Supporting Information

One-pot Synthesis of Dithiocarbamates is Accelerated in Water

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General Experimental Methods: ^1H NMR spectra were recorded on 500 MHz NMR spectrometer and ^{13}C NMR spectra were recorded on 125 MHz NMR spectrometer respectively using $\text{CDCl}_3/\text{CCl}_4$ or $\text{CDCl}_3/\text{DMSO}$, as a solvent, Chemical shifts have been expressed in (ppm). All amines, Michael acceptor, CS_2 and solvent are commercially available and were purchased and used without further purification; water and other solvent were distilled before used. All the reactions are monitored by thin layer chromatography (TLC) carried out on silica gel with UV light and iodine, as detecting agents. Silica gel and petroleum ether and ethyl acetate are used for column chromatography.

General procedure for the one-pot reaction of amines, CS_2 and α - β unsaturated olefins in water: the carbon disulfide (8 mmol), the Michael acceptor (6 mmol) and the amines (5 mmol) were added to water (10 ml) the reaction mixture were stirred under vigorous magnetic stirring at room temperature for 5- 18 h. organic materials were extracted with diethyl ether or ethyl acetate (2 x 10 mL). The organic layer was separated and dried over anhydrous Na_2SO_4 . The solvent was removed under reduced pressure to give desired products, and the crude product was purified by flash column chromatography and in some cases crystallized from ethanol or diethyl ether to provide the corresponding product. All compounds were characterized on the basis of NMR spectroscopic data.

Table 1, Entry 1: ^1H NMR (500 MHz, CDCl_3) δ 2.71 (2H, t, $J = 6.8$ Hz), 3.36-3.41 (4H, m), 3.51-3.54 (4H, m), 3.59-4.12 (4H, m). ^{13}C NMR (125 MHz; CDCl_3) δ 31.8, 34.1, 44.1, 48.3, 51.4, 51.8, 52.9, 53.8, 172.4, 194.1; Anal. (Found: C, 43.58; N, 5.58; H, 6.08. $\text{C}_9\text{H}_{15}\text{NO}_3\text{S}_2$ requires C, 43.37; N, 5.62; H, 6.02%)

Table 1, Entry 2: ^1H NMR (500 MHz, CDCl_3) δ 1.41-1.47 (6H, m), 2.53 (2H, t, $J = 6.4$ Hz), 3.42-4.01 (9H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 24.5, 25.8, 31.8, 34.0, 44.3, 51.5, 51.8, 52.9, 172.1, 194.5; Anal. (Found: C, 48.70; N, 5.79; H, 6.95. $\text{C}_{10}\text{H}_{17}\text{NO}_2\text{S}_2$ requires C, 48.55; N, 5.66; H, 6.93%)

Table 1, Entry 3: ^1H NMR (500 MHz, CDCl_3) δ 1.76-1.86 (4H, m), 2.57 (2H, t, $J = 6.7$ Hz), 3.28-3.46 (7H, m), 3.64-3.66 (2H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 24.5, 26.3, 31.2, 34.1, 50.8, 51.8, 55.2, 172.3, 191.7

Table 1, Entry 4: ^1H NMR (500 MHz, CDCl_3) δ 0.93- 0.99 (6H, m), 2.47 (2H, t, $J = 6.4$ Hz), 3.20 (2H, t, $J = 6.5$ Hz), 3.44 (3H, s), 3.45 (2H, q, $J = 6.9$ Hz), 3.70 (2H, q, $J = 6.9$ Hz); ^{13}C NMR (125 MHz; CDCl_3) δ 11.7, 12.9, 31.7, 33.9, 46.9, 49.6, 51.6, 171.9, 194.4.

