Supplementary Material

A New and Practical One-Pot Access to Sulfonimides

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Sulfonimides. General Procedure A: $\text{PhI}=\text{O}^1$ (165 mg, 0.75 mmol, 1 equiv.) was added at room temp. to a solution of sulfonamide (116 mg, 0.75 mmol) in alcohol (2 mL). After 15 min, excess alcohol was removed in vacuo. The crude mixture was purified by flash chromatography.

Sulfonimides. General Procedure B: Alcohol (2.25 mmol, 3 equiv.) and $\text{PhI}=\text{O}$ (165 mg, 0.75 mmol, 1 equiv.) were added at room temp. To a solution of sulfonamide (116 mg, 0.75 mmol) in acetonitrile (2 mL). After 15 min, the solvent was evaporated. The crude mixture was purified by flash chromatography. When diols were used, the evaporated mixture was diluted in CH_2Cl_2 and washed with water to get rid of excess alcohol before chromatography.

Following General Procedure A, chromatography (PE/EA, 70 :30) afforded 126 mg (91%) of sulfonimide as a white solid.

Following General Procedure B, chromatography (PE/EA, from 80:20 to 70:30) afforded 118 mg (85%) of sulfonimide along with 8 mg (5%) of sulfonamide.

M.p. 45-47°C. – IR (neat) 3300, 3020, 2905, 1180, 1040, 850, 730 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 2.35 (s, 3H, CH_3), 3.36 (s, 1H, NH), 3.35 (s, 3H, OCH_3), 7.25 (d, J = 8.1 Hz, 2H, arom.), 7.81 (d, J = 8.1 Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.3 (CH_3), 55.3 (CH_3), 127.6 (2 CH arom.), 129.4 (2 CH arom.), 133.9 (C arom.), 143.8 (C arom.). – $\text{C}_8\text{H}_{11}\text{NO}_2\text{S}$ (185.24) : calcd. C 51.87, H 5.99, N 7.56 ; found : C 51.84, H 6.17, N 7.45.

Following General Procedure A, chromatography (PE/EA, 70 :30) afforded 140 mg (94%) of sulfonimide as a pale yellow oil.

Following General Procedure B, chromatography (PE/EA, from 80:20 to 70:30) afforded 100 mg (67%) of sulfonimide along with 30 mg (23%) of sulfonamide.

IR (neat) : 3280, 2960, 1590, 730 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 1.22 (t, J = 7.1 Hz, 3H, CH_3), 2.41 (s, 3H, CH_3), 3.20 (s, 1H, NH), 3.95 (m, 2H, OCH_2), 7.29 (d, J = 8.2 Hz, 2H, arom.), 7.86 (d, J = 8.4 Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 14.9 (CH_3), 21.6 (CH_3), 65.7 (CH_2), 127.7 (2 CH arom.), 129.6 (2 CH arom.), 135.3 (C arom.), 143.9 (C

¹ Saltzman, H.; Sharefkin, J. G. Organic Syntheses; Wiley: New York, 1973; Collect. Vol. V, pp 658-659.

arom.). – C₉H₁₃NO₂S (199.27) : calcd. C 54.25, H 6.58, N 7.03 ; found : C 54.17, H 6.87, N 6.75.

Following General Procedure A, chromatography (Pentane/AE, 70 :30) afforded 115 mg (73%) of sulfonimidate as a colorless oil.

Following General Procedure B, chromatography (PE/AE, from 80:20 to 70:30) afforded 28 mg (18%) of sulfonimidate along with 84 mg (74%) of sulfonamide.

IR (neat) : 3280, 2960, 2920, 1590, 740 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) : δ 1.03 (d, *J* = 6.2 Hz, 3H, CH₃), 1.07 (d, *J* = 6.2 Hz, 3H, CH₃), 2.28 (s, 3H, CH₃), 3.09 (s, 1H, NH), 4.46 (sept, *J* = 6.2 Hz, 2H, OCH(CH₃)₂), 7.16 (d, *J* = 8.2 Hz, 2H, arom.), 7.74 (d, *J* = 8.2 Hz, 2H, arom.). ¹³C NMR (100 MHz, CDCl₃) : δ 21.6 (CH₃), 22.9 (CH₃), 23.9 (CH₃), 75.1 (CH), 127.4 (2 CH arom.), 129.5 (2 CH arom.), 136.5 (C arom.), 143.6 (C arom.). – C₁₀H₁₅NO₂S (213.30) : calcd. C 56.31, H 7.09, N 6.57 ; found : C 56.02, H 7.37, N 6.31.

