SUPPORTING INFORMATION

Catalyst-free chemoselective *N*-*tert*-butyloxycarbonylation of amines in water

Sunay V. Chankeshwara and Asit K. Chakraborti*

National Institute of Pharmaceutical Education and Research (NIPER),
Sector 67, S. A. S. Nagar, Punjab – 160062, India. Fax +91(172)2214692.
E-mail: akchakraborti@niper.ac.in

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Aniline Vs Benzylamine: GCMS (crude product)	S49; S50
(S)-(a)-Methylbenzylamine Vs	
(S)- Phenylglycinemethyl ester: ^1H NMR (crude product)	S51
(S)-(a)-Methylbenzylamine Vs	
(S)- Phenylalaninol: ^1H NMR (crude product)	S52

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: IR (crude product) S54

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and pure product) S55: Comparative IR (*N*-Boc-dicyclohexylamine;
N-Boc-cyclohexylamine crude and pure product) S56**Experimental** S57

NAME	PQ
EXPNO	40
PROCNO	1

F2 - Acquisition Parameters

Date_	20041005
Time	14.45
INSTRUM	dpx300
PROBHD	5 mm GNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	16
DM	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPMCM	0.45333 ppm/cm
HZCM	136.05893 Hz/cm

NHBoc

Table 1, Entry 1

Table 1, Entry 1

Current Data Parameters
NAME CO
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041005
Time 15.02
INSTRUM gpc300
PROBHD 5 mm GNP 1H
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1909
DS 0
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 11585.2
DN 22.050 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec

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

NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 75.4782545 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
SFO2 300.1313735 MHz

F2 - Processing parameters

SI 16384
SF 75.4677517 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
F1P 170.000 ppm
F1 12829.52 Hz
F2P -2.000 ppm
F2 -150.94 Hz
PPNOM 7.81818 ppm/cm
HZCM 590.02057 Hz/cm

ppm

Table 1, Entry 2

Table 1, Entry 2

Current Data Parameters
NAME CS
EXPNO 73
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040927
Time 9.51
INSTRUM dpx300
PROBHD 5mm GNP 1H
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2880
DS 0
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 11585.2
DW 22.000 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SFO1 75.4782845 MHz

===== CHANNEL f2 =====
PULPROG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
SFO2 300.1313735 MHz

F2 - Processing parameters
SI 16384
SF 75.4677503 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00

13 NMR plot parameters
CX 22.00 cm
F1P 200.000 ppm
F1 15093.55 Hz
F2P -2.000 ppm
F2 150.93 Hz
F1-HZ 300.1313735 MHz
F2-HZ 150.93 Hz

ppm

Table 1, Entry 3

Current Data Parameters
 NAME PD
 EXPNO 132
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20041223
 Time 12.32
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6313.131 Hz
 FIDRES 0.192661 Hz
 AQ 2.5952756 sec
 RG 35.9
 DH 79.200 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

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

NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
 SF 300.1300115 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 22.50 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.200 ppm
 F2 -60.03 Hz
 PPMCM 0.45333 ppm/cm
 HZCM 136.05893 Hz/cm

Current Data Parameters

NAME	P0
EXPNO	97
PROCNO	1

F2 - Acquisition Parameters

Date_	20041013
Time	14.08
INSTRUM	opx300
PROBHD	5 mm Multinu
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	4
DS	0
SWH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	35.9
OW	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	7.80 usec
PL1	-4.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	1096
SF	300.1300180 MHz
WDW	EM
SSB	0
LB	0.70 Hz
GB	0
PC	4.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPMCM	0.45333 ppm/cm
HZCM	136.05893 Hz/cm

ppm

Table 1 Entry 5

7.26051

6.86949

2.25231

2.22059

1.58274

1.49237

0.00000

Current Data Parameters
 NAME P0
 EXPNO 156
 PROCNO 1

F2 - Acquisition Parameters

Date 20041020
 Time 16.54
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6313.131 Hz
 FIDRES 0.192661 Hz
 AQ 2.5952756 sec
 RG 1149.4
 DW 79.200 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

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

NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SF01 300.1329005 MHz

F2 - Processing parameters

SI 8192
 SF 300.1300060 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

10 NMR plot parameters

CX 22.50 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.200 ppm
 F2 -60.03 Hz
 PPMCM 0.45333 ppm/cm
 HZCM 136.05893 Hz/cm

S10

ppm

Table 1 Entry 6

Current Data Parameters
 NAME PMAY
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060502
 Time 10.19
 INSTRUM dpx300
 PROBHD 5 mm GNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 11990.407 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 41.700 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SFO1 300.1329005 MHz

F2 - Processing parameters
 SI 8192
 SF 300.1300531 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07803 Hz/cm

s14

Table 1, Entry 7

Current Data Parameters

NAME PJ
EXPNO 76
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050110
Time 17.14
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6313.131 Hz
FIDRES 0.192661 Hz
AQ 2.5952756 sec
RG 128
DW 79.200 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