Table 1, Entry 5: ^1H NMR (500 MHz, CDCl_3) δ 2.82 (2H, t, $J = 6.7$ Hz), 3.52 (2H, t, $J = 6.7$ Hz), 3.67 (3H, s), 4.90 (2H, s), 7.33-7.35 (5H, m), 7.90 (1H, br s, NH); ^{13}C NMR (125 MHz; CDCl_3) δ 30.3, 34.6, 51.4, 52.3, 128.3, 128.6, 129.3, 135.7, 172.8, 197.7

Table 1, Entry 6: ^1H NMR (500 MHz, CDCl_3) δ 0.89 (3H, t, $J = 7.2$ Hz), 1.19 (3H, d, $J = 5.3$ Hz), 1.51-1.61 (2H, m), 2.74 (2H, t, $J = 6.8$ Hz), 3.44 (2H, t, $J = 6.8$ Hz), 3.66 (3H, s), 4.52 (1H, m), 7.38 (1H, br s, NH); ^{13}C NMR (125 MHz; CDCl_3); δ 10.6, 20.9, 29.1, 30.9, 34.2, 52.1, 54.7, 54.8, 172.8, 196.0

Table 1, Entry 7: ^1H NMR (500 MHz, CDCl_3) δ 1.43 (9H, s) 2.60 (2H, t, $J = 6.1$ Hz), 3.28 (2H, t, $J = 6.2$ Hz), 3.56 (3H, s); ^{13}C NMR (125 MHz; CDCl_3) δ 27.9, 28.4, 34.5, 52.0, 57.6, 172.6, 194.6.

Table 1, Entry 8: ^1H NMR (500 MHz, CDCl_3) δ 1.59 (3H, d, $J = 7.1$ Hz), 2.77 (2H, t, $J = 6.5$ Hz), 3.50 (2H, t, $J = 6.4$ Hz), 3.67 (3H, s), 5.82 (1H, q, $J = 7.1$ Hz), 7.27-7.36 (5H, m), 7.97 (1H, br, NH); ^{13}C NMR (125 MHz; CDCl_3) δ 21.2, 30.2, 34.1, 52.3, 56.3, 141.7, 173.0, 196.3.

Table 1, Entry 12: ^1H NMR (500 MHz, CDCl_3) δ 1.30-1.51 (6H, m), 2.74 (2H, t, $J = 6.2$ Hz), 3.39 (2H, t, $J = 6.3$ Hz), 3.75 (2H, m), 4.12 (2H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 18.5, 25.9, 32.2, 51.9, 53.4, 54.2, 118.7, 193.0; Anal. (Found: C, 50.80; N, 12.92; H, 6.62. $\text{C}_9\text{H}_{14}\text{N}_2\text{S}_2$ requires C, 50.43; H, 6.58; N, 13.07%)

Table 1, Entry 13: ^1H NMR (500 MHz, CDCl_3) δ 1.72- 1.92 (4H, m), 2.66 (2H, t, $J = 6.5$ Hz), 3.29 (2H, t, $J = 6.5$ Hz), 3.43 (2H, t, $J = 6.7$ Hz), 3.64 (2H, t, $J = 6.7$ Hz); ^{13}C NMR (125 MHz; CDCl_3) δ 18.6, 24.5, 26.2, 31.6, 51.1, 53.9, 55.5, 118.7, 190.0; Anal. (Found: C,

48.30; H, 5.82, N, 13.69; C₈H₁₂N₂S₂ requires C, 47.97; H, 6.04; N, 13.98%).

Table 1, Entry 14: ¹H NMR (500 MHz, CDCl₃); δ 0.92-0.96 (6H, m), 2.53 (2H, t, *J* = 6.7 Hz), 3.12 (2H, t, *J* = 6.2 Hz), 3.42 (2H, q, *J* = 6.7 Hz), 3.67 (2H, t, *J* = 6.7 Hz), ¹³C NMR (125 MHz; CDCl₃) δ 9.4, 11.7, 18.2, 32.0, 47.2, 49.9, 118.6, 192.7

Table 1, Entry 15: ¹H NMR (500 MHz, CDCl₃) δ 2.82 (2H, t, *J* = 6.2 Hz), 3.46 (2H, t, *J* = 6.3 Hz), 4.88 (2H, s), 7.26-7.39 (5H, m), 8.02 (1H, br s, NH); ¹³C NMR (125 MHz; CDCl₃) δ 18.9, 31.4, 51.5, 119.0, 128.3, 128.8, 129.7, 136.5, 196.0.

