Regioespecific Synthesis of 4-Alkoxy and 4-Amino Substituted 2-Trifluoro-methyl Pyrroles

Nilo Zanatta,^{*,†} Juliana M. F. M. Schneider,^{†,‡} Paulo H. Schneider,^{†,‡} Ana D. Wouters,[†]
Helio G. Bonacorso,[†] Marcos A. P. Martins,[†] and Ludger A. Wessjohann[‡]

[†] Núcleo de Química de Heterociclos (NUQUIMHE), Departamento de Química, Universidade Federal de Santa Maria, CEP – 97105-900, Santa Maria, RS, Brazil.

[‡] Leibniz Institute of Plant Biochemistry, Weinberg 3, D-06120 Halle (Saale), Germany.

zanatta@base.ufsm.br

Additional Supporting Information

¹H and ¹³C NMR Spectra of compounds 2	S2
¹H and ¹³C NMR Spectra of compounds 3	S8
¹H and ¹³C NMR Spectra of compounds 4	S12
¹H and ¹³C NMR Spectra of compounds 5	S18
¹H and ¹³C NMR Spectra of compounds 6	S28

GSP287_3/CDCl3/1H
Schneider 040903.08
Thu Sep 4 17:24 2003

exp4 std1h

SAMPLE

date Sep 4 2003

solvent CDCl3

file exp

ACQUISITION

instrum g300

probe atb5

seqfil s2pu1

sfrq 300.225

tn H1

et 2.733

np 32768

sw 5995.2

bs 8

tpwr 61

pw 2.0

d1 0.267

d2 0

tof 46.0

nt 64

ct 64

alock n

gain not used

FLAGS

il n

in n

dp y

DEC. & VT

dn H1

dfrq 300.225

homo n

dpwr 30

dof 0.0

dm nnn

dms c

dmf 200

PROCESSING

lb 8.30

wtfile

proc ft

fn 65536

DISPLAY

sp -150.2

wp 2401.8

vs 170

sc 65

wc 225

hzmm 10.67

ls 400.00

rfl 1495.2

rflp 0

th 1.9

ins 100.000

rp 127.7

lp -195.3

nm ph

GSP287.3/CDC13/13C
Schneider 050903.05
Fri Sep 5 18:13 2003

exp6 std13c

SAMPLE
date Sep 5 2003
solvent CDC13
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 75.500
tn C13
et 1.747
np 65906
sw 18867.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 1e+06
ct 66304
atlock n
gain not used

FLAGS
il n
in n
dp y

DEC. & VT
dn H1
dfrq 300.225
homo n
dpwr 37
dof 0
dm yyy
dmm w
dmf 7900
pp 17.5

PROCESSING
lb 1.00
wtfite ft
proc fn 65536

DISPLAY
sp- 754.5
wp 13212.2
vs 200
sc 65
wc 225
hzmm 58.72
rfi 6947.0
rfp 5812.0
th 1.9
rp 131.2
lp -198.5
na no ph

```

GSP298_3/CDCl3/1H
Schneider 040903_07
Thu Sep 4 17:18 2003

exp3 stdih

SAMPLE
Date Sep 4 2003
solvent CDCl3
file exp
-ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 300.225
in H1
at 2.733
np 32768
sw 5995.2
bs 8
tpwr 61
pw 2.0
d1 0.287
d2 0
tof 46.0
nt 64
ct 64
alock n
gain not used
il n
in n
dp y
DEC. & VT
dn H1
dfrq 300.225
homo n
dpwr 30
dof 0.0
ds nm
dm c
dnt PROCESSING 200
lb 0.30
wtfile ft
proc
fn 65536

DISPLAY
sp -150.1
vp 2401.6
vs 170
sc 65
vc 225
hzmm 10.67
ip 805.86
rf1 1495.3
rfp 0
th 1.9
ins 100.000
rp 125.2
ip -105.3
nm ph