Following General Procedure A, chromatography (PE/EA, 80:20) afforded 112 mg (71%) of sulfonimidate as a colorless oil.

Following General Procedure B, chromatography (PE/EA, from 80:20 to 70:30) afforded 95mg (60%) of sulfonimidate along with 47 mg (36%) of sulfonamide.

IR (neat) : 3300, 2920, 1650, 1600, 780 cm⁻¹. ¹H NMR (400 MHz, CDCl₃) : δ 2.41 (s, 3H, CH₃), 3.28 (s, 1H, =NH), 4.39 (m, 2H, OCH₂), 5.24 (m, 2H, =CH₂), 5.79 (m, 1H, =CH), 7.30 (d, *J* = 8.1 Hz, 2H, arom.), 7.87 (d, *J* = 8.1 Hz, 2H, arom.). ¹³C NMR (100 MHz, CDCl₃) : δ 21.5 (CH₃), 69.9 (CH₂), 119.3 (=CH₂), 127.6 (2 CH arom.), 129.6 (2 CH arom.), 131.2 (CH), 135.0 (C arom.), 143.6 (C arom.). – C₁₀H₁₃NO₂S (211.28) : calcd. C 56.85, H 6.20, N 6.63 ; found : C 56.92, H 6.19, N 6.58.

Following General Procedure A, chromatography (Pentane/AE, 70 :30) afforded 145 mg (92%) of sulfonimide as a pale yellow oil.

Following General Procedure B, chromatography (PE/AE, from 80:20 to 70:30) afforded 110 mg (70%) of sulfonimide along with 5 mg (4%) of sulfonamide.

IR (neat) : 3280, 2220, 1590, 920, 730 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 2.40 (s, 3H, CH_3), 2.42 (t, $J = 2.1$ Hz, 1H), 3.43 (s, 1H, NH), 4.51 (d, $J = 2.1$ Hz, 2H, OCH_2), 7.29 (d, $J = 8.3$ Hz, 2H, arom.), 7.87 (d, $J = 8.3$ Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.7 (CH_3), 56.7 (CH_2), 76.5 (CH), 76.7 (C), 128.0 (2 CH arom.), 129.8 (2 CH arom.), 134.5 (C arom.), 144.5 (C arom.). – $\text{C}_{10}\text{H}_{11}\text{NO}_2\text{S}$ (209.27) : calcd. C 57.39, H 5.30, N 6.69 ; found : C 57.38, H 5.28, N 6.71.

Following General Procedure A, chromatography (Pentane/EA, 80 :20) afforded 143 mg (85%) of sulfonimide as a colorless oil.

Following General Procedure B, chromatography (Pentane/EA, from 80:20 to 70:30) afforded 91mg (53%) of sulfonimide along with 50 mg (39%) of sulfonamide.

IR (neat) : 3300, 2960, 1600, 730 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 2.31 (m, 2H), 2.39 (s, 3H, CH_3), 3.30 (s, 1H, NH), 3.90 (m, 2H, OCH_2), 4.09 (m, 2H, $=\text{CH}_2$), 5.63 (m, 1H, $=\text{CH}$), 7.28 (d, $J = 8.0$ Hz, 2H, arom.), 7.85 (d, $J = 8.0$ Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.6 (CH_3), 33.3 (CH_2), 68.5 (CH_2), 129.6 (2 CH arom.), 133.1 (2 CH arom.), 135.1 (C arom.), 143.9 (C arom.). – $\text{C}_{11}\text{H}_{15}\text{NO}_2\text{S}$ (225.31) : calcd. C 58.64, H 6.71, N 6.22 ; found : C 58.72, H 6.81, N 6.04.

Following General Procedure B, chromatography (PE/EA, from 80:20 to 60:40) afforded 130 mg (57%) of sulfonimide along with 35 mg (27%) of sulfonamide.