Table 1, Entry 16: ¹H NMR (500 MHz, CDCl₃); δ 0.77 (3H, t, *J* = 7.3 Hz), 1.07 (3H, d, *J* = 6.4 Hz), 1.41-1.51 (4H, m), 2.65 (2H, t, *J* = 6.6 Hz), 3.35 (2H, *J* = 6.7 Hz), 4.37-4.38 (1H, m), 7.73 (1H, br s, NH); ¹³C NMR (125 MHz; CDCl₃) δ 10.8, 18.5, 19.4, 29.7, 31.1, 55.1, 55.2, 119.1, 194.3.

Table 1, Entry 18: ¹H NMR (500 MHz, CDCl₃) δ 1.57 (3H, d, *J* = 6.8 Hz), 2.73 (2H, t, *J* = 6.7 Hz), 3.40 (2H, t, *J* = 6.7 Hz), 5.79 (1H, q, *J* = 6.7 Hz), 7.29-7.37 (5H, m), 8.37 (1H, br s, NH); ¹³C NMR (125 MHz; CDCl₃) δ 18.2, 21.8, 31.5, 57.5, 119.3, 127.1, 128.8, 129.5, 141.7, 194.9.

Table 1, Entry 23 ¹H NMR (CD₃NO₂/CCl₄) δ 1.78-1.82 (6H, m), 2.71 (2H, t, *J* = 7.1 Hz), 3.56 (2H, t, *J* = 7.1 Hz), 3.96-4.33 (4H, m), 6.34 (2H, br, NH₂).

Table 1, Entry 24 ^1H NMR (DMSO/ CDCl_3) δ 1.04 (3H, t, $J = 7.1$ Hz), 1.14 (3H, t, $J = 7.1$ Hz), 2.49 (2H, t, $J = 7.1$ Hz), 3.36 (2H, t, $J = 7.0$ Hz), 3.63 (2H, q, $J = 7.1$ Hz,), 3.83 (2H, q, $J = 7.1$ Hz), 4.98- 5.41 (2H, br, NH_2).

Table 1, Entry 27: ^1H NMR (500 MHz, CDCl_3) δ 1.34-1.62 (6H, m), 2.08 (3H, s), 2.87 (2H, t, $J = 6.6$ Hz), 3.42 (2H, t, $J = 6.6$ Hz), 3.77-3.79 (2H, m), 4.12-4.19 (2H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 24.8, 25.1, 30.1, 43.1, 50.7, 55.6, 191.1, 206.8.

Table 1, Entry 28: ^1H NMR (500 MHz, CDCl_3) δ 1.38-1.76 (7H, m), 2.53 (2H, t, $J = 6.1$ Hz), 3.01-3.44 (6H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 23.8, 25.9, 29.9, 43.1, 50.7, 55.1, 191.7, 206.3. Anal. (Found: C, 49.53; H, 6.82; N = 6.61. $\text{C}_9\text{H}_{15}\text{NOS}_2$ requires C, 49.73; H, 6.96; N, 6.44%).

Table 1, Entry 29: ^1H NMR (500 MHz, CDCl_3) δ 1.01-1.06 (6H, m), 1.94 (3H, s), 2.72 (2H, t, $J = 6.6$ Hz), 3.23 (2H, t, $J = 6.6$ Hz), 3.52 (2H, q, $J = 7.1$ Hz), 3.79 (2H, q, $J = 7.1$ Hz); ^{13}C NMR (125 MHz; CDCl_3) δ 11.8, 12.7, 30.1, 30.6, 43.3, 46.9, 49.6, 195.2, 206.9.

Table 1, Entry 32: ^1H NMR (500 MHz, CDCl_3 / CCl_4) δ 1.58 (3H, d, $J = 6.8$ Hz), 2.14 (3H, s), 2.89 (2H, t, $J = 6.1$ Hz), 3.40 (2H, t, $J = 6.1$ Hz), 5.81 (1H, q, $J = 6.8$ Hz), 7.26-7.35 (5H, m), 8.18 (1H, br s, NH); ^{13}C NMR (125 MHz; CDCl_3) δ 21.3, 29.0, 30.4, 43.3, 56.4, 127.0, 128.2, 129.3, 141.7, 196.8, 207.6.