```

[illegible]

```

GSP244_3/CDCl3/1H
Schneider 040903_09
Thu Sep  4 17:30 2003

exp6 std1h

SAMPLE
date: Sep  4 2003
solvent: CDCl3
file: exp
ACQUISITION
instrum: g300
probe: atb5
seqfil: s2pul
sfrq: 300.225
tn: H1
at: 2.733
np: 32765
sw: 5995.2
bs: 5
tpwr: 61
pw: 2.0
d1: 0.267
d2: 0
tof: 46.0
nt: 64
ct: 64
alock: n
gain: not used
FLAGS
il: n
in: n
dp: y
DEC. & VT
dn: H1
dfrq: 300.225
homo: n
dpwr: 30
dof: 0.0
dm: nnn
dnn: c
dmf: 200
PROCESSING
lb: 0.30
wtfile: ft
proc: ft
fn: 65536
DISPLAY
sp: -150.2
wp: 2401.8
vs: 170
sc: 85
wc: 225
hzmn: 10.67
is: 400.00
rf1: 1495.5
rtp: 0
th: 1.6
ins: 100.000
rs: 127.2
lp: -133.6
nm: ph

```

Compound 2d

GSP244/CDC13/13C
Juliana 080903
Mon Sep 8 20:01 2003

expl std13c

SAMPLE
date Sep 8 2003
solvent CDC13
file exp

ACQUISITION
instrum m400
probe asw5
seqfil 52pul
sfrq 100.374
tn C13
at 1.311
np 67216
sw 25641.0
bs 15
tpwr 61
pw 4.0
d1 1.689
d2 0
tof 1327.2
nt 15000
ct 15000
alock n
gain not used

FLAGS
il n
in nw
dp y

DEC. & VT
dn H1
dfrq 399.936
homo n
dpwr 40
dof 0
dm yyy
dss w
dmf 9350
pp 17.5

PROCESSING
lb 1.00
wtfile
proc ft
fn 65536

DISPLAY
sp -0.3
wp 20114.8
vs 200
sc 65
wc 225
hzmm 89.40
rfi 9673.4
rfp 7743.4
th 1.0
rp 62.1
lp -312.9
nm no ph

```

GSP292_2/CDC13/1H
Schneider 110903_05
Thu Sep 11 15:24 2003

exp7 std1h

SAMPLE
date Sep 11 2003
solvent CDC13
file exp
ACQUISITION
instrum g300
probe atb5
seqfil s2pu1
sfrq 300.225
tn H1
at 2.733
np 32768
sw 5995.2
bs 0
tpwr 62
pw 2.0
d1 0.267
d2 0
tcf 46.0
nt 64
ct 64
elock n
gain not used
FLAGS
il n
in n
dp y
DEC. & VT H1
dn
dfrq 300.225
homo n
dpr 30
dof 0.0
dm nnn
dmm c
dnt 200
PROCESSING
lb 0.30
wtfile ft
proc
fn 65536
DISPLAY
sp -150.2
wp 2401.8
vs 170
sc 65
wc 225
hzmm 10.67
ls 300.00
rf1 1494.5
rfp 0
th 30.0
ins 100.000
rp 124.5
lp -103.3
nm ph

```

GSP292_2/CDC13/13C
Schneider 120903_06
Fri Sep 12, 16:18 2003

exp3 std13c

SAMPLE
date Sep 12 2003
solvent CDC13
file exp

ACQUISITION
instrum g300
probe atb5
seqfil 52pul
sfrq 75.500
tn C18
at 1.747
np 65906
sw 18867.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 1e+06
ct 60720

alock n
gain not used
FLAGS
f1 n
in n
dp y

DEC. & VT H1
dn
dfrq 300.225
homo n
dpwr 37
dof 0
dm yyy
dmm w
dmf 7900
pp 17.5

PROCESSING
lb 1.00
wtfile ft
proc
fn 65536

DISPLAY
sp 754.6
wp 13212.2
vs 256
sc 65
wc 225
hzmm 58.72
rfl 6947.3
rfp 5812.0
th 1.6
rp 149.7
lp -235.4
na no ph