IR (neat) : 3300, 3040, 2950, 1600, 930, 730 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 1.59–1.63 (m, 4H, $-(\text{CH}_2)_2-$), 2.40 (s, 3H, CH_3), 2.53 (t, $J = 6.9$ Hz, 2H, CH_2), 3.19 (s, 1H, NH), 3.88 (m, 2H, OCH_2), 7.09 (d, $J = 7.1$ Hz, 2H, arom.), 7.16 (t, $J = 7.1$ Hz, 1H, arom.), 7.24 (t, $J = 7.1$ Hz, 2H, arom.), 7.28 (d, $J = 8.1$ Hz, 2H, arom.), 7.87 (d, $J = 8.1$ Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.6 (CH_3), 27.3 (CH_2), 28.6 (CH_2), 35.3 (CH_2), 69.4 (CH_2), 125.9 (1 CH arom.), 127.7 (2 CH arom.), 128.4 (4 CH arom.), 129.6 (2 CH arom.), 135.2 (1C arom.), 141.8 (1C arom.), 143.9 (C arom.). – $\text{C}_{17}\text{H}_{21}\text{NO}_2\text{S}$ (303.42) : calcd. C 67.29, H 6.98, N 4.62; found : C 67.44, H 7.06, N 4.53.

Following modified (using 5 equiv. alcohol) General Procedure B, chromatography (PE/EA, from 80:20 to 70:30) afforded 184mg (95%) of sulfonimide as a colorless oil along with 4 mg (3%) of sulfonamide.

IR (neat) : 3250, 2900, 2840, 1580, 800, 720 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 1.28 (m, 2H), 1.40 (m, 2H), 1.52 (m, 2H), 2.34 (s, 3H, CH_3), 3.09 (s, 1H, NH), 3.45 (t, $J = 6.4$ Hz, 2H), 3.82 (m, 2H), 7.24 (d, $J = 8.1$ Hz, 2H, arom.), 7.78 (d, $J = 8.1$ Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.4 (CH_3), 21.7 (CH_2), 28.5 (CH_2), 31.8 (CH_2), 61.9 (HOCH_2), 69.3 (HNOCH_2), 127.4 (2 CH arom.), 129.5 (2 CH arom.), 134.9 (C arom.), 143.9 (C arom.).— $\text{C}_{12}\text{H}_{19}\text{NO}_3\text{S}$ (257.35) : calcd. C 56.00, H 7.44, N 5.44; found : C 55.58, H 7.58, N 5.31.

Following modified General Procedure B, chromatography (PE/EA, from 80:20 to 20:80) afforded 88 mg (51%) of sulfonimide as white crystals along with 8 mg (6%) of sulfonamide.

M.p. 52-54°C. IR (neat) : 3300, 2960, 2950, 1600, 820, 740 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 1.82 (m, 2H, CH_2), 2.42 (s, 3H, CH_3), 2.48 (t, $J = 5.6$ Hz, OH), 3.34 (s, 1H, NH), 3.61 (m, 2H, CH_2OH), 4.08 (m, 2H, $-\text{OCH}_2-$), 7.31 (d, $J = 7.6$ Hz, 2H, arom.), 7.86 (d, $J = 7.6$ Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.4 (CH_3), 31.6 (CH_2), 57.8 (CH_2), 66.3 (CH_2), 127.4 (2 CH arom.), 129.5 (2 CH arom.), 134.8 (C arom.), 143.9 (C arom.).— $\text{C}_{10}\text{H}_{15}\text{NO}_3\text{S}$ (229.30) : calcd. C 52.38, H 6.59, N 6.11; found : C 52.51, H 6.57, N 6.18.

Following General Procedure B, chromatography (PE/EA from 100:0 to 70:30) afforded 128.6 mg (62%) of sulfonimide as a colorless oil along with 14 mg (11%) of sulfonamide.

IR (neat) : 3280, 1590, 860, 810, 730 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 2.42 (s, 3H, CH_3), 3.41 (t, 3H, $J = 6.1$ Hz, $\text{CH}_2\text{Br} + \text{NH}$), 4.14 (t, $J = 6.1$ Hz, 2H, OCH_2), 7.31 (d, $J = 8.6$ Hz, 2H, arom.), 7.88 (d, $J = 8.6$ Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 21.7 (CH_3), 28.2 (CH_2), 68.1 (CH_2), 127.7 (2 CH arom.), 129.8 (2 CH arom.), 134.4 (C arom.), 144.4 (C arom.).