Table 1, Entry 36: ^1H NMR (500 MHz, CDCl_3) δ 1.52-2.20 (8H, m), 2.72- 3.02 (4H, m), 3.41-3.43 (4H, m),

3.86 (1H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 24.3, 24.7, 26.1, 29.3, 30.1, 39.1, 53.8, 54.9, 190.0, 207.0

Table 1, Entry 37: ^1H NMR (500 MHz, CDCl_3) δ 0.99-1.04 (6H, m), 1.62-2.32 (7H, m), 2.62 (1H, dd, $J = 4.8, 4.8$ Hz), 3.48 (2H, q, $J = 7.0$ Hz), 3.74 (2H, q, $J = 7.0$ Hz), 4.02-4.05 (1H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 11.8, 12.8, 24.6, 31.0, 41.1, 47.2, 49.3, 49.4, 193.2, 207.9

Table 1, Entry 39: ^1H NMR (500 MHz, CDCl_3) δ 1.93-2.05 (4H, m), 3.58-4.02 (6H, m), 5.83 (1H, dd, $J = 4.4, 4.4$ Hz), 7.27-7.56 (8H, m), 8.00 (2H, d, $J = 7.3$ Hz); ^{13}C NMR (125 MHz; CDCl_3) δ 24.6, 26.5, 51.0, 54.6, 55.3, 128.0, 128.6, 128.8, 129.0, 129.4, 133.6, 137.0, 140.0, 191.5, 197.4.

Table 1, Entry 40: ^1H NMR (500 MHz, CDCl_3) δ 1.26-1.31 (6H, m), 3.68-4.21 (6H, m), 5.76 (1H, dd, $J = 4.1, 4.1$ Hz), 7.24-7.69 (8H, m), 8.00-8.01 (2H, m); ^{13}C NMR (125 MHz; CDCl_3) δ 127.9, 128.5, 128.7, 129.1, 129.6, 134.1, 137.6, 140.8, 190.8, 197.4.

a-196 1H NMR in CDCl3 at 298 K 84/8/24

Table 1 Entry 2

Current Data Parameters
NAME AZ121
EXPNO 63
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051115
Time 15.06
INSTRUM spect
PROBHD 5 mm BBI 1H-9B
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 2
SWH 10000.000 Hz
FIDRES 0.306176 Hz
AQ 1.6385000 sec
RG 5
DM 50.000 usec
DE 6.50 usec
TE 291.1 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 2.00 dB
SFO1 500.130095 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 18.00 cm
CY 12.41 cm
F1P 10.253 ppm
F1 5127.98 Hz
F2P 0.015 ppm
F2 7.37 Hz
PPMCK 0.56981 ppm/cm
HZCK 284.47958 Hz/cm

Table 1, Entry 3

a-205 ¹HNMR in CDCl₃ at 298 K 84/8/24

Current Data Parameters
NAME AZ11
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051115
Time 14.51
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 4
DS 2
SWH 10000.000 Hz
FIDRES 0.305175 Hz
AQ 1.6395000 sec
RG 5
DM 50.000 usec
DE 6.50 usec
TE 293.0 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 10.30 usec
PL1 2.00 dB
SF01 500.130085 MHz

F2 - Processing parameters
SI 32768
SF 500.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 18.00 cm
CY 15.36 cm
F1P 3.805 ppm
F1 1902.82 Hz
F2P 1.517 ppm
F2 788.46 Hz
PPMCK 0.12373 ppm/cm
HZCM 61.50866 Hz/cm

g-205 130NMR in CDCl3 at 298 K 04/0/24

Table 1 Entry 3

Current Data Parameters
NAME: g-205
EXPNO: 60
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 0005115
Time : 14.53
INSTRUM: spect
PROBHD: 5 mm BBI 1H-BB
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 38
DS: 2
SWH: 40000.000 Hz
FIDRES: 0.161258 Hz
AQ: 0.161258 sec
RG: 32768
GB: 3
PC: 12.500 usec
DE: 6.50 usec
TE: 293.15 K
D1: 3.00000000 sec
d11: 0.03000000 sec
DELTA: 2.90000010 sec
WDELT: 0.03000000 sec
KORST: 0.01000000 sec