DSP294_2/CDCl3/1H
Schneider 120903.94
Fri Sep 12 16:25 2003

expl std1h

SAMPLE

date Sep 12 2003

solvent CDCl3

file exp

ACQUISITION

instrum g300

probe atb5

seqfil s2pu1

sfrq 300.225

tn H1

at 2.733

np 32768

sw 5995.2

bs 6

tpwr 61

pw 2.0

d1 0.267

d2 0

tot 46.0

nt 64

ct 64

alock n

gain not used

il n

in n

dp y

DEC. & VT

dn H1

dfrq 300.225

homo n

dpwr 30

dof 0.0

de nmh

dmm c

dnt 200

PROCESSING

lb 0.30

wtfile

proc ft

fn 65536

DISPLAY

sp -150.2

wp 2591.6

vs 170

sc 65

wc 225

hzmm 11.34

is 400.00

rfl 1495.4

rtp 0

th 2.0

ins 100.000

rp 120.7

lp -102.2

nm ph

Compound 3c

GSP294_2/CDC13/13C
Schneider 150903_04
Mon Sep 15 17:45 2003
exp7 std13c

SAMPLE
date Sep 15 2003
solvent CDC13
file exp
ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 75.500
tn C13
at 1.747
np 65906
sw 18867.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.0
nt 15000
ct 14080
alock n
gain not used
fl1 FLADS n
in n
dp y
DEC. & VT
dn M1
dfrq 300.225
homo n
dpwr 37
dot 0
dm vvy
dmm w
dmf 7900
pp 17.5
PROCESSING
lb 1.00
wtfile
proc ft
fn 65536
DISPLAY
sp 1132.3
wp 12834.5
vs 300
sc 65
wc 225
hcam 57.04
rf1 6947.0
rfp 5812.8
th 20.0
rp 142.4
lp -214.1
nm no ph

GSP301_2/CDC13/1H
Schneider 220903_03
Mon Sep 22 11:04 2003

exp8 std1h

SAMPLE
date Sep 22 2003
solvent CDC13
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 300.225
tn H1
at 2.733
np 32768
sw 5895.2
bs 8
tpwr 61
pw 2.0
d1 0.267
d2 0
tof 46.0
nt 64
ct 64
alock n
gain not used
f1 FLAGS
in n
dp y

DEC. & VT
dn H1
dfrq 300.225
homo n
dpwr 30
dot 0.0
dm nm
dmm c
dmt 200

PROCESSING
lb 0.30
wtfile
proc ft
fn 65536

DISPLAY
sp -150.2
wp 3002.1
vs 170
sc 65
wc 225
hzmm 13.34
ts 300.00
rf1 1497.0
rfp 0
th 30.0
ins 100.000
rp -125.6
lp -194.5
nm ph

GSP301_2/CDC13/13C
 Schneider 230903_09
 Tue Sep 23 17:27 2003

exp6 std13c

SAMPLE
 date Sep 23 2003
 solvent CDC13
 file exp

ACQUISITION
 instrum g300
 probe atb5
 seqfil s2pul
 sfrq 75.500
 tn C13
 at 1.747
 np 65506
 sw 18867.9
 bs 16
 tpwr 56
 pw 3.5
 d1 2.000
 d2 0
 tof 767.8
 nt 15000
 ct 14208

clock n
 gain not used
 FLAGS

il n
 in mw
 dp y

DEC. & VT
 dn H1
 dfrq 300.225
 homo n
 dpwr 37
 dot 0
 dm yvy
 dam w
 dmf 7900
 pp 17.5

PROCESSING
 lb 1.00
 wtfle ft
 proc ft
 fn 65536

DISPLAY
 sp 37.6
 wp 13551.9
 vs 150
 sc 65
 wc 225
 hzmm 60.23
 rft 6946.5
 rtp 5812.8
 th 20.0
 rp 144.8
 lp -225.5