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

NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.40 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.45333 ppm/cm
HZCM 136.05893 Hz/cm

ppm

s 12

Table 1, Entry 7

Current Data Parameters
 NAME PJ
 EXPNO 124
 PROCNO 4

F2 - Acquisition Parameters

Date_ 20050117
 Time 10.35
 INSTRUM cpx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6313.131 Hz
 FIDRES 0.192661 Hz
 AQ 2.5952756 sec
 RG 456.1
 OH 79.200 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

----- CHANNEL f1 -----

NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SFO1 300.1329005 MHz

F2 - Processing parameters

SI 16384
 SF 300.1300051 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 22.50 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.200 ppm
 F2 -60.03 Hz
 PPMCM 0.45333 ppm/cm
 HZCM 136.05893 Hz/cm

ppm

Table 1, Entry 8

Current Data Parameters
 NAME
 EXPNO 87
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041215
 Time 12.27
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6313.131 Hz
 FIDRES 0.192661 Hz
 AQ 2.5952759 sec
 RG 181
 DW 79.200 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SFO1 300.1328731 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1311726 MHz
 NDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 10.000 ppm
 F1 3001.31 Hz
 F2P -0.200 ppm
 F2 -60.03 Hz
 PPMCM 0.45333 ppm/cm
 HZCM 136.05946 Hz/cm

Table 1, Entry 9

Current Data Parameters
NAME PN
EXPNO 184
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041122
Time 16.52
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6313.131 Hz
FIDRES 0.192661 Hz
AQ 2.5952756 sec
RG 128
DW 79.200 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters
SI 8192
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.50 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.54222 ppm/cm
HZCM 162.73715 Hz/cm

ppm

Table 1, Entry 10

Current Data Parameters

NAME	PMAY
EXPNO	7
PROCNO	1

F2 - Acquisition Parameters

Date_	20060502
Time	10.04
INSTRUM	dpx300
PROBHD	5 mm GNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	0
SWH	11990.407 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	228.1
DW	41.700 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300505 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	11.000 ppm
F1	3301.43 Hz
F2P	-1.000 ppm
F2	-300.13 Hz
PPMCM	0.60000 ppm/cm
HZCM	180.07802 Hz/cm

Integral

Table 1, Entry 11

Table 1, Entry 13

Current Data Parameters
NAME PHAY
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060502
Time 10.08
INSTRUM dpx300
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT b
NS 16
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 57
DW 41.700 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters
SI 8192
SF 300.1300505 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.60000 ppm/cm
HZCM 180.07802 Hz/cm

ppm

Table 1, Entry 13

Chemical shift values (ppm) for the compound:

- 155.368
- 137.646
- 132.308
- 129.135
- 128.502
- 128.060
- 121.117
- 115.825
- 80.796
- 78.113
- 77.690
- 77.266
- 70.882
- 28.965

Current Data Parameter
NAME C
EXPNO
PROCNO

F2 - Acquisition Parameter
Date_ 20060
Time 10
INSTRUM dpx
PROBHD 5 mm QNP
PULPROG z
TD 32
SOLVENT CD
NS
DS
SWH 22675.
FIDRES 0.692
AQ 0.7225
RG 919
DN 22.
DE 4
TE 30
D1 2.00000
d11 0.03000

===== CHANNEL
NUC1
P1 6
PL1 -6
SF01 75.4777

===== CHANNEL
CPDPRG2 waltz
NUC2
PCPD2 100
PL2 120
PL12 17
SF02 300.1313

F2 - Processing parameter
SI 16
SF 75.4677
WDW
SSB
LB 3
GB
PC 1

1D NMR plot parameter
CX 22
F1P 240.
F1 18112
F2P -5.
F2 -377
PPMCH 10.86
HZCH 821.75

Current Data Parameters

NAME PMAY
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060501
Time 16.49
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 64
DW 41.700 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

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

NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
SF 300.1300740 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.60000 ppm/cm
HZCM 180.07803 Hz/cm

ppm

```

1D NMR plot parameters
CX          2
F1P         240
F1          1611
F2P         -5
F2          -37
PPMCM       10.8
HZCM        821.7

```

Table 1, Entry 15

Current Data Parameters

NAME	PC
EXPNO	8
PROCNO	1

F2 - Acquisition Parameters

Date_	20041001
Time	12.09
INSTRUM	gpc300
PROBHD	5 mm GNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	16
DW	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

===== CHANNEL #1 =====

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300173 MHz
WOW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	4.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPNCM	0.45333 ppm/cm
HZCM	136.05693 Hz/cm

ppm

Table 1, Entry 15

S24

Current Data Parameters
 NAME CD
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041001
 Time 12.12
 INSTRUM dpx300
 PROBHD 5 mm GNP 1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 128
 DS 0
 SWH 22675.736 Hz
 FIDRES 0.692009 Hz
 AQ 0.7225844 sec
 RG 1585.2
 OW 22.050 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 D11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 6.30 usec
 PL1 -6.00 dB
 SF01 75.4782845 MHz

===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 17.00 dB
 SF02 300.1313735 MHz