===== CHANNEL f2 =====
NUC1: 13C
P1: 10.50 usec
PL1: 0.00 dB
SFO1: 125.760343 MHz

===== CHANNEL f1 =====
NUC2: 1H
P2: 67.00 usec
PL2: 0.00 dB
SFO2: 500.130000 MHz

F2 - Processing parameters
SI: 32768
SF: 125.760343 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR data parameters
EX: 30.00 sec
C1: 12.21 sec
F1p: 200.810 GHz
T1: 200.000 usec
F2p: 500.130 MHz
H2: 145.75 Hz
SFOH: 125.760343 MHz
SFOH: 500.130000 MHz

a-200 ¹HNMR in CDCl₃ at 298 K 84/8/24

Table 1 Entry 4

Current Data Parameters
NAME A2121
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051115
Time 15.25
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 2
SWH 10000.000 Hz
FIDRES 0.306176 Hz
AQ 1.636500 sec
RG 3.6
DM 50.000 usec
DE 6.50 usec
TE 291.1 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCNCR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 2.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 18.00 cm
CY 15.52 cm
F1P 10.166 ppm
F1 5084.12 Hz
F2P -0.161 ppm
F2 -80.35 Hz
FREQM 0.57366 ppm/cm
HZCM 286.91522 Hz/cm

8-200 13C NMR in CDCl3 at 298 K B4/B/24

Table 1 Eentry 4

Current Data Parameters
NAME Az121
EXPNO 70
PROCNO 1
F2 - Acquisition Parameters
Date_ 20051127
Time 15:27
INSTRUM spect
PROBHD 5 mm BBI 1H-13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29
DS 2
SWH 42000.000 Hz
FIDRES 0.610362 Hz
AQ 0.610362 sec
RG 327.500
DWDW 12.500
DE 5.50 usec
TE 291.2 K
D1 3.00000000 sec
D11 0.03000000 sec
DELTA 2.90000010 sec
DELT14 0.00000000 sec
ACQRES 0.01000000 sec
MCLOCK 0.01000000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
SFO1 125.7703143 MHz
----- CHANNEL f2 -----
GPROG2 waltz16
NUC2 1H
P2 9.70 usec
PL2 -6.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577580 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
SD NMR 210C parameters:
CX 20.00 cm
CY 12.81 cm
F1P 416.455.000 MHz
F2P 200.141.910 MHz
F3P 200.141.910 MHz
F4P 200.141.910 MHz
PCW 363.31 Hz
PWCW 10.00000000 Hz/cm
H2CW 13379.106889 Hz/cm

197 JHNMR in CDCl₃ at 298K 84/9/28

Table 1 Entry 5

Current Data Parameters
NAME Az121
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date 20051220
Time 16.11
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 8
DS 0
SWH 10030.578 Hz
FIDRES 0.315544 Hz
AQ 1.2860595 sec
RG 71.8
DM 48.400 usec
DE 6.50 usec
TE 293.2 K
D1 2.00000000 sec
WDELTA 0.00000000 sec
WDELT 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 10.30 usec
PL1 2.00 dB
SFO1 500.130000 MHz

F2 - Processing parameters
SI 32768
SF 500.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR data parameters
CX 18.40 cm
CY 11.64 cm
F1P 9.726 ppm
F1 4064.07 Hz
F2P 1.934 ppm
F2 567.05 Hz
FREQM 0.43285 ppm/cm
HZCM 218.5045 Hz/cm

Table 1 Entry 7

Current Data Parameters

NAME	A2121
EXPNO	57
PROCNO	1

F2 - Acquisition Parameters

Date_	20051115
Time	14.46
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zg
TD	32768
SOLVENT	DMSO
NS	4
DS	2
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	1.6365000 sec
RG	5
DM	50.000 usec
DE	6.50 usec
TE	291.0 K
D1	3.00000000 sec
MCHEST	0.00000000 sec
KCMR	0.01500000 sec

===== CHANNEL f1 =====

NUC1	1H
P1	10.30 usec
PL1	2.00 dB
SFO1	500.1330885 MHz

F2 - Processing parameters

SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	18.00 cm
CY	14.85 cm
F1P	9.047 ppm
F1	4824.91 Hz
F2P	0.089 ppm
F2	20.30 Hz
POWCK	0.49336 ppm/cm
HZCM	249.75036 Hz/cm

B-204 130NMH in CDCl3 at 298 K 84/8/24

Table 1 Entry 7

Current Data Parameters
NAME: A111
TYPE: 50
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20011125
Time_: 14:17
INSTRUM: spect
PROBHD: 5 mm BBI 1H-50
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 31
DS: 2
SWH: 40000.000 Hz
FIDRES: 0.610100 Hz
AQ: 0.619000 sec
RG: 2560.3
DM: 12.5000 sec
DE: 6.5000000
TE: 291.2 K
D1: 3.00000000 sec
D11: 0.05000000 sec
DELTA: 2.50000010 sec
DELTA: 0.00000000 sec
MPCST: 0.01500000 sec
MORF: 0.01500000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 125.761140 MHz
----- CHANNEL f2 -----
DIAPHR: IR

CTDPRG2: M011218
NAC2: 1H
PCPRG2: 87.00 usec
PL2: -6.00 dB
PL12: 12.00 dB
PL13: 12.00 dB
SFO2: 500.135000 MHz
F2 - Processing parameters
SI: 32768
SF: 125.767700 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
SD NMR F1 F2 Parameters
EX 20.00 cm
CX 12.21 cm
CY 2.14 usec
CZ 2.14 usec
F1 500.135000 MHz
F2 125.767700 MHz
F3 -40.16 Hz
F4 11.7431100000 Hz
F5 1412.47331 Hz/Hz

232 ¹H NMR in CDCl₃ at 298 K 84/9/12

Table 1 Entry 28

Current Data Parameters
NAME AZ121
EXPNO 103
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051203
Time 13.49
INSTRUM spect
PROBHD 5 mm BB1 1H-9B
PULPROG zg
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.305178 Hz
AQ 1.6386000 sec
RG 6.3
DM 50.000 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
MCHEST 0.00000000 sec
MCNKR 0.01500000 sec

***** CHANNEL f1 *****
NUC1 ¹H
P1 10.30 usec
PL1 2.00 dB
SFO1 500.1330085 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 16.00 cm
CY 16.16 cm
F1P 8.807 ppm
F1 4404.88 Hz
F2P -0.084 ppm
F2 -42.02 Hz
PPMCM 0.49387 ppm/cm
HZCM 247.05013 Hz/cm

232 13C NMR in CDCl₃ at 298 K B4/S/12

Table 1 Entry 28

233 1H NMR in CDCl3 at 298 K 84/9/12

Current Data Parameters

NAME	AZ121
EXPNO	37
PROCNO	1

F2 - Acquisition Parameters

Date_	20051203
Time	13.28
INSTRUM	spect
PROBHD	5 mm BBI 1H-9B
PULPROG	zg
TD	32768
SOLVENT	DMF50
NS	4
DS	1
SWH	10000.000 Hz
FIDRES	0.305176 Hz
AQ	1.638500 sec
RG	6.3
DM	50.000 usec
DE	6.50 usec
TE	291.6 K
D1	2.0000000 sec
WREST	0.0000000 sec
WOMRK	0.01500000 sec

===== CHANNEL f1 =====

NUC1	1H
P1	10.30 usec
PL1	2.00 dB
SFO1	500.130085 MHz

F2 - Processing parameters

SI	32768
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	18.00 cm
CY	16.15 cm
F1P	10.864 ppm
F1	5633.64 Hz
F2P	0.049 ppm
F2	24.35 Hz
PPMCK	0.60088 ppm/cm
HZCM	300.51624 Hz/cm

233 130NMR in CDCl3 at 298 K 84/9/12

Current Data Parameters

NAME	Az121
EXPNO	98
PROCNO	1

F2 - Acquisition Parameters

Date_	20051203
Time	13.31
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	35
DS	3
SWH	40000.000 Hz
FIDRES	0.010352 Hz
AQ	0.019525 sec
RG	2560.3
DM	12.500 usec
DE	6.50 usec
TE	292.2 K
D1	3.0000000 sec
d11	0.0300000 sec
DELTA	2.0000000 sec
DELTA2	0.0000000 sec
MCLOCK	0.01560000 sec

===== CHANNEL f1 =====

NUC1	13C
P1	10.50 usec
PL1	0.00 dB
SFO1	125.770143 MHz

===== CHANNEL f2 =====

CPDPRG2	zgpg30
NUC2	1H
PCPD2	87.00 usec
PL2	-6.00 dB
PL12	12.00 dB
PL13	12.00 dB
SFO2	500.130000 MHz

F2 - Processing parameters

SI	32768
SS	125.757750 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

IX	20.00 cm
QX	1.00 cm
F1P	222.088 ppm
F2P	27929.28 Hz
F2P	-3.096 ppm
FPMCK	-389.31 Hz
HZCM	11.25918 ppm/cm
HZCM	1415.92820 Hz/cm

Table 1 Entry 32

Current Data Parameters
NAME: A2121
EXPNO: 30
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20051220
Time: 16.17
INSTRUM: spect
PROBHD: 5 mm BBI 1H-BB
PULPROG: zgpg30
TD: 4030
SOLVENT: CDCl₃
NS: 0
DS: 0
SWH: 10330.578 Hz
FIDRES: 0.315264 Hz
AQ: 1.586026 sec
RG: 11.0
DN: 48.400 usec
DE: 0.50 usec
TE: 293.1 K
D1: 2.00000000 sec
MDELST: 0.00000000 sec
MDELK: 0.01500000 sec
F2 - Processing parameters
CH1: 1H
NUC1: 1H
P1: 10.30 usec
PL1: 2.00 dB
SFO1: 500.135095 MHz
F2 - Processing parameters
SI: 32768
SF: 500.1350000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
F2 - NMR plot parameters
CX: 18.00 cm
CY: 11.84 cm
F1P: 10.321 ppm
F1: 5186.51 Hz
F2P: -0.095 ppm
F2: 42.56 Hz
FREQCK: 0.58146 ppm/Hz
FTOL: 290.80374 Hz/cm

241 1HMR in CDCl3 at 298K 84/9/28

Table 1 Entry 37

Current Data Parameters
NAME Az121
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20031219
Time 8.08
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860595 sec
RG 16
DM 49.400 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
MCHREST 0.00000000 sec
MCHRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 2.00 dB
SFO1 500.1330085 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 16.00 cm
CY 11.54 cm
F1p 10.878 ppm
F1 5440.56 Hz
F2p -0.210 ppm
F2 -105.21 Hz
PPMCK 0.61604 ppm/cm
HZCM 308.03824 Hz/cm

Table 1 Entry 39

400 MHz CDCl₃ at 298K 04/9/28

ppm

Current Data Parameters
NAME Az121
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081220
Time 15:59
INSTRUM spect
PROBHD 5 mm BBI 1H-13C
PULPROG zgpg30
TO 30758
SOLVENT CDCl₃
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.318564 Hz
AQ 1.5880856 sec
RG 161.3
DM 48.400 usec
DE 8.50 usec
TE 291.1 K
D1 2.00000000 sec
MCREST 0.00000000 usec
MCWPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 2.00 dB
SFO1 500.1330685 MHz

F2 - Processing parameters
SI 32768
SF 500.1330685 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13 NMR p10t parameters
CX 18.00 cm
CY 7.83 cm
F1P 10.440 ppm
F1 5321.45 Hz
F2P 0.020 ppm
F2 10.09 Hz
RGWCK 0.57899 ppm/cm
HZCK 298.32758 Hz/cm