nm no ph

Compound 4b

GSP277_2/CDCl3/13C
Ruijter 150808
Fri Aug 15 17:51 2003

expl std13c

SAMPLE

date Aug 15 2003

solvent CDCl3

file exp

ACQUISITION

instrum m400

probe asw5

seqfil s2pu1

strq 100.574

tn C13

at 1.311

np 67216

sw 25641.0

bs 16

tpwr 61

pw 4.0

d1 1.689

d2 0

tof 1327.2

nt 15000

ct 15000

alock n

gain not used

il FLAGS

in n

dp nw

DEC. & VT y

dn H1

dfrq 399.836

homo n

dpwr 40

dof 0

dm yyy

dmm w

daf 9350

pp 17.5

PROCESSING

lb 1.00

wtfile

proc ft

Tn 65536

DISPLAY

sp -0.5

wp 16091.9

vs 125

sc 65

wc 225

hzmm 71.52

rfl 9740.8

rfp 7743.4

th 20.0

rp 68.6

lp -345.3

na no ph

GSP293_2/CDC13/1H
 Schneider 050903_05
 Fri Sep 5 16:34 2003

exp2 std1h

SAMPLE

date Sep 5 2003

solvent CDC13

file exp

ACQUISITION

instrum g300

probe atb5

seqfil s2pul

sfrq 300.225

tn H1

at 2.733

np 32768

sw 5995.2

bs 8

tpwr 61

pw 2.0

d1 0.267

d2 0

tof 46.0

nt 64

ct 64

alock n

gain not used

fl FLAGS

in n

dp n

DEC. & VT y

dn H1

dfrq 300.225

homo n

dpwr 30

dof 0.0

dm nnn

dmm C

daf 200

PROCESSING

lb 0.30

wtfile

proc ft

fn 65536

DISPLAY

sp -150.2

wp 2702.0

vs 100

sc 65

wc 225

hzmm 12.01

is 425.68

rfl 1496.5

rtp 0

th 3.7

ins 100.000

rp 130.4

lp -213.0

na ph

Compound 4d

Compound 4d

GSP293/CDCl3/13C
Koeper 050903
Fri Sep 5 18:36 2003

exp3 std13c

SAMPLE
date Sep 5 2003
solvent CDCl3
file exp

ACQUISITION
instrum m400
probe agw5
seqfil s2p01
sfrq 100.624
tn C13
at 1.311
np 67216
sw 25641.0
bs 16
tpwr 61
pw 4.0
d1 1.689
d2 0
tof 1327.2
nt 15000
ct 15000
alock n
gain not used

11 n
1n nw
dp y

DEC. & VT
dn H1
dfrq 399.936
homo n
dpwr 40
dor 0
dm yyy
dmm w
dmf 9350
pp 17.5

PROCESSING
lb 1.00
wtfile ft
proc
fn 65536

DISPLAY
sp -566.8
wp 17781.3
vs 250
sc 65
wc 225
hzmm 79.03
rfl 1970.6
rfp 0
th 20.0
rp 48.1
lp -295.4
nm no ph

QSP252.2/CDCl3/1H
Schneider 250803_05
Mon Aug 25 14:27 2003

exp6 std1h

SAMPLE
date Aug 25 2003
solvent CDCl3
file exp

ACQUISITION

instrum g300
probe atb5
seqfil s2pu1
sfrq 300.225
tn H1
at 2.733
np 32768
sw 5995.2
bs 0
tpwr 61
pw 2.0
d1 0.267
d2 0
tof 46.0
nt 64
ct 64
elock n
gain not used

FLAGS
il n
in n
dp y

DEC. & VT HI

dn dfrq 300.225
homo n
dpwr 30
dof 0.0
dm nnn
dmm c
dof 200

PROCESSING 0.30

wtfile
proc ft
fn 65536

DISPLAY

sp -150.2
wp 2401.0
vs 162
sc 65
wc 225
hzmm 10.67
is 749.04
rfl 1487.7
rfp 0
th 2.9
ins 100.000
rp 150.7
lp -222.4
na ph

GSP252_2/CDCl3/13C
Schneider 250803_05
Mon Aug 25 17:41 2003

exp8 std13c

SAMPLE
date Aug 25 2003
solvent CDCl3
file exp

ACQUISITION
instrum g300
probe atb5
seqfl1 s2pul
sfrq 75.500
tn C13
at 1.747
np 65906
sw 18867.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 15000
ct 14752
alock n
gain not used

FLAGS
f1 n
in nw
dp y

DEC. & VT H1
dfrq 300.225
homo n
dpwr 37
dot 0
dm yvy
dca - w
def 7900
pp 17.5

PROCESSING
lb 1.00
wtfile
proc ft
fn 65536

DISPLAY
sp 1132.0
wp 12834.5
vs 150
sc 65
wc 225
hcam 57.04
rfl 6951.9
rfp 5812.8
th 4.0
rp 159.9
lp -250.9
nm no ph

GSP205.2/CDCl3/1H
Schneider 020603.85
Mon Jun 2 16:36 2003

exp6 std1h

SAMPLE
date Jun 2 2003
solvent CDCl3
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 300.225
in H1
at 2.733
np 32768
sw 5995.2
bs 8
tpwr 61
pw 2.0
d1 0.267
d2 0
tof 46.0
nt 64
ct 64
alock n
gain not used
f1 n
in n
dp y
DEC. & VT
dn H1
dfrq 300.225
homo n
dpwr 30
dof 0.0
dm nnn
dmm c
dmf 200

PROCESSING
lb 0.30
wtfile ft
proc 65536

DISPLAY
sp -150.2
wp 2401.8
vs 170
sc 65
wc 225
hzmm 10.67
is 300.00
rf1 1494.6
rfp 0
th 30.0
ins 100.000
rp 105.0
lp -190.4
nm ph

GSP205_2/CDC13/13C
Schneider 020603_05
Mon Jun 2 16:42 2003

exp7 std13c

SAMPLE
date Jun 2 2003
solvent CDC13
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 75.500
tn C13
at 1.747
np 65906
sw 16867.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 2000
ct 1184
alock n
gain not used

FLAGS
il n
in n
dp y

DEC. & VT H1
dn
dfrq 300.225
homo n
dpr 37
dof 0
dm yyy
dmm w
dmf 7900
pp 17.5

PROCESSING
lb 1.00
wtfile
proc ft
fn 65536

DISPLAY
sp 37.2
wp 13551.9
vs 200
sc 65
wc 225
hzmm 60.23
rf1 6947.4
rfp 5812.8
th 20.0
rp 155.9
lp -215.7
nm no ph

```

GR0212_2/CDC13/1H
Schneider 190603_03
Thu Jun 19 16:13 2003

exp3 std1h

SAMPLE
date Jun 19 2003
solvent CDC13
file exp
ACQUISITION
instrum m400
probe asw5
seqfil s2pul
sfrq 399.937
tn H1
at 2.562
np 65536
sw 12787.7
bs 8
tpwr 50
pw 2.5
d1 1.000
d2 0
tof 826.3
nt 40
ct 40
alock n
gain not used
FLAGS
fl n
in n
dp y
DEC. & VT
dn H1
dfrq 399.936
homo n
dpwr 30
dot 0.9
dm nnn
dmn c
dmf 200
PROCESSING
lb 0.40
wtfile
proc ft
tn 65536
DISPLAY
sp -200.2
wp 3193.4
vs 170
sc 65
wc 225
hzmm 14.22
fs 300.00
rf1 3542.4
rfp 0
th 25.0
ins 100.000
rp -27.8
lp -185.5
nm cdc ph

```

GRD212_2/CDC13/13C
 Schneider 190603.03
 Thu Jun 19 16:15 2003

exp4 std13c
 SAMPLE
 date Jun 19 2003
 solvent CDC13
 file exp
 ACQUISITION
 instrum m400
 probe asw5
 seqfil s2pul
 srfq 100.574
 tn C13
 at 1.311
 np 67216
 sw 25641.0
 hs 16
 tpwr 61
 pw 4.0
 d1 1.663
 d2 0
 tof 1327.2
 nt 1000
 ct 816
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DEC. & VT
 dn H1
 dfrq 399.936
 homo n
 dpwr 40
 dot 0
 dm yyy
 dmm w
 dmf 3350
 pp 17.5
 PROCESSING
 lb 1.00
 wtfile ft
 proc ft
 fn 65536
 DISPLAY
 sp 2011.1
 wp 16091.9
 vs 170
 sc 65
 wc 225
 hzmm 71.52
 rfi 9742.6
 rfp 7743.4
 th 2.6
 rp 77.8
 lp -302.1
 nm no ph

GSP213_2/CDCl3/1H
 Schneider 190803_04
 Tue Aug 19 12:26 2003

exp4 std1h

SAMPLE
 date Aug 19 2003
 solvent CDCl3
 file exp

ACQUISITION
 instrum g300
 probe atb5
 seqfil 52p01
 sfrq 300.225
 tn H1
 at 2.733
 np 32768
 sw 5395.2
 bs 8
 tpwr 61
 pw 2.0
 d1 0.267
 d2 0
 tof 46.0
 nt 64
 ct 64
 alock n
 gain not used

ll
 tn
 dp

DEC. & VT
 dn H1
 dfrq 300.225
 homo n
 dpwr 30
 dof 0.0
 dm nnn
 dmm c
 dmt 200

PROCESSING
 lb 0.30
 wtfile
 proc ft
 fn 65536

DISPLAY
 sp -150.3
 wp 2401.8
 vs 170
 sc 65
 wc 225
 hzmm 10.67
 is 500.00
 rfl 1494.2
 rtp 0
 th 30.0
 ins 100.000
 rp 137.2
 lp -202.6
 nm ph

GSP218_2/CDC13/13C
Schneider 200803_07
Wed Aug 20 17:39 2003
expB std13c

SAMPLE
date Aug 20 2003
solvent CDC13
file exp

ACQUISITION
instrum g300
probe eth5
seqfil s2pul
sfrq 75.500
in C13
at 1.747
np 65906
sw 10067.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 15000
ct 13936
alock n
gain not used

FLAGS
il n
in n
dp y

DEC. & VT
dn H1
dfrq 300.225
homo n
dpwr 37
dof 0
da yyy
dss w
def 7900
pp 17.5

PROCESSING
lb 1.00
wtfile ft
proc ft
fn 65536

DISPLAY
sp 3019.9
wp 10946.9
vs 170
sc 65
wc 225
hzmm 48.65
rfl 6948.1
rfp 5812.8
th 2.2
rp 138.6
lp -233.6
nm no ph

GSP273_2/CDCl3/1H
Schneider 250803_03
Mon Aug 25 14:08 2003

exp3 std1h

SAMPLE
date Aug 25 2003
solvent CDCl3
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfreq 300.225
in H1
at 2.733
np 32768
sw 5995.2
bs 8
tpwr 61
pw 2.0
d1 0.267
d2 0
tof 46.0
nt 64
ct 64
alock n
gain not used

FLAGS
il n
in n
dp y

DEC. & VT
dn H1
dfrq 300.225
homo n
dpr 30
dot 0.0
dm nnn
dnn c
dnf 200

PROCESSING
lb 0.30
wtfile f
proc 65536

DISPLAY
sp -150.2
wp 3382.3
vs 162
sc 65
wc 225
hzmm 14.68
is 500.00
rf1 1497.7
rfp 0
th 2.1
ins 100.000
rp 149.9
lp -219.1
nm ph

Compound 5f

GSP273_2/CDCl3/13C
Schneider 260803_02
Tue Aug 26 16:51 2003

exp2 std13c

SAMPLE
date Aug 26 2003
solvent CDCl3
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 75.500
tn C13
at 1.747
np 65906
sw 18867.9
hs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 15000
ct 15000
alock n
gain not used

il FLAGS n
in nw
dp y

DEC. & VT H1
dn dfrq 300.225
homo n
dpwr 37
dof 0
da yyy
dca w
daf 7900
pp 17.5

PROCESSING
lb 1.00
wtfile
proc ft
fn 65536

DISPLAY
sp 3019.6
wp 10946.3
vs 250
sc 65
wc 225
hzmm 48.65
rf1 6947.8
rfp 5812.8
tn 20.0
rp 155.4
lp -270.5
nm no ph

```

GSP264_2/CDCl3/1H
Schneider 110803_12
Mon Aug 11 19:18 2003

exp6 std1h

SAMPLE
date Aug 11 2003
solvent CDCl3
file exp6
ACQUISITION
instrum g300
probe atb5
sqgfil s2pu1
sfrq 300.225
tn H1
at 2.733
np 32768
sw 5995.2
bs 6
ipwr 61
pw 2.0
d1 0.267
d2 0
tof 46.0
nt 64
ct 64
alock n
gain not used
il n
in n
dp y
DEC. & VT H1
dn dfrq 300.225
homo n
dpwr 30
dof 0.0
ds nnn
dnn c
daf 200
PROCESSING
lb 0.30
wtfile ft
proc ft
fn 65536
DISPLAY
sp -150.2
wp 3002.1
vs 1708
sc 65
wc 225
hzmm 13.34
is 300.00
rf1 1496.6
rfp 0
th 4.0
ins 100.000
rp 131.9
lp -205.7
nm ph

```

OSP264.2/CDCl3/13C
 Schneider 110803.12
 Mon Aug 11 19:22 2003

exp7 std13c

SAMPLE
 date Aug 11 2003
 solvent CDCl3
 file exp

ACQUISITION
 instrum p300
 probe eth5
 seqfil s2pul
 sfrq 75.500
 tn C13
 at 1.747
 np 65906
 sw 18867.9
 bs 16
 tpwr 56
 pw 3.5
 d1 2.000
 d2 0
 tof 767.6
 nt 15000
 ct 13552
 alock n
 gain not used

FLAGS
 il n
 in n
 dp y

DEC. & VT
 dn H1
 dfrq 300.225
 homo n
 apwr 37
 dof 0
 dm yyy
 dmm w
 dmf 7900
 pp 17.5

PROCESSING
 lb not used
 wtfile
 proc ft
 fn 65536

DISPLAY
 sp 2642.1
 wp 8304.5
 vs 170
 sc 65
 wc 225
 hzmm 36.91
 rfl 6947.0
 rfp 5812.6
 th 1.5
 rp 147.0
 lp -246.0
 nm no ph

GSP215_2/CDCl3/1H
Schneider 030603_08
Tue Jun 3 16:12 2003

exp8 std1h

SAMPLE

date Jun 3 2003

solvent CDCl3

file exp

ACQUISITION

instrum g300

probe atb5

seqfil s2pu1

sfrq 300.225

tn H1

at 2.733

np 32768

sw 5995.2

bs 8

tpwr 61

pw 2.0

d1 0.267

d2 0

tof 46.0

nt 64

ct 64

alock n

gain not used

FLAGS

il n

in nw

dp y

DEC. & VT

dp H1

dfrq 300.225

homo n

dpwr 30

dof 0.0

dm nnn

dmm c

dmf 200

PROCESSING

lb 0.30

wtfile ft

proc 65536

tn

DISPLAY

sp -150.2

wp 2702.0

vs 170

sc 65

wc 225

hzmm 12.01

ls 469.63

rfl 1497.0

rpf 0

th 2.1

ins 100.000

rp 100.4

lp -150.0

nm ph

GSP200_2/CDC13/13C
Schneider 230503
Fri May 23 17:35 2003

exp1 std13c

SAMPLE
date May 23 2003
solvent CDC13
file exp

ACQUISITION
instrum m400
probe asw5
seqfil s2pul
sfrq 100.574
tn C13
at 1.311
np 67216
sw 25641.0
bs 16
tpwr 61
pw 4.0
d1 1.689
d2 0
tof 1327.2
nt 20000
ct 20000
alock n
gain not used

fl flags
il n
in nw
dp y

DEC. & VT
dn H1
dfrq 399.936
homo n
dpwr 40
dof 0
dm yyy
dem w
dof 9350
pp 17.5

PROCESSING
lb 1.00
wtfile
proc ft
fn 65536

DISPLAY
sp -358.7
wp 15354.7
vs 120
sc 65
wc 225
hzmm 68.24
rfl 9741.7
rtfp 7743.4
th 20.0
rp 62.4
lp -823.8
nm no ph

GSP238_2/CDC13/1H
 Schneider 160703.08
 Wed Jul 16 17:01 2003

exp7 std1h
 SAMPLE
 date Jul 16 2003
 solvent CDC13
 file exp
 ACQUISITION
 instrum g300
 probe_ atb5
 seqfil s2p01
 sfrq 300.225
 tn H1
 at 2.733
 np 32768
 sw 5985.2
 bs 8
 tpwr 61
 pw 2.0
 d1 0.267
 d2 0
 tof 46.0
 nt 64
 ct 64
 alock n
 gain not used
 FLAGS
 fl n
 in n
 dp y
 DEC. & VT
 dn H1
 dfrq 300.225
 homo n
 dpwr 30
 dot 0.0
 dm nnn
 dmm c
 dmf 200
 PROCESSING
 lb 0.30
 wtfile
 proc ft
 fn 65536
 DISPLAY
 sp -150.2
 wp 2852.1
 vs 162
 sc 65
 wc 225
 hzmm 12.60
 is 556.19
 rfi 1498.5
 rfp 0
 th 2.1
 ins 100.000
 rp 104.4
 lp -195.9
 na ph

GSP238_2/CDCl3/13C
Ruijter 160703
Wed Jul 16 16:04 2003

exp2 std13c

SAMPLE
date Jul 16 2003
solvent CDCl3
file exp

ACQUISITION
instrum m400
probe asv5
seqf11 s2pul
sfrq 100.574
tn C13
et 1.311
np 67216
sw 25641.0
bs 16
tpwr 61
pw 4.0
d1 1.689
d2 0
tof 1327.2
nt 15000
ct 15000
alock n
gain not used

FLAGS
il n
in nw
dp y

DEC. & VT
dn H1
dfrq 399.936
homo n
dpwr 40
dof 0
dm yyy
dnn w
dmf 9350
pp 17.5

PROCESSING
lb 1.00
wtfile ft
proc ft
fn 65536

DISPLAY
sp -0.5
wp 16091.9
vs 120
sc 65
wc 225
hzmm 71.52
rf1 9741.7
rfp 7743.4
th 28.0
rp 62.5
lp -331.3
nm no ph