F2 - Processing parameters
 SI 16384
 SF 75.4677559 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 F1P 200.000 ppm
 F1 15093.55 Hz
 F2P -2.000 ppm
 F2 -150.94 Hz
 PRMCM 9.18182 ppm/cm
 HZCM 692.93121 Hz/cm

Table 1, Entry 16

NAME PA
EXPNO 83
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050408
Time 17.01
INSTRUM dpx300
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6313.131 Hz
FIDRES 0.192661 Hz
AQ 2.5952756 sec
RG 466.1
DW 79.200 usec
DE 4.50 usec
TE 300.0 K
D1 0.1000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
SF 300.1300049 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 2.00

1D NMR plot parameters

CX 22.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.45333 ppm/cm
HZCM 136.05893 Hz/cm

Table 1, Entry 17

Current Data Parameters

NAME	PA
EXPNO	72
PROCNO	1

F2 - Acquisition Parameters

Date_	20050408
Time	15.10
INSTRUM	gpc300
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	0
SWH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	406.4
DW	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300058 MHz
WDW	EM
SSB	0
LB	0.40 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPMCM	0.45333 ppm/cm
HZCM	136.05893 Hz/cm

Table 1, Entry 18

Current Data Parameters
NAME PS
EXPNO 174
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040927
Time 14.19
INSTRUM opx300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 4
DS 0
SWH 6313.131 Hz
FIDRES 0.192661 Hz
AQ 2.5952756 sec
RG 57
OW 79.200 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters
SI 16384
SF 300.1300102 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.45333 ppm/cm
HZCM 136.05893 Hz/cm

Table 1, Entry 18

Table 1, Entry 19

NAME	PN
EXPNO	103
PROCNO	1

F2 - Acquisition Parameters

Date_	20041109
Time	17.09
INSTRUM	dpx300
PROBHD	5 mm Multinu
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	18
DW	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	16384
SF	300.1299872 MHz
WDM	EM
SSB	0
LB	0.20 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPMCM	0.45333 ppm/cm
HZCM	136.05891 Hz/cm

N
Boc

Table 1, Entry 20

ppm

Table 1, Entry 21

Current Data Parameters

NAME	PQ
EXPNO	131
PROCNO	1

F2 - Acquisition Parameters

Date_	20041223
Time	12.29
INSTRUM	gpx300
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	35.9
DW	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1299912 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPMCM	0.45333 ppm/cm
HZCM	136.05893 Hz/cm

ppm

N
Boc

Table 1, Entry 21

154.885

79.030
77.460
77.035
76.612

44.533

28.409
25.675
24.436

ppm

160

140

120

100

80

60

40

20

S32

ppm

Table 1, Entry 22

7.31352

3.64743
3.63221
3.61510
3.41955
3.40278
3.38753

1.46495

Integral

0.2674

4.0738

4.0341

8.9954

S33

Current Data Parameters
NAME PN
EXPNO 104
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041109
Time 17.15
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6313.131 Hz
FIDRES 0.192661 Hz
AQ 2.5952756 sec
RG 18
DM 79.200 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters

SI 16384
SF 300.1299899 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00

1D NMR plot parameters

CX 22.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.45333 ppm/cm
HZCM 136.05893 Hz/cm

ppm

NHBoc

Table 1, Entry 23

5.04144
3.71897
3.70630
3.69219
3.24458
3.22790
2.45803
1.45663

Integral

1.000
4.904
2.555
7.871
10.907

ppm

10

8

6

S34

4

2

0

Current Data Parameters

NAME PMAY
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060502
Time 9.03
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 40.3
DW 41.700 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

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

NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
SF 300.1300394 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.60000 ppm/cm
HZCM 180.07802 Hz/cm

ppm

Table 1, Entry 23

S35

Current Data Parameters
 NAME CAPR
 EXPNO 100
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060418
 Time 10.15
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H
 PULPROG zgdc
 TD 32768
 SOLVENT CDCl3
 NS 284
 DS 0
 SWH 22675.736 Hz
 FIDRES 0.692009 Hz
 AQ 0.7225844 sec
 RG 8192
 DW 22.050 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 6.30 usec
 PL1 -6.00 dB
 SF01 75.4777562 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 17.00 dB
 SF02 300.1313735 MHz

F2 - Processing parameters
 SI 16384
 SF 75.4677190 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 240.000 ppm
 F1 18112.25 Hz
 F2P -5.000 ppm
 F2 -377.34 Hz
 PPMCH 12.25000 ppm/cm
 HZCH 924.47955 Hz/cm

ppm

Table 1, Entry 24

Current Data Parameters

NAME PMAY
EXPNO 183
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060524
Time 14.33
INSTRUM dpx300
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 7485.030 Hz
FIDRES 0.228425 Hz
AQ 2.1889524 sec
RG 812.7
DW 66.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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

NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters

SI 16384
SF 300.1300516 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.60000 ppm/
HZCM 180.07803 Hz/c

1.93839
1.90328
1.71680
1.67188
1.65200
1.61041
1.59583
1.57031
1.44263
1.34996
1.30872
1.26638
1.15329
1.11324
1.07395
0.00000

Integral

1.000

0.965

1.435

2.891

5.192

12.763

2.011

0.857

3.765

ppm

10

8

6

4

2

0

S37

ppm

7.8248

7.2650

1.7811
1.7407
1.5839
1.4731
1.3060
1.2611
1.1289
1.0860
1.0424
0.0001

Table 1, Entry 25

S39

Current Data Parameters

NAME	PMAY
EXPNO	196
PROCNO	1

F2 - Acquisition Parameters

Date_	20060524
Time	17.16
INSTRUM	dpx300
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	7485.030 Hz
FIDRES	0.228425 Hz
AQ	2.1889524 sec
RG	1625.5
DW	66.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SF01	300.1324010 MHz

F2 - Processing parameters

SI	16384
SF	300.1300526 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	11.000 ppm
F1	3301.43 Hz
F2P	-1.000 ppm
F2	-300.13 Hz
PPMCM	0.60000 ppm/
HZCM	180.07803 Hz/c

Table 1, Entry 25

ppm

Table 1, Entry 26

Current Data Parameters
 NAME PMAY
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060502
 Time 12.55
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 11990.407 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 40.3
 DW 41.700 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SFO1 300.1329005 MHz

F2 - Processing parameters
 SI 8192
 SF 300.1300359 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07802 Hz/cm

Table 1, Entry 26

Table 1, Entry 27

NAME PS
EXPNO 191
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040929
Time 15.03
INSTRUM dpx300
PROBHD 5 mm GNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 8
DS 0
SWH 6313.131 Hz
FIDRES 0.192661 Hz
AQ 2.5952756 sec
RG 40.3
DW 79.200 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters
SI 8192
SF 300.1300108 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.45333 ppm/cm
HZCM 136.05893 Hz/cm

Table 1, Entry 27

Current Data Parameters
NAME CS
EXPNO 92
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040929
Time 15.08
INSTRUM dpx300
PROBHD 5 mm GNP 1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 240
DS 0
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 11585.2
DN 22.050 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 6.30 usec
PL1 -6.00 dB
SF01 75.4782645 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
SF02 300.1313735 MHz

F2 - Processing parameters
SI 16384
SF 75.4677572 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 200.000 ppm
F1 15093.55 Hz
F2P -2.000 ppm
F2 -150.93 Hz
PPMCM 9.18182 ppm/cm
HZCM 692.93121 Hz/cm

Current Data Parameters

NAME	PA
EXPNO	71
PROCNO	1

F2 - Acquisition Parameters

Date_	20050408
Time	15.06
INSTRUM	gpx300
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SHH	6313.131 Hz
FIDRES	0.192661 Hz
AQ	2.5952756 sec
RG	101.6
DW	79.200 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300058 MHz
WDW	EM
SSB	0
LB	0.40 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.50 cm
F1P	10.000 ppm
F1	3001.30 Hz
F2P	-0.200 ppm
F2	-60.03 Hz
PPMCM	0.45333 ppm/cm
HZCM	136.05893 Hz/cm

Current Data Parameters
 NAME PMAY
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060502
 Time 8.52
 INSTRUM dpx300
 PROBHD 5 mm GNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 11990.407 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 90.5
 DW 41.700 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SF01 300.1329005 MHz

F2 - Processing parameters
 SI 8192
 SF 300.1300523 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07803 Hz/cm

Current Data Parameters

NAME PMAY
EXPNO 119
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060505
Time 15.31
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 90.5
DW 41.700 usec
DE 4.50 usec
TE 300.0 K
D1 0.10000000 sec

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

NUC1 1H
P1 11.00 usec
PL1 -6.00 dB
SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
SF 300.1300495 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.60000 ppm/cm
HZCM 180.07802 Hz/cm

Current Data Parameters

NAME	PMAR
EXPNO	171
PROCNO	1

F2 - Acquisition Parameters

Date_	20060310
Time	10.15
INSTRUM	dpx300
PROBHD	5 mm GNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	8992.806 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	203.2
DW	55.600 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300530 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	11.000 ppm
F1	3301.43 Hz
F2P	-1.000 ppm
F2	-300.13 Hz
PPMCM	0.60000 ppm/c
HZCM	180.07803 Hz/cm

Scheme 2: Intermolecular competition between Aniline and Benzylamine

Sample : svc1
 ID :
 Type : Unknown
 Operator :
 Method File Name : SHA4-EI.MET

*** Chromatogram ***

*** Peak Report ***

PKNO	R.Time	I.Time	F.Time	Area	Height	A/H(sec)	MK	%Total	Name
1	3.093	3.025	3.275	10590697	2533644	4.180		1.00	
2	6.778	6.592	6.925	188038652	42679101	4.406		17.68	
3	7.182	7.092	7.475	73816796	33190183	2.224		6.94	
4	7.631	7.575	7.892	3548988	639257	5.552		0.33	
5	11.326	11.175	11.425	214886516	67785735	3.170		20.21	
6	11.707	11.525	12.008	569091760	96905052	5.873		53.52	
7	12.545	12.442	12.725	3309089	860500	3.846		0.31	
Total				1063282497				100.00	

PKNO : 2 Peak # : 13 Ret. Time : 6.783
 Scan # : 527
 Base Peak : 93 (14729648)

PKNO : 3 Peak # : 23 Ret. Time : 7.183
Scan # : 575
Base Peak : 105 (16107074)

PKNO : 4 Peak # : 16 Ret. Time : 7.633
Scan # : 629
Base Peak : 42 (373674)

PKNO : 5 Peak # : 33 Ret. Time : 11.333
Scan # : 1073
Base Peak : 56 (30459336)

PKNO : 6 Peak # : 30 Ret. Time : 11.708
Scan # : 1118
Base Peak : 56 (35545616)

Current Data Parameters
 NAME PMAY
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20060502
 Time 10.25
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 11990.407 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 203.2
 DW 41.700 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.10000000 sec

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

NUC1 1H
 P1 11.00 usec
 PL1 -6.00 dB
 SFO1 300.1329005 MHz

F2 - Processing parameters

SI 8192
 SF 300.1300483 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07802 Hz/cm

Current Data Parameters

NAME	PMAY
EXPNO	29
PROCNO	1

F2 - Acquisition Parameters

Date_	20060502
Time	15.24
INSTRUM	dpx300
PROBHD	5 mm GNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	0
SWH	11990.407 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	128
DW	41.700 usec
DE	4.50 usec
TE	300.0 K
D1	0.10000000 sec

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

NUC1	1H
P1	11.00 usec
PL1	-6.00 dB
SFO1	300.1329005 MHz

F2 - Processing parameters

SI	8192
SF	300.1300523 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	11.000 ppm
F1	3301.43 Hz
F2P	-1.000 ppm
F2	-300.13 Hz
PPMCM	0.60000 ppm/cm
HZCM	180.07803 Hz/cm

Current Data Parameters
 NAME PMAY
 EXPNO 155
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060523
 Time 10.02
 INSTRUM dpx300
 PROBHD 5 mm GNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7485.030 Hz
 FIDRES 0.228425 Hz
 AQ 2.1889524 sec
 RG 181
 DW 66.800 user
 DE 6.00 user
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 user
 PL1 -6.00 dB
 SF01 300.1324010 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300514 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/
 HZCM 180.07803 Hz/c

c:\pel_data\spectra\5-24-svcdycy.001

c:\pel_data\spectra\5-24-svccy.001

c:\pel_data\spectra\5-24-svcdcy.001
c:\pel_data\spectra\5-24-svccy.001
c:\pel_data\spectra\5-24-svcdcy.001

Experimental

General details

The ^1H and ^{13}C NMR spectra were recorded on 300 MHz spectrometer in CDCl_3 using TMS as internal standard. The IR spectra were recorded as KBr pellets for solid samples and neat for liquid samples. The reactions were monitored by TLC (Merck). MS spectral data were recorded on EI and APCI. Evaporation of solvents was performed at reduced pressure, using a rotary evaporator.

Typical procedure for *N-tert*-butoxycarbonylation of amines:

Reaction with liquid amine. Phenyl-carbamic acid *tert*-butyl ester (Table 1, Entry 1): To a magnetically stirred mixture of aniline (0.235 g, 2.5 mmol) in water (2.5 mL) was added $(\text{Boc})_2\text{O}$ (0.60 g, 2.75 mmol, 1.1 equiv) at room temperature (30-35°C). Transperant liquid droplets were formed and after stirring the reaction mixture a white emulsion appeared on the surface of the walls of the reaction vessel with slow effervescence. A white solid settled down and indicated completion of the reaction (30 min: TLC, IR), the supernatant water was decanted off. Water (2×5 mL) was added to the solid residue, the mixture was stirred for a few minutes, and after each addition, the water was decanted off. The residue was dried under vacuum to provide the desired product as a white solid, 0.46 g, 95 %, Mp: 132-133°C. IR (KBr) ν : 1689 cm^{-1} . ^1H NMR (300 MHz, CDCl_3) δ : 1.51 (s, 9H), 6.55 (bs, 1H), 6.99-7.04 (m, 1H), 7.24-7.36 (m, 4H); ^{13}C NMR (CDCl_3 , 75 MHz) δ : 28.3, 80.4, 118.5, 122.9, 128.9, 138.3, 152.7. MS (ESI): m/z = 193 (M^+), identical with those of an authentic sample of phenyl-carbamic acid *tert*-butyl ester.¹

Reaction with solid amine. 4-Benzyloxyphenyl)carbamic acid *tert*-butyl ester (Table 1, Entry 13): To a magnetically stirred suspension of 4-benzyloxy aniline (0.5 g, 2.5 mmol) in water (2.5 mL) was added $(\text{Boc})_2\text{O}$ (0.60 g, 2.75 mmol, 1.1 equiv) at rt (30-35°C). A clear solution was formed with concomitant slow effervescence. After stirring the reaction mixture for some time transperant liquid droplets appeared that were converted to a white emulsion on further stirring. Finally a white solid settled down and indicated completion of the reaction (60 min: TLC, IR), the supernatant water was

¹ Bartoli, G.; Bosco, M.; Locatelli, M.; Marcantoni, E.; Massaccesi, M.; Melchiorre, P.; Sambri, L. *Synlett* **2004**, 1794.

decanted off. Water (2 × 5 mL) was added to the solid residue, the mixture was stirred for a few minutes, and after each addition, the water was decanted off. The residue was dried under vacuum to provide the desired product as a off-white solid, yield 90 %; Mp: 114-115 °C. IR (KBr) ν : 3428, 3294, 2986, 1696, 1590, 1527, 1450, 1326, 1228, 1152, 1055, 750 cm^{-1} . ^1H NMR (CDCl_3 , 300 MHz) δ : 1.55 (s, 9H), 5.04 (s, 2H), 6.54 (bs, 1H), 6.93 (d, J = 8.33 Hz, 2H), 7.28-7.46 (m, 6H); ^{13}C NMR (CDCl_3 , 75 MHz) δ : 28.9, 70.9, 80.8, 115.9, 121.1, 128.1, 128.5, 129.1, 132.3, 137.6, 153.8, 155.3. MS (EI): m/z 299 (M^+). Anal. Calcd. For (%) $\text{C}_{18}\text{H}_{21}\text{NO}_3$ C, 72.22; H, 7.07; N, 4.68. Found: C, 71.99; H, 7.14; N, 4.71.

The remaining reactions were carried out following this general procedure. In case of liquid products, the reaction mixture was extracted with EtOAc (2 × 5 mL), dried (Na_2SO_4) and evaporated to yield product. The physical data (mp, IR, NMR and MS) of all reported compounds were identical with those of the literature reports.

***p*-Tolyl-carbamic acid *tert*-butyl ester² (Table 1, Entry 2):** White Solid, yield 96 %; IR (KBr) ν : 1690 cm^{-1} ; ^1H NMR (CDCl_3 , 300 MHz) δ : 1.50 (s, 9H), 2.28 (s, 3H), 6.42 (bs, 1H), 7.08 (d, J = 7.8 Hz, 2H), 7.23 (d, J = 10.53 Hz, 2H); ^{13}C NMR (75 MHz) δ : 20.7, 28.3, 80.2, 118.6, 129.4, 132.5, 135.7, 152.9; MS (EI): m/z 207 (M^+).

***o*-Tolyl-carbamic acid *tert*-butyl ester³ (Table 1, Entry 3):** White Solid, yield 92 %; IR (KBr) ν : 1693 cm^{-1} ; ^1H NMR (CDCl_3 , 300 MHz) δ : 1.52 (s, 9H), 2.23 (s, 3H), 6.26 (bs, 1H), 6.95-7.06 (m, 1H), 7.11-7.20 (m, 2H), 7.78 (d, J = 7.5 Hz, 1H). MS (EI): m/z 207 (M^+).

(2, 4-Dimethylphenyl)carbamic acid *tert*-butyl ester³ (Table 1, Entry 4): White solid, yield 90 %; Mp: 84 - 85 °C; IR (KBr) ν : 1699 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ : 1.50 (s, 9H), 2.17 (s, 3H), 2.24 (s, 3H), 6.22 (bs, 1H), 6.95 (d, J = 11.4 Hz, 2H), 7.56 (d, J = 6.9 Hz, 1H). MS (EI): m/z 221 (M^+).

(2, 4, 6-Trimethyl-phenyl)-carbamic acid *tert*-butyl ester¹ (Table 1, Entry 5): White solid, yield 90 %; ^1H NMR (CDCl_3 , 300 MHz) δ : 1.49 (s, 9H), 2.22 (s, 6H), 2.25 (s, 3H), 6.86 (s, 2H); MS (EI): m/z 235 (M^+).

² Pandey, R. K.; Dagade, S. P.; Upadhyay, R. K.; Dongare, M. K.; Kumar, P. *ARKIVOC* **2002** (vii), 28.

³ Chankeshwara, S. V.; Chakraborti, A. K. *Tetrahedron Lett.* **2006**, 47, 1087.

(4-Hydroxy-phenyl)-carbamic acid *tert*-butyl ester⁴ (Table 1, Entry 6) : Off-White solid, yield 87 %; Mp: 146° C. IR (KBr) ν : 1690 cm^{-1} . ¹H NMR (CDCl₃, 300 MHz) δ : 1.54 (s, 9H), 4.96 (bs, 1H), 6.50 (bs, 1H), 6.75 (d, J = 8.50 Hz, 2H), 7.18 (d, J = 8.17 Hz, 2H); MS (EI): m/z 209 (M^+).

(2-Hydroxy-phenyl)-carbamic acid *tert*-butyl ester² (Table 1, Entry 7): Off-White solid, yield 90 %; Mp: 142 °C. IR (KBr) ν : 1696 cm^{-1} . ¹H NMR (CDCl₃, 300 MHz) δ : 1.52 (s, 9H), 6.73 (bs, 1H), 6.82-7.13 (m, 4H), 8.20 (bs, 1H). MS (EI): m/z 209 (M^+).

4-Mercaptophenylcarbamic acid *tert*-butyl ester³ (Table1, Entry 8): Off-white solid, yield 83 %; Mp: 179-180° C. IR (KBr): ν : 1704 cm^{-1} . ¹H NMR (300 MHz; CDCl₃) δ : 1.51 (s, 9H), 4.25 (bs, 1H) 4.65 (bs, 1H), 7.19 - 7.49 (m, 4 H). MS (EI): m/z 225 (M^+).

4-Fluorophenylcarbamic acid *tert*-butyl ester³ (Table 1, Entry 9): White solid, yield 90 %; Mp: 124-125°C. IR (KBr) ν : 1694 cm^{-1} . ¹H NMR (300 MHz; CDCl₃) δ : 1.50 (s, 9H), 6.52 (bs, 1H), 6.94-6.99 (m, 2H), 7.28-7.32 (m, 2H). MS (EI): m/z 211 (M^+).

(4-Bromophenyl)-carbamic acid *tert* -butyl ester⁴ (Table 1, Entry 10): White solid, yield 90 %; Mp: 102 °C. IR (KBr) ν : 1690 cm^{-1} . ¹H NMR (CDCl₃, 300 MHz) δ : 1.51 (s, 9H), 6.50 (bs, 1H), 7.25 (d, J = 7.53 Hz, 2H), 7.38 (d, J = 7.10 Hz, 2H). MS (EI): m/z 272 (M^+).

(4-Bromo-2-methylphenyl)carbamic acid *tert*-butyl ester³ (Table 1, Entry 11): Off-White solid, yield 90 %; Mp: 97 °C. ¹H NMR (300 MHz; CDCl₃) δ : 1.51 (s, 9H), 2.21 (s, 3H), 6.21 (bs, 1H), 7.27-7.30 (m, 2H), 7.72 (d, J = 8.05 Hz, 1H). MS (EI): m/z 286 (M^+).

(3-Chloro-4-fluoro-phenyl)-carbamic acid *tert*-butyl ester⁵ (Table 1, Entry 12): Off-White solid, yield 92 %; Mp: 91-92 °C. ¹H NMR (CDCl₃, 300 MHz) δ : 1.51 (s, 9H), 6.46 (bs, 1H), 7.00-7.13 (m, 2H), 7.56 (d, J = 4.88 Hz, 1H). MS (EI): m/z 245 (M^+).

(9-Ethyl-9H-carbazol-3-yl)-carbamic acid *tert*-butyl ester (Table 1, Entry 14): Yellow solid, yield 92 %; Mp: 161-162° C. IR (KBr) ν : 3165, 2960, 1726, 1608, 1526, 1332, 1255, 1158, 1045, 999, 820 cm^{-1} . ¹H NMR (300 MHz, CDCl₃): δ = 1.31 (t, J = 6.82 Hz, 3H), 1.54 (s, 9H), 4.21 (q, J = 6.98 Hz, 2H), 6.65 (bs, 1H), 7.12-7.43 (m, 5H), 7.99-8.13 (m, 2H). ¹³C NMR (75 MHz, CDCl₃) δ : 13.7, 28.4, 37.4, 80.0, 108.4, 111.4, 118.4,

⁴ Aldrich Catalogue, India 2005-2006

⁵ Chandrasekhar, S.; Reddy, R. C.; Rao, J. R. *Synlett*, **2001**, 1561.

120.6, 122.7, 123.0, 125.6, 130.1, 136.6, 140.3, 153.6. MS (EI): m/z 310 (M^+); Anal. Calcd. for $C_{19}H_{22}N_2O_2$ C, 73.52; H, 7.14; N, 9.03; O, 10.31 Anal. Found: C, 73.51; H, 7.15; N, 8.96; O, 10.24.

Pyridin-4-yl-carbamic acid tert-butyl ester⁶ (Table 1, Entry 15): White solid, yield 92 %; 1H NMR ($CDCl_3$, 300 MHz) δ : 1.41 (s, 9H), 7.36 (bs, 2H), 8.36 (bs, 2H), 8.75 (bs, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ : 28.1, 81.0, 112.5, 146.6, 149.8, 152.5. MS (EI): m/z 194 (M^+).

(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)carbamic acid tert-butyl ester (Table 1, Entry 16)³: Yellow solid; , yield 90 %; Mp 196 – 197 °C; IR (KBr) ν : 1716 cm^{-1} ; 1H NMR (300 MHz; $CDCl_3$) δ : 1.48 (s, 9H), 2.26 (s, 3H), 3.03 (s, 3H), 5.95 (brs, 1H), 7.28- 7.47 (m, 5H); MS (EI) m/z 303: (M^+); Anal. calcd. for (%) for C, 63.35; H, 6.98; N, 13.85. Found C, 63.26; H, 6.95; N, 13.89.

(1H-Benzoimidazol-2-yl)carbamic acid tert-butyl ester³ (Table 1, Entry 17) : White solid; , yield 92 %; Mp 210°C (d). IR (KBr) ν : 1732 cm^{-1} . 1H NMR (300 MHz; $CDCl_3$) δ : 1.71 (s, 9H), 7.06 (brs, 1H) 7.20 - 7.35 (m, 4H), 7.66 (bs, 1 H). MS (EI) m/z : 233 (M^+); Anal. Calcd. For $C_{12}H_{15}N_3O_2$: C, 61.79; H, 6.48; N, 18.01. Found: C, 61.68; H, 6.50; N, 18.12.

Benzyl-carbamic acid tert-butyl ester¹ (Table 1, Entry 18): Colorless oil, yield 96 %; IR (Neat) ν : 1700 cm^{-1} . 1H NMR ($CDCl_3$, 300 MHz) δ : 1.45 (s, 9H), 4.29 (bs, 2H), 4.94 (bs, 1H), 7.24-7.33 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ : 28.3, 44.5, 127.2, 127.3, 128.4, 138.8, 155.8. MS (EI): m/z 150 (M^+ -57).

Furan-2-ylmethylcarbamic acid tert-butyl ester (Table 1, Entry 19) : Yellow oil, yield 95 %; IR (neat) ν : 3346, 2979, 2932, 1702, 1508, 1367, 1250, 1171, 1006, 753 cm^{-1} . 1H NMR (300 MHz; $CDCl_3$) δ : 1.45 (s, 9H), 4.29 (d, 2H, J = 5.04 Hz), 4.86 (bs, 1H), 6.20 (s, 1H), 6.30 (s, 1H), 7.34 (s, 1H). MS (EI) m/z : 197 (M^+); Anal. Calcd. for $C_{10}H_{15}NO_3$: C, 60.90; H, 7.67; N, 7.10. Found: C, 60.73; H, 7.69; N, 7.12.

Pyrrolidine-1-carboxylic acid tert-butyl ester⁴ (Table 1, Entry 20): Colorless oil, yield 95 %; IR (neat) ν : 1695 cm^{-1} . 1H NMR ($CDCl_3$, 300 MHz) δ : 1.45 (s, 9H), 1.82 (bs, 4H), 3.30 (bs, 4H). MS (EI): m/z 171 (M^+).

⁶ Kelly, T. A.; McNeil, D. W. *Tetrahedron Lett.* **1994**, 35, 9003.

Piperidine-1-carboxylic acid *tert*-butyl ester⁷ (Table 1, Entry 21): Colorless oil, yield 95 %; IR (Neat)v: 1690 cm⁻¹. ¹H NMR (CDCl₃, 300 MHz) δ : 1.45-1.51 (m, 15H), 3.34-3.37 (m, 4H); ¹³C NMR (CDCl₃, 75 MHz) δ : 24.4, 25.6, 28.4, 44.5, 79.0, 154.8. MS (EI): *m/z* 185 (M)⁺.

Morpholine-4-carboxylic acid *tert*-butyl ester⁸ (Table 1, Entry 22): Colorless oil, yield 98 %; IR (Neat) v: 1701 cm⁻¹. ¹H NMR (CDCl₃, 300 MHz) δ : 1.46 (s, 9H), 3.38-3.41 (m, 2H), 3.61-3.64 (m, 2 H). MS (EI): *m/z* 187 (M⁺).

(2-Morpholin-4-yl-ethyl)-carbamic acid *tert*-butyl ester (Table 1, Entry 23): Yellow oil, yield 90 %; IR (neat) v: 2974, 2875, 1695, 1407, 1255, 1266, 1128 cm⁻¹. ¹H NMR (CDCl₃, 300 MHz) δ : 1.45 (s, 9H), 2.20-2.45 (m, 6H), 2.69-3.71 (m, 4H), 3.22-3.24 (m, 2H), 5.04 (s, 1H); ¹³C NMR (75 MHz, CDCl₃): δ : 28.9, 37.3, 53.9, 58.1, 67.4, 79.1, 156.47. MS (EI): *m/z* 230 (M⁺). Anal. Calcd. For (%) C₁₁H₂₂N₂O₃ C, 57.37; H, 9.63; N, 12.16. Found: C, 57.14; H, 9.75; N, 12.04.

Cyclohexylcarbamic acid *tert*-butyl ester⁷ (Table 1, Entry 24): Colourless solid, yield 90 %; IR (CCl₄) v: 3364, 2973, 2934, 2854, 1681, 1520 1448, 1366, 1315, 1251, 1233, 1168 cm⁻¹. ¹H NMR (300 MHz; CDCl₃) δ : 1.04-1.15 (m, 3H), 1.26-1.34 (m, 2H), 1.44 (s, 9H), 1.57- 1.71 (m, 3H), 1.90-1.93 (m, 2H), 3.43 (bs, 1H), 4.43 (bs, 1H).

Dicyclohexylcarbamic acid *tert*-butyl ester (Table 1, Entry 25): Colourless solid, yield 90 %; mp 58 -59 °C. IR (CCl₄) v: 2929, 2854, 1686, 1436, 1365, 1295, 1177, 1159 cm⁻¹. ¹H NMR (300 MHz; CDCl₃) δ : 1.04-1.12 (m, 3H), 1.2-1.3 (m, 5H), 1.47-1.58 (m, 18H), 1.74-1.78 (m, 5H) ¹³C NMR (CDCl₃, 75 MