lp -159.3

DECOUPLER
dn H1 wc 250
dof 0 sc 0
dm yyy vs 62607
dmm w th 3
dpwr 44 ai cdc ph
dmf 10400

INDEX	FREQUENCY	PPM	HEIGHT
1	20171.629	200.570	28.5
2	17377.346	172.786	38.2
3	10162.894	101.052	4.3
4	7776.740	77.326	28.4
5	7744.326	77.003	29.5
6	7712.648	76.688	30.0
7	6818.300	67.796	10.0
8	6756.418	67.180	151.2
9	3674.087	36.532	75.8
10	3004.432	29.874	117.6
11	2947.706	29.310	63.5
12	2454.858	24.409	7.7
13	2434.230	24.204	109.3
14	2372.348	23.589	7.8
15	2174.914	21.626	4.6
16	2171.967	21.596	4.3
17	1643.020	16.337	9.8

220 200 180 160 140 120 100 80 60 40 20 0 ppm

1LLW202-f27-40

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
INOVA-400 "Zr"
PULSE SEQUENCE
Pulse 38.8 degrees
Acq. time 2.666 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1 398.9649498 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32788
Total time 0 min, 42 sec

Std Carbon

exp3 Carbon

SAMPLE SPECIAL
gate Jul 9 2006 temp not used
solvent CDC13 gain 30
file /home/tw/lyons- spin 20
/vnmr/sys/data/1nov- hst 0.008
a.400/tw1-1-132-ca- pw90 12.100
rbon.t1d a1fa 10.000

ACQUISITION FLAGS
sw 24140 0 11 n
at 1.300 1m n
np 62786 dp y
fb 13000 hs n
bs 32 PROCESSING
ss 2 1b 1.00
dl 0.100 fn not used
nt 1000 DISPLAY
ct 448 sp 50.8
TRANSMITTER
tn C13 rfi 21163.8
sfrq 100.582 rfp 9252.9
tot 1028.5 rp 7744.8
tpwr 54 1p 36.5
pw 6.050 PLOT
DECOUPLER
an H1 sc 250
dof 0 vs 42792
dm yyy th 8
dmm w at cdc ph
dpwr 39
dnt 9090

tw1-2-53

File: Proton

Pulse Sequence: szpul

Solvent: cdcl3

Ambient temperature

Operator: twlyons

INOVA-500 "Sn.Chem,LSA,UMich,Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1, 499.9042701 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 55 sec

Acquisition date: Jan 24 2007

Standard Carbon

exp2 Carbon

SAMPLE SPECIAL
date Jan 24 2007 temp not used
solvent cdcl3 gain 40
file /home/twilyons- spin 20
/vnmr/sys/data/Inov- hst 0.008
a.500/twl-2-53-CAR- pw30 14.700
BON. fid alfa 10.000

INDEX	FREQUENCY	PPM	HEIGHT
1	25048.580	199.271	35.5
2	21846.766	173.799	22.0
3	9711.080	77.255	17.5
4	9679.320	77.003	19.0
5	9647.099	76.746	18.9
6	9061.143	72.085	135.6
7	5076.827	40.388	26.0
8	4924.470	39.176	49.5
9	3779.715	30.069	97.3
10	3388.464	26.957	149.2
11	1649.469	13.122	120.9

ACQUISITION FLAGS
sw 30165.9 il n
at 1.300 in n
np 78460 dp y
fb 17000 hs nm
bs 16 PROCESSING
ss 2 lb 1.00
d1 0.100 fn not used
nt 2000 DISPLAY
ct 272 sp -1900.8
TRANSMITTER
tn C13 rfi 30165.5
sfreq 125.714 rfp 11580.6
tof 1285.6 rp 9679.3
tpwr 57 lp -14.6
pw 7.350 PLOT -226.5
DECOUPLER
dn H1 sc 250
dof 0 vs 0
dm yyy th 7145
dmm w al cdc ph 16
dpmr 31
dmf 12200

220 200 180 160 140 120 100 80 60 40 20 0 ppm

Std proton
Std proton

File: 21LW112-f66-93H
exp2 Proton

Pulse Sequence: szpul

SAMPLE

SPECIAL

date Nov 9 2005 temp not used
solvent cdcl3 gain not used
file /home/lwelbes- spin 20
/vnmr/sys/data/Inov- hst 0.008
a.400/21LW112-f66-~ pw90 11.100
93H.fid a1fa 6.600

ACQUISITION

FLAGS

sw 4799.6 il n
at 3.500 in nw
np 33598 dp y
fb 3000 hs nm
bs 8 PROCESSING
ss 2 lb 0.20
di 0.100 fn not used
nt 16 DISPLAY

ct 16 sp -391.8
TRANSMITTER wp 4799.5
tn h1 rfi 3287.7
sfreq 399.967 rfp 2895.8
tof -0.0 rp -95.4
tpwr 59 lp 6.5
pw 5.550 PLOT

DECOUPLER wc 250
dn C13 sc 0
dof 0 vs 48
dm nnn th 13
dmm c ai cdc ph
dpwr 36
dmf 29412

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

1.84 2.04
0.99

1.05
1.08

2.98

1.00
0.92

Std Carbon
Std Carbon

File: 21M112-f66-93C1
exp2 Carbon
Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Nov 9 2005 temp not used
solvent cdcl3 gain 30
file /home/lwlbef-spin 20
/vnmrsys/data/Inov~ hst 0.008
a.400/21M112-f66~ pw90 14.100
93C1.fid alfa 10.000

ACQUISITION

FLAGS

sw 24140.0 z1 n
at 1.300 in n
np 62786 dp y
fb 13000 hs nm
bs 16 PROCESSING
ss 2 lb 1.00
dl 0.100 fn not used
nt 5000 DISPLAY
ct 624 sp -1505.3
TRANSMITTER wp 24139.3
tn C13 refi 1506.0
sfreq 100.582 rfp 0
toe 1028.5 rp 163.1
tpwr 58 lp -171.1
pw 7.050 PLOT
DECOUPLER wc 250
dn H1 sc 0
dof 0 vs 20618
dm yyy th 3
dnu w ai cdc ph
dpr 38
dmf 9600

INDEX	FREQUENCY	PPM	HEIGHT
1	19124.385	190.158	19.5
2	17074.900	169.779	9.7
3	16779.486	166.842	16.1
4	13556.446	134.794	16.9
5	13493.090	134.164	58.5
6	13023.079	129.491	151.2
7	12991.401	129.176	6.2
8	12942.780	128.693	128.2
9	7790.337	77.461	12.6
10	7757.922	77.139	12.9
11	7726.244	76.824	12.1
12	6564.477	65.272	70.1
13	5320.199	52.900	34.8
14	4268.936	42.447	25.2
15	3248.614	32.302	60.4
16	3030.552	30.133	71.4
17	2920.048	29.035	2.9

220 200 180 160 140 120 100 80 60 40 20 0 ppm

115

Automatic un directory:
Sample : 1k2748 f38-A0

Acq Sequence: s2pu1

Solvent: cdk13

Ambient temperature

Operator: tweldes

INOVA-500 "Sn.Chem.LSA-17Mch Edu"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 4999.1 Hz
16 repetitions
OBSERVE 11 459.9042607 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 1 min, 3 sec

Automation directory:
Sample : 1kac48 f30-48

Pulse Sequence: szpu1

Solvent: ccd13

Ambient temperature

Operator: twelbes

INOVA-500 150. Chemical shift (ppm)

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

16816 repetitions

OBSERVE C13, 125.7010263 MHz

DECOUPLE H1, 499.9072532 MHz

Power 41 dB

off during acquisition

on during delay

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 11 hr, 44 min 41 sec

514

O=C1C2C(C1)OC2

date	Dec 10 2005	temp	not used
solvent	cdcl3	gain	not used
file	/home/lvelbes- spin		20
/vnmrsws/data/1novr_008			
a.500/211WT160mzfor- p930			5.700
pdth.fid	alfa		6.600

FLAGS

DISPLAY

PLANT

•
•
•
•

dc
ph

Standard carbon
Standard carbon

File: 21LM160majorpdc
exp2 Carbon

Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Dec 10 2005 temp not used
solvent CDCl3 gain 50
file /home/1welpes~ spin 20
/vnmrsws/data/Inov~ hst 0.008
a.500/21LM160majorp~ pw90 12.500
pdc.fnd alfa 10.000

ACQUISITION

FLAGS

sw 30165.9 il n
st 1.300 in n
np 78460 dp y
fb 17000 hs nn
bs 16
d1 0.100 lb 1.00
nt 2000 fn not used
ct 1056

PROCESSING

TRANSMITTER

DISPLAY

tn C13 sp -1902.4
sfreq 125.714 wf 30165.5
toif 1285.5 rfp 11582.9
tpwr 59 rp 9680.0
pw 6.250 ip 163.5
-203.8

DECOUPLER

PLOT

dn H1 wg 250
dof 500.0 sc 0
dm YY vs 1026
dnu w th 2
dpwr 31 ai cdc ph
dmf 12200

INDEX	FREQUENCY	PPM	HEIGHT
1	25174.472	200.273	10.2
2	17361.880	138.120	22.3
3	16628.169	132.283	74.7
4	16322.533	129.852	2.8
5	16137.954	128.384	121.7
6	16119.543	128.237	4.2
7	16049.578	127.681	151.2
8	9712.232	77.265	6.1
9	9680.011	77.008	6.3
10	9647.791	76.752	6.4
11	8816.497	70.139	58.3
12	8624.094	68.608	65.6
13	4863.942	38.695	25.0
14	3714.124	29.547	10.9
15	3684.205	29.309	76.9
16	2361.777	18.789	72.3

220 200 180 160 140 120 100 80 60 40 20 0 ppm

S15

Standard proton

01/14/06

Automation directory:
Sample 2116196p

Pulse Sequence: zgpg30

Solvent: cdcl3

Ambient temperature

Operator: jwe1bes

INOVA-500 "St. Chem. LSA. Litch. Edin"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 5998.8 Hz
16 repetitions
OBSERVE H1, 499.9042607 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 3 sec

Standard carbon

Automation directory:

Sample : 211116p

Pulse Sequence: s2pul

Solvent: cdc13

Amplifier temperature

Operator: twelbes

INOVA-500 "St. Chem. LSA. Ulrich. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

4816 repetitions

OBSERVE C13, 125.7010263 MHz

DECUPLE H1, 499.9072532 MHz

Power 31 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 1 hr. 57 min. 26 sec

Std Fluorine experiment

File: Fluorine

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: twlyons

INOVA-400 "Zr.Chem.LSA DMich.Edu"

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 1.133 sec

Width 75258.7 Hz

16 repetitions

OBSERVE F19, 376.3430704 MHz

DATA PROCESSING

Line broadening 0.9 Hz

Gauss apodization 0.462 sec

FT size 262144

Total time 0 min, 38 sec

Acquisition date: Jan 26 2007

INDEX	FREQUENCY	PPM	HEIGHT
1	-23600.082	-62.709	2.1
2	-23635.107	-62.802	0.8
3	-23651.184	-62.845	0.7
4	-23668.983	-62.892	1.6
5	-23694.821	-62.961	0.7
6	-23708.027	-62.996	0.9
7	-23739.607	-63.080	3.4
8	-23743.626	-63.090	2.5
9	-23756.258	-63.124	151.2
10	-23776.355	-63.177	2.7
11	-23780.948	-63.190	2.8
12	-23791.857	-63.219	8.5
13	-23795.877	-63.229	14.1
14	-23800.470	-63.241	40.4
15	-23818.270	-63.289	5.3
16	-23821.715	-63.298	4.6
17	-23833.198	-63.328	4.8
18	-23838.940	-63.344	3.3
19	-23864.778	-63.412	1.5
20	-23871.094	-63.429	2.2
21	-23941.144	-63.615	0.9

-40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

Standard proton
Standard proton

File: ZHLM162-F102-132H
exp2 Proton

Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Dec 10 2005 temp not used
solvent cdc13 gain not used
file /home/lwelbes~ spin 20
/vnmrsws/data/Inov~ hst 0.008
a.500/2HLM162-F102~ pw90 5.700
-132H.fid alfa 6.600

ACQUISITION

FLAGS

sw 5998.8 al h
at 3.000 in nw
np 35992 dp y
fb 3000 hs nm

PROCESSING

ss 2 lb 0.20
d1 0.500 fm not used
nt 16 DISPLAY

ct 16 sp -516.2
TRANSMITTER wp 5998.6

tn H1 rfi 4135.7

sfxy 499.907 rfp 3619.3

tof 0.0 rp -171.1

tpwr 56 lp -18.6

pw 2.850 FLOT

DECOUPLER

wc 250

dn C13 sc 0

dof 1285.0 vs 64

dm nm th 25

dmm p al cdc ph

dpwr 41

dntf 32258

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

1.87

2.12

1.02114
1.0115

0.95

0.98
1.00

Standard carbon
Standard carbon

File: 21LM162-f102-132C
exp2 Carbon

Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Dec 10 2005 temp not used

solvent CDC13 gain 50

file /home/jwelbes- spin 20

/vnmr/sy/data/Inov- hst 0.008

a.500/21LM162-f102- pm90 12.500

-132C.fid alfa 10.000

ACQUISITION

FLAGS

sw 30165.9 il n

at 1.300 in n

np 78460 dp y

fb 17000 hs nn

PROCESSING

bs 16

dl 0.100 lb 1.00

nt 3000 fn not used

ct 464 DISPLAY

TRANSMITTER

sp -1897.4

tn C13 mp 30165.5

sfreq 125.714 rfl 11577.8

tof 1285.5 rfp 9680.0

tpwr 59 rp 165.5

pw 6.250 lp -206.2

DECOUPLER

plot

dn H1 wc 250

doe 500.0 sc 0

dm yyy vs 1729

dmm w th 3

dpwr 31 ai cdc ph

dmf 12200

INDEX	FREQUENCY	PPM	HEIGHT
1	24895.978	198.057	14.4
2	20495.555	163.050	26.5
3	16426.084	130.676	17.1
4	16379.594	130.306	147.1
5	16351.056	130.079	4.4
6	14284.330	113.637	151.2
7	14270.521	113.527	7.1
8	9712.217	77.264	12.0
9	9679.996	77.008	12.1
10	9648.236	76.755	12.0
11	8861.591	70.497	68.1
12	8640.649	68.740	70.9
13	6958.270	55.356	69.0
14	4832.626	38.445	32.6
15	3719.172	29.587	4.4
16	3559.450	28.317	81.1
17	2319.874	18.455	73.9

Standard proton
Standard proton

File: 21LM138-f69-90H
exp2 proton

Pulse Sequence: szpu1

SAMPLE

SPECIAL

date Nov 20 2005 temp not used
solvent cdc13 gain not used
file /home/lwelbes~ spin 20
/vnmrsws/data/Inov~ hst 0.008
a.500/21LM138-f69- pw90 5.500
90H.fid alfa 6.600

ACQUISITION

FLAGS

sw 5998.8 il n
at 3.000 in nw
np 35992 dp y
fb 3000 hs nm
bs 8
ss 2 lb
d1 0.500 fn not used
nt 16
ct 16 sp -516.4
TRANSMITTER wp 5998.6
tn H1 rfl 4135.9
sfrq 499.907 rfp 3619.3
tof 0.0 xp -171.8
tpwr 56 lp 3.7
pw 2.750
DECOUPLER wc 250
dn C13 sc 0
dof 1285.0 vs 66
dm non th 50
dnn p al cdc ph
dpr 41
dmf 32258

PROCESSING

DISPLAY

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

1.82 1.89 2.05 1.01 1.03 1.00 2.99 2.84 1.25

Standard carbon

exp2 Carbon

SAMPLE SPECIAL
date Nov 20 2005 temp not used
solvent cdc13 gain 50
file /home/lwlbac~ spin 20
/vnmrsws/data/Inov~ hat 0.008
a.500/ZLW138f69-9~ pw90 12.500
DC.fid alfa 10.000
ACQUISITION FLAGS
sw 30165.9 il n
at 1.300 in n
np 78460 dp y
fb 17000 hs nm
bs 16 PROCESSING
d1 0.100 lb 1.00
nt 5000 fn not used
ct 864 DISPLAY
TRANSMITTER
tn C13 sp -1885.6
sfreq 125.714 fF1 30165.5
tof 1285.5 rfp 0
tpwr 59 ip 172.4
pw 6.250 lp -220.0
DECOUPLER PLOT
dn H1 wc 250
dof 500.0 sc 0
dm yyy vs 3201
dmm w th 4
dpr 31 ai cdc ph
dmf 12200

INDEX	FREQUENCY	PPM	HEIGHT
1	25702.687	204.475	12.6
2	18085.261	143.875	29.4
3	16676.297	132.666	12.9
4	16314.505	129.788	151.2
5	16043.391	127.631	127.0
6	9719.394	77.322	25.8
7	9687.173	77.065	26.8
8	9654.952	76.809	26.1
9	6167.295	49.063	78.8
10	6138.756	48.836	82.3
11	4888.594	38.891	27.4
12	3419.792	27.206	76.3
13	3206.215	25.507	44.7
14	2707.715	21.541	50.3
15	2204.152	17.535	72.7

220 200 180 160 140 120 100 80 60 40 20 0 ppm

Standard Proton
Standard Proton

File: tw1-2-89f68-96a
exp2 Proton

Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Dec 13 2006 temp not used
solvent cdc13 gain not used
file /home/twlyons~ spin 20
/vnmrsys/data/Inov~ hst 0.008
a.500/tw1-2-89f68~ pw90 7.100
96a.fid alfa 6.600

ACQUISITION

FLAGS

sw 7998.4 11 n
at 3.000 in n
np 47990 dp y
fb 4000 hs nm
bs 8 PROCESSING
ss 2 lb 0.20
dl 0.100 fm not used
nt 16 DISPLAY
ct 16 sp -1016.1
TRANSMITTER wp 7998.2
tn h1 rfi 4635.7
sfreq 499.907 xfp 3619.3
tof 499.9 rp -74.4
tpwr 53 lp 1.8
pw 3.550 PLOT
DECOUPLER wc 250
dn c13 sc 0
dof 0 vs 24
dm nm th 13
dum c al cdc ph
dpwr 40
dmf 32258

INDEX	FREQUENCY	PPM	HEIGHT
1	3925.491	7.852	20.5
2	3924.515	7.851	22.7
3	3917.436	7.836	26.1
4	3915.972	7.833	21.0
5	3755.115	7.512	14.6
6	3711.667	7.425	19.7
7	3703.612	7.409	28.2
8	3696.289	7.394	12.8
9	1681.067	3.363	19.7
10	1670.327	3.341	17.8
11	1399.629	2.800	151.2
12	549.701	1.100	22.4

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

1.611.71
0.85
0.96
2.73
1.00
0.92

Std Carbon

File: Carbon

Pulse Sequence: s2pul1

Solvent: cdcl3

Ambient temperature

Operator: twlyons

INOVA-400 "Zr.Chem.ISA,UMich,Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 2440.0 Hz

352 repetitions

OBSERVE C13, 100.5712703 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 8 min, 16 sec

Acquisition date: Jan 26 2007

INDEX	FREQUENCY	PPM	HEIGHT
1	19585.220	194.740	10.0
2	17241.794	171.439	10.6
3	13730.707	136.527	16.2
4	13383.724	133.077	76.0
5	12975.595	129.019	162.0
6	12900.452	128.272	161.7
7	7784.897	77.377	31.9
8	7750.219	77.062	32.1
9	7717.805	76.740	31.5
10	5020.029	49.915	64.0
11	3875.942	38.539	20.3
12	2988.225	29.713	38.5
13	2233.113	22.204	76.7
14	1931.804	19.208	85.6

Standard proton
Standard proton

File: 21LM256c013H
exp2 Proton

Pulse Sequence: s2pul

SAMPLE

SPECIAL

date Feb 26 2006 temp not used
solvent cdcl3 gain not used
file /home/lwelbes/spin 20
/vnmrSYS/data/Inov-nst 0.008
a.500/21LM256c013H-pw90 53.000
.fid alfa 6.600

ACQUISITION

FLAGS

sw 5998.8 11 n
at 3.000 in nw
np 35992 dp y
fb 3000 hs m
bs 8 PROCESSING
ss 2 lb 0.20
d1 0.500 fn not used
nt 16 DISPLAY
ct 16 sp -516.6
tn H1 xfl 5998.6
stfq 499.907 xfp 4136.1
tof -0.0 xp 3619.3
tpwr 59 lp -171.0
pw 26.500 PLOT -7.0
DECOUPLER WC 250
dn C13 sc 0
dof 499.9 vs 128
dm nm th 50
dmm c al cdc ph
dpr 41
dmf 32258

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

1.10 1.36 0.65
1.10 1.36 0.65
0.96 1.00 0.59 0.66 3.46 0.28

Standard carbon

exp2 Carbon

SAMPLE

SPECIAL

date Feb 26 2006 temp not used
solvent CDC13 gain 50
file /home/lvalbes/spin 20
/vnmr/sys/data/Inov-hst 0.008
a.500/ZLHM256COL3C-pw90 12.500
.fid alfa 10.000

ACQUISITION

FLAGS

sw 30165.9 il n
at 1.300 in n
np 78460 dp y
fb 17000 hs nm
bs 16
dl 0.100 lb 1.00
nt 5000 fn not used
ct 5000 DISPLAY

TRANSMITTER

DISPLAY

tn C13 sp -1889.5
sfreq 125.714 xfl 30165.5
tof 1285.5 xfp 11570.0
tpwr 59 rp 9680.0
pw 6.250 lp -71.9
-203.7

DECOUPLER

PILOT

dn H1 wg 250
dof 500.0 sc 0
dm yyy vs 5204
dmm w th 6
dpr 41 ai cdc ph
dntf 2600

INDEX	FREQUENCY	PPM	HEIGHT
1	24072.969	191.510	13.0
2	21606.247	171.886	9.3
3	17099.495	136.033	14.5
4	16833.445	133.917	60.7
5	16351.976	130.086	151.2
6	16276.027	129.482	10.1
7	16256.695	129.328	11.2
8	16143.002	128.424	150.3
9	16089.608	127.999	9.9
10	9711.756	77.261	45.2
11	9679.996	77.008	46.1
12	9647.775	76.752	46.7
13	8520.051	67.780	83.8
14	5185.672	41.254	25.9
15	4008.237	31.887	7.9
16	3785.454	30.115	6.7
17	3728.377	29.661	88.0
18	3695.236	29.397	6.6
19	3685.570	29.320	8.3
20	3664.857	29.155	67.9
21	3552.545	28.262	56.5
22	2847.372	22.652	8.3
23	1770.281	14.083	7.7
24	1568.212	12.476	62.3

220 200 180 160 140 120 100 80 60 40 20 0 ppm

tw1-2-39-f134-end

File: tw1-2-39f134-end

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: twlyons

File: tw1-2-39f134-end

INOVA-500 "Md.Chem.ISA.UMich.Edu"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 7998.4 Hz
16 repetitions
OBSERVE H1, 499.9042709 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 3 sec
Acquisition date: Oct 3 2006

Std Carbon
Std Carbon

File: tw1-2-39f134-Car
exp2 Carbon
Pulse Sequence: szpul

SAMPLE

SPECIAL

date Oct 4 2006 temp not used
solvent CDC13 gain 30
file /home/twlyons~ spin 20
/vnmr/s/data/Inov~ hst 0.008
a.400/tw1-2-39f134~ pw90 12.100
-Car.fid alfa 10.000

ACQUISITION

FLAGS

sv 24140.0 il n
at 1.300 in n
np 62786 dp y
fb 13000 hs nm
bs 32 PROCESSING
ss 2 lb 1.00
dl 0.100 fn not used
nt 1000 DISPLAY

DISPLAY

ct 544 sp -1518.1
TRANSMITTER wp 24139.3
tn C13 rfi 9263.7
sfrq 100.582 rfp 7744.8
tof 1028.5 rp 32.5
tpwr 54 lp -153.7
pw 6.050 PLOT

DECOUPLER wc 250
dn H1 sc 0
dof 0 vs 19464
dm yyy th 3
dmm w ai cdc ph
dppwr 39
dmf 9090

INDEX	FREQUENCY	PPM	HEIGHT
1	17146.020	170.486	17.1
2	16929.431	168.333	19.4
3	16877.863	167.820	15.9
4	15450.885	153.631	18.5
5	13444.129	133.678	24.6
6	13128.823	130.542	71.1
7	12941.703	128.682	132.3
8	12843.722	127.708	151.2
9	11824.874	117.577	31.5
10	7776.736	77.326	18.0
11	7744.322	77.003	19.1
12	7712.644	76.688	18.6
13	7003.207	69.634	79.7
14	6152.324	61.174	75.6
15	4909.520	48.816	3.1
16	3566.526	35.463	76.5
17	3391.929	33.727	8.0
18	3221.016	32.027	73.4
19	2562.411	25.479	5.2
20	2495.372	24.812	6.6
21	2081.349	20.695	55.1
22	2071.772	20.600	44.9
23	1412.431	14.044	2.8

528

tw1-2-114af31-36a

File: Proton

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: twlyons

INOVA-500 "Sn.Chem.USA,Mich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1, 499.9042706 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 55 sec

Acquisition date: Jan 31 2007

INDEX	FREQUENCY	PPM	HEIGHT
1	3780.917	7.563	15.4
2	3779.697	7.561	18.9
3	3773.106	7.548	23.0
4	3771.398	7.544	18.2
5	3701.343	7.404	14.7
6	3696.462	7.394	24.5
7	3690.848	7.383	13.0
8	3689.139	7.380	25.1
9	3619.329	7.240	37.0
10	2202.376	4.406	13.7
11	2200.423	4.402	13.6
12	2135.006	4.271	13.1
13	1144.726	2.290	148.8
14	1025.121	2.051	151.2
15	621.637	1.244	64.7
16	618.952	1.238	13.4
17	615.047	1.230	66.8

629

tw1-2-114aE31-36

File: Carbon

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: twlyons

INOVA-400 "Zr.Chem.USA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

560 repetitions

OBSERVE C13, 100.5712703 MHz

DECOUPLE H1, 399.9669644 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.8 Hz

FT size 65536

Total time 13 min, 9 sec

Acquisition date: Jan 30 2007

INDEX	FREQUENCY	PPM	BRIGHT
1	17126.133	170.289	33.4
2	16901.441	168.054	23.4
3	16894.811	167.988	27.5
4	15923.110	158.327	18.9
5	13239.331	131.641	17.5
6	13156.822	130.821	72.6
7	12971.911	128.982	162.0
8	12868.037	127.949	125.6
9	11577.348	115.116	35.8
10	7774.530	77.304	143.9
11	7742.852	76.989	161.6
12	7711.174	76.674	157.1
13	6989.214	69.495	67.6
14	6561.931	65.247	81.2
15	4296.594	42.722	73.2
16	2983.804	29.669	74.4
17	2129.239	21.171	52.7
18	2099.771	20.878	51.4
19	1454.426	14.462	75.8

220 200 180 160 140 120 100 80 60 40 20 0 ppm

Standard proton

Automation directory:
Sample : 2LLW214p-2

Pulse Sequence: szpul

Solvent: cdcl3

Ambient temperature

Operator: twelbes

INOVA-500 "Sr.Chem.LSA.Umich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 5998.8 Hz

16 repetitions

OBSERVE H1, 499.9042605 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Standard carbon

exp2 Carbon

SAMPLE

SPECIAL

date Jan 28 2006 temp not used
solvent CDCl3 gain 50
file /home/1welbes~ spin 20
/vnmr/s/data/Inov~ hst 0.008
a.500/211W214p-2-C~ pw90 12.500
fid alfa 10.000

ACQUISITION

FLAGS

sw 30165.9 il n
at 1.300 in n
np 78460 dp y
fb 17000 hs m
bs 16
d1 0.100 lb 1.00
nt 10000 en not used
ct 2672
TRANSMITTER sp -1900.1
tn C13 wp 30165.5
freq 125.714 rfi 11580.6
tof 1285.5 rfp 9680.0
tpwr 59 ip 156.4
pw 6.250 lp -193.3

DISPLAY

DECOUPLER

PLOT

dn H1 wc 250
dof 500.0 sc 0
dm yyy vs 1851
dmm w th 6
dpmr 31 ai cdc ph
dmf 12200

INDEX	FREQUENCY	PPM	HEIGHT
1	24227.629	192.740	21.2
2	21506.824	171.095	14.1
3	17044.261	135.594	17.0
4	16824.700	133.847	6.4
5	16779.131	133.484	79.0
6	16340.009	129.991	13.9
7	16242.887	129.218	151.2
8	16131.495	128.332	136.2
9	9712.217	77.264	17.0
10	9679.996	77.008	18.1
11	9647.776	76.752	17.9
12	8513.608	67.729	6.7
13	8093.359	64.386	84.9
14	5244.131	41.719	34.7
15	3876.133	30.836	80.1
16	3717.791	29.576	23.1
17	3653.810	29.067	7.0
18	3542.879	28.185	6.1
19	3141.041	24.988	79.1
20	1559.007	12.402	6.9
21	967.067	7.693	63.0

220 200 180 160 140 120 100 80 60 40 20 0 ppm