GSP239_2/CDCl3/1H
Schneider 110703_04
Mon Jul 14 15:37 2003

exp3 - std1h

SAMPLE	
date	Jul 14 2003
solvent	CDCl3
file	exp3
ACQUISITION	
instrum	g300
probe	atb5
seqfil	s2pul
sfrq	300.225
tn	H1
at	2.733
np	32768
sw	5995.2
bs	8
tpwr	61
pw	2.0
d1	0.267
d2	0
tof	46.0
nt	64
ct	64
alock	n
gain	not used
FLAGS	
s1	n
in	n
dp	y
dn	DEC. & VT H1
dfrq	300.225
homo	n
dpwr	30
dof	0.0
dm	nnn
dmm	c
dmf	200
PROCESSING	
lb	0.30
wtfile	ft
proc	
fn	65536
DISPLAY	
sp	-150.2
wp	2852.1
vs	162
sc	65
wc	225
hzmm	12.60
is	500.00
rfl	1496.5
rfp	0
th	2.1
ins	100.000
rp	106.0
lp	-201.3
nm	ph

GSP239_2/CDCl3/13C
Schneider 110703_04
Fri Jul 11 23:33 2003

exp7 std13c

SAMPLE
date Jul 11 2003
solvent CDCl3
file exp

ACQUISITION
instrum g300
probe atb5
seqfil s2pul
sfrq 75.500
tn C13
at 1.747
np 65906
sw 18867.9
bs 16
tpwr 56
pw 3.5
d1 2.000
d2 0
tof 767.8
nt 60000
ct 55648
alock n
gain not used

FLAGS
s1 n
in n
dp y

DEC. & VT
dn H1
dfrq 300.225
homo n
dpwr 37
dof 0
dm yvy
dse w
def 7900
pp 17.5

PROCESSING
lb 1.00
wifile
proc ft
fn 65536

DISPLAY
sp 754.7
wp 10192.0
vs 170
sc 65
wc 225
hzm 45.30
rfl 6946.0
rfp 5812.6
th 20.0
rp 157.3
lp -242.4
nm no ph

GSP289_2/CDC13/1H
 Schneider 170903_02
 Wed Sep 17 12:25 2003

exp4 stdih

SAMPLE
 date Sep 17 2003
 solvent CDC13
 file exp

ACQUISITION
 instrua g300
 probe atb5
 seqfil szpul
 sfrq 300.225
 tn H1
 at 2.733
 np 32768
 sw 5895.2
 bs 8
 spwr 61
 pw 2.0
 d1 0.267
 d2 0
 tof 46.0
 nt 64
 ct 64
 alock n
 gain not used
 fls
 fl n
 tn n
 dp y
 DEC. & VT
 dn H1
 dfrq 300.225
 homo n
 dpwr 30
 dcf 0.0
 dm nnn
 dmm c
 dmt 200

PROCESSING
 lb 0.30
 wtfile
 proc ft
 fn 65536

DISPLAY
 sp -150.2
 wp 2052.1
 vs 170
 sc 65
 wc 225
 hzmm 12.68
 fs 300.00
 rfi 1498.5
 rfp 6
 th 30.0
 ins 100.000
 rp 107.4
 lp -157.2
 nm ph

GSP203_2/CDCl3/13C
 Schneider 250903_04
 Thu Sep 25 18:09 2003

exp? std13c

SAMPLE
 date Sep 25 2003
 solvent CDCl3
 file exp

ACQUISITION

instrum g300
 probe atb5
 seqfit s2pu7
 srfq 75.500
 rn C13
 at 1.747
 ap 65906
 sw 16867.9
 bs 16
 tpuw 56
 pw 3.5
 d1 2.000
 d2 0
 tof 767.8
 nt 13500
 cl 13500
 alock n
 gain not used

FLACS
 il n
 in n
 dp y

DEC. & VT
 dn H1
 dfrq 300.225
 hmc n
 dsw 37
 dcf 0
 dm yyy
 den w
 dmf 7900
 pp 17.5

PROCESSING
 lb 1.00
 wfile ft
 proc ft
 fn 65536

DISPLAY
 sp 1510.0
 wp 9437.1
 vs 150
 sc 65
 wt 225
 h2mm 41.94
 rll 6948.2
 rfp 5812.8
 th 20.0
 rd 172.1
 lp -284.4
 nm nc ph