Following General Procedure B starting from of 230 mg (1.09 mmol) substituted sulfinamide chromatography (Pentane/EA, from 90:10 to 60:40) afforded 135mg (52%) of sulfonimide along with 54 mg (22%) of sulfonamide.

IR (neat) : 2920, 2850, 1450, 980, 810, 700 cm^{-1} . ^1H NMR (400 MHz, CDCl_3) : δ 0.92, (t, J = 7.4 Hz, 3H, CH_3), 1.41 (m, 2H, CH_2), 1.60 (m, 2H, CH_2), 2.40 (s, 3H, CH_3), 3.19 (m, 1H, NCH), 3.29 (m, 1H, NCH), 3.54 (s, 3H, CH_3), 7.28 (d, J = 8.1 Hz, 2H, arom.), 7.83 (d, J = 8.1 Hz, 2H, arom.). ^{13}C NMR (100 MHz, CDCl_3) : δ 13.9 (CH_3), 20.4 (CH_2), 21.6 (CH_3), 34.7 (CH_2), 42.5 (NCH_2), 55.4 (OCH_3), 127.9 (2 CH arom.), 129.2 (2 CH arom.), 134.2 (C arom.), 143.6 (C arom.).— $\text{C}_{10}\text{H}_{15}\text{NO}_3\text{S}$ (229.30) : calcd. C 59.72, H 7.93, N 5.80; found : C 59.71, H 7.89, N 5.78.

CRYSTAL DATA for $\text{C}_{10}\text{H}_{15}\text{NO}_3\text{S}$:

Fw	229.29
a (Å)	9.369(2)
b (Å)	10.196(5)
c (Å)	12.334(4)
α (°)	78.99(3)
β (°)	88.77(2)
γ (°)	78.92(3)
V (Å ³)	1134.9(7)
Z	4
Crystal system	triclinic
Space group	P -1
Linear absorption coefficient μ (cm^{-1})	2.6
Density ρ (g.cm^{-3})	1.34
Diffractometer	MACH-3 Enraf-Nonius
Radiation	MoK α (λ = 0.71069 Å)
Scan type	$\omega/2\theta$
Scan range (°)	0.8 + 0.345 $\text{tg}\theta$
θ Limits (°)	1 - 26
Temperature of measurement	295K
Octants collected	0,11 ; -12,12 ; -15,15
Decay %	none
Nb of data collected	4753
Nb of unique data collected	4461 (R_{int} =0.03)
Nb of unique data used for refinement	3223 ($\text{Fo}^2 > 3\sigma(\text{Fo})^2$)
$R = \Sigma \text{Fo} - \text{Fc} / \Sigma \text{Fo} $	0.0524
$Rw^* = [\Sigma w(\text{Fo} - \text{Fc})^2 / \Sigma w \text{Fo} ^2]^{1/2}$	0.0612

S	1.12
Extinction parameter	599
Nb of variables	273
$\Delta\rho_{\min}$ (e.Å ⁻³)	-0.58
$\Delta\rho_{\max}$ (e.Å ⁻³)	0.32

* $w = w'[1 - ((|F_o| - |F_c|)/6 \cdot \sigma(F_o))^2]^2$ with $w' = 1/\sum_r A_r T_r(X)$ with 3 coefficients 7.20, 0.173 and 5.55 for a Chebyshev Series, for which X is $F_c/F_c(\max)$

Current Data Parameters
 NAME 01121
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020208
 Time 15.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 184
 DS 2
 SWH 3333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830900 sec
 RG 32768
 DW 15.000 us
 DE 21.43 us
 TE 300.0 K
 O12 0.0000200 sec
 DL6 120.00 dB
 D1 1.00000000 sec
 CPDPRG waitz16
 P31 100.00 us
 D11 0.0300000 sec
 DL5 16.00 dB
 P1 7.75 us
 SF01 100.6250730 MHz
 NUCLEUS 13C

F2 - Processing parameters
 SI 16384
 SF 100.6127598 MHz
 NQM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 24.00 cm
 F1P 160.379 DP
 F1 16136.19 Hz
 F2P -5.000 DP
 F2 -503.06 Hz
 PPMCH 6.89060 DP
 NZCH 693.30206 Hz

Current Data Parameters
 NAME J82401108
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020124
 Time 16.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 8333.333 Hz
 FIDRES 0.254313 Hz
 AQ 1.9661300 sec
 RG 512
 DW 60.000 us
 DE 85.71 us
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.75 us
 SFO1 400.1324508 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 400.1299981 MHz
 MO 16
 SS 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 23.50 cm
 FIP 8.500 dp
 FI 3401.10 Hz
 F2P 0.000 dp
 F2 0.00 Hz
 PMCH 0.35170 dp
 HZCH 144.72787 Hz

Current Data Parameters

NAME	1a20199
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20020122
Time	16.37
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	171
DS	2
SWH	3333.332 Hz
FIDRES	0.508626 Hz
AQ	0.983090 s
RG	32768
DW	15.000 us
DE	21.43 us
TE	300.0 K
D12	0.000200 s
DL6	120.00 dB
D1	1.0000000 s
CPDPRG	waltz16
P31	100.00 us
D13	0.030000 s
DL5	15.00 dB
P1	7.75 us
SFO1	100.6250730 MHz
NUCLEUS	13C

F2 - Processing parameters

SI	16384
SF	100.6127687 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	24.00 cm
F1P	153.999 pp
F1	15494.25 Hz
F2P	12.808 pp
F2	1288.63 Hz
PPMCM	5.88296 pp
HZCM	591.50076 Hz

Current Data Parameters	
NAME	OC170114
EXPNO	1
PROCNO	1
F2 - Acquisition Parameter	
Date_	20011217
Time	9.28
INSTRUM	9.28
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SH	833.333 Hz
FIDRES	0.254313 Hz
AQ	1.5961300 sec
RG	360
DM	60.000 us
DE	85.71 us
TE	300.0 K
P1	1.00000000 sec
P2	10.75 us
SFO1	400.1324508 MHz
NUCLEUS	
1H	
F2 - Processing parameters	
SF	16984
WDW	400.1300488 MHz
SSB	no
LB	0
GB	0.00 Hz
PC	0
1.00	
10 NMR plot parameters	
CX	23.50 cm
F1P	7.996 pp
F1	3199.37 Hz
F2P	0.454 pp
F2	181.83 Hz
PUNCH	0.32091 pp
HCCH	128.40599 Hz

Current Data Parameters
 NAME dc170170
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011217
 Time 9.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 245
 DS 2
 SMH 3333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830900 se
 RG 32768
 DK 15.000 us
 DE 21.43 us
 TE 300.0 K
 012 0.0000200 se
 016 120.00 dB
 01 1.00000000 se
 CPOPRG waltz16
 P31 100.00 us
 011 0.0300000 se
 015 16.00 dB
 P1 7.75 us
 SF01 100.6250730 MHz
 NUCLEUS 13C

F2 - Processing Parameters
 SI 16384
 SF 100.6127598 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 24.00 cm
 F1P 157.396 DD
 F1 15836.06 Hz
 F2P 4.514 DD
 F2 454.19 Hz
 PMCH 6.37008 DD
 HZCH 640.91101 Hz

Current Data Parameters
NAME d160
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011206
Time 10.31

INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 193
DS 2

SMH 333.332 Hz
FIDRES 0.50826 Hz
AQ 0.9830500 sec

RG 32768
DM 15.000 us
DE 21.43 us

TE 300.0 K
D12 0.0000200 sec
DL6 120.00 dB

D1 1.00000000 sec
CPDPRG waltz16
P31 100.00 us

D11 0.0300000 sec
DL5 16.00 dB
P1 7.75 us

SFO1 100.6250730 MHz
NUCLEUS 13C

F2 - Processing parameters

SF 16384

SF 100.6127598 MHz

KON no

SSB 0

LB 0.00 Hz

GB 0

PC 1.00

10 NMR plot parameters

CX 24.00 cm

F1P 156.088 pp

F1 15704.47 Hz

F2P -6.221 pp

F2 -625.68 Hz

PPMCH 6.76287 pp

HZCH 680.43103 Hz

Current Data Parameters

NAME	EXPNO	DIRX	PROCNO
NAME	1		1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TO	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	OW	DE	TE	O1	SF01	NUCLEUS
20020507	16.07	5 mm QNP 1H	1930	zgpg30	32768	CDCl3	16	2	8333.333 Hz	0.254313 Hz	1.9661300 s	1024	60.000 us	85.71 us	300.0 K	1.00000000 s	10.75 us	400.1324508 MHz

F2 - Processing Parameters

SI	SF	WDW	SSB	LB	GB	PC
16384	400.130093 MHz	NO	0	0.00 Hz	0	1.00

1D NMR plot parameters

CX	F1P	F1	F2P	F2	PPMCM	HZCM
23.50 cm	8.708 DP	3484.42 Hz	0.000 DP	0.00 Hz	0.37056 DP	148.27318 Hz

Current Data Parameters
 NAME d1158
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020320
 Time 10.35
 INSTRUM spect
 PROBO 5 mm QNP 1H
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 35
 DS 2
 SWH 3333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.983090 sec
 RG 32768
 DW 15.000 us
 DE 21.43 us
 TE 300.0 K
 D12 0.0000200 sec
 DL6 120.00 dB
 D1 1.00000000 sec
 CPDPRG waitz16
 P31 100.00 us
 D11 0.0300000 sec
 DL5 16.00 dB
 P1 7.75 us
 SFO1 100.6250730 MHz
 NUCLEUS 13C

F2 - Processing parameters
 SI 16384
 SF 100.6127809 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 24.00 cm
 F1P 160.000 DP
 F1 16098.04 Hz
 F2P 0.000 DP
 F2 0.00 Hz
 PPMCH 6.66667 DP
 HZCM 670.75183 Hz

Current Data Parameters
NAME d153
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011210
Time 14.29
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 833.333 Hz
FIDRES 0.254313 Hz
AQ 1.9661300 sec
RG 512
DM 60.000 us
DE 85.71 us
TE 300.0 K
D1 1.00000000 sec
P1 10.75 us
SFO1 400.1324508 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 16384
SF 400.130000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 23.50 cm
F1P 8.084 dB
F1 3234.64 Hz
F2P -0.019 dB
F2 -7.47 Hz
PPHCH 0.34479 dB
HZCH 137.96204 Hz

Current Data Parameters

NAME	d163
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20011210
Time	14.32
INSTRUM	spect
PROBHD	5 mm DNP 1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	122
DS	2
SWH	33333.332 Hz
FIDRES	0.508626 Hz
AQ	0.9830900 sec
RG	32768
OW	15.000 us
DE	21.43 us
TE	300.0 K
D12	0.0000200 sec
DL6	120.00 dB
D1	1.00000000 sec
CPDPRG	waltz16
P31	100.00 us
D11	0.0300000 sec
DL5	16.00 dB
P1	7.75 us
SFO1	100.6250730 MHz
NUCLEUS	¹³ C

F2 - Processing parameters

SI	16384
SF	100.6127598 MHz
MDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	24.00 cm
F1P	147.673 pp
F1	14857.80 Hz
F2P	-1.656 pp
F2	-156.58 Hz
PPMCH	6.22203 pp
HZCM	626.01562 Hz

Current Data Parameters
 NAME d1122-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020208
 Time 15.29
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8333.333 Hz
 FIDRES 0.254313 Hz
 AQ 1.9661300 sec
 RG 512
 DW 60.000 us
 DE 65.71 us
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.75 us
 SFO1 400.1324508 MHz
 NUCLEUS 1H

F2 - Processing Parameters
 SI 16384
 SF 400.1300164 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 23.50 cm
 F1P 8.278 pp
 F1 3312.20 Hz
 F2P 0.133 pp
 F2 53.10 Hz
 PPMCK 0.34650 pp
 HZCK 138.58492 Hz

Current Data Parameters

NAME	d1122-1
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20020208
Time	15.11
INSTRUM	spect
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	383
DS	2
SWH	33333.332 Hz
FIDRES	0.506626 Hz
AQ	0.9830900 s
RG	32768
DM	15.000 us
DE	21.43 us
TE	300.0 K
DT2	0.000200 s
DL6	120.00 dB
DI	1.00000000 s
CPDPRG	waltz16
P31	100.00 us
DI1	0.0300000 s
DL5	16.00 dB
P1	7.75 us
SFO1	100.6250730 MHz
NUCLEUS	¹³ C

F2 - Processing parameters

SI	16384
SF	100.6127626 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	24.00 cm
F1P	159.602 DP
F1	16058.05 Hz
F2P	-2.118 DP
F2	-213.14 Hz
PPMCM	6.73837 DP
HZCM	677.96606 Hz