224 13C NMR in CDCl3 at 298K BA/9/28

Table 1 Entry 39

Current Data Parameters
 Name: 224 13C NMR
 Date: 09/28
 Time: 11:00
 F2 - Acquisition Parameters
 Date_: 20051220
 Time: 16:02
 Instrument: spect
 Processed: 16 mm HLL 1H 80
 PULPROG: zgpg30
 TD: 65536
 SO: 2
 EX: 125.130 MHz
 NS: 2
 DS: 4
 SWH: 40000.000 MHz
 FIDRES: 0.1617052 MHz
 AQ: 0.8119026 SEC
 RG: 6560.3
 DW: 12.000 usec
 DE: 6.50 usec
 TE: 300.2 K
 D1: 3.0000000 SEC
 d11: 0.0500000 SEC
 DELTA: 2.0000000 SEC
 WDELT: 0.0000000 SEC
 KICK: 0.0100000 SEC

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 10.00 usec
 PL1: 0.00 dB
 SFO: 125.130143 MHz

===== CHANNEL f2 =====
 NUC2: 1H
 P2: 0.00 usec
 PL2: 0.00 dB
 SFO: 500.136000 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.27290 MHz
 DS: 4
 SW: 0
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR 2D NMR parameters
 EX: 40.00 C°
 CY: 15.21 C°
 F1P: 200.272 MHz
 F2P: 500.136 MHz
 F3: 500.136 MHz
 F4: 500.136 MHz
 F5: 500.136 MHz
 F6: 500.136 MHz
 F7: 500.136 MHz
 F8: 500.136 MHz
 F9: 500.136 MHz
 F10: 500.136 MHz
 F11: 500.136 MHz
 F12: 500.136 MHz
 F13: 500.136 MHz
 F14: 500.136 MHz
 F15: 500.136 MHz
 F16: 500.136 MHz
 F17: 500.136 MHz
 F18: 500.136 MHz
 F19: 500.136 MHz
 F20: 500.136 MHz
 F21: 500.136 MHz
 F22: 500.136 MHz
 F23: 500.136 MHz
 F24: 500.136 MHz
 F25: 500.136 MHz
 F26: 500.136 MHz
 F27: 500.136 MHz
 F28: 500.136 MHz
 F29: 500.136 MHz
 F30: 500.136 MHz
 F31: 500.136 MHz
 F32: 500.136 MHz
 F33: 500.136 MHz
 F34: 500.136 MHz
 F35: 500.136 MHz
 F36: 500.136 MHz
 F37: 500.136 MHz
 F38: 500.136 MHz
 F39: 500.136 MHz
 F40: 500.136 MHz
 F41: 500.136 MHz
 F42: 500.136 MHz
 F43: 500.136 MHz
 F44: 500.136 MHz
 F45: 500.136 MHz
 F46: 500.136 MHz
 F47: 500.136 MHz
 F48: 500.136 MHz
 F49: 500.136 MHz
 F50: 500.136 MHz
 F51: 500.136 MHz
 F52: 500.136 MHz
 F53: 500.136 MHz
 F54: 500.136 MHz
 F55: 500.136 MHz
 F56: 500.136 MHz
 F57: 500.136 MHz
 F58: 500.136 MHz
 F59: 500.136 MHz
 F60: 500.136 MHz
 F61: 500.136 MHz
 F62: 500.136 MHz
 F63: 500.136 MHz
 F64: 500.136 MHz
 F65: 500.136 MHz
 F66: 500.136 MHz
 F67: 500.136 MHz
 F68: 500.136 MHz
 F69: 500.136 MHz
 F70: 500.136 MHz
 F71: 500.136 MHz
 F72: 500.136 MHz
 F73: 500.136 MHz
 F74: 500.136 MHz
 F75: 500.136 MHz
 F76: 500.136 MHz
 F77: 500.136 MHz
 F78: 500.136 MHz
 F79: 500.136 MHz
 F80: 500.136 MHz
 F81: 500.136 MHz
 F82: 500.136 MHz
 F83: 500.136 MHz
 F84: 500.136 MHz
 F85: 500.136 MHz
 F86: 500.136 MHz
 F87: 500.136 MHz
 F88: 500.136 MHz
 F89: 500.136 MHz
 F90: 500.136 MHz
 F91: 500.136 MHz
 F92: 500.136 MHz
 F93: 500.136 MHz
 F94: 500.136 MHz
 F95: 500.136 MHz
 F96: 500.136 MHz
 F97: 500.136 MHz
 F98: 500.136 MHz
 F99: 500.136 MHz
 F100: 500.136 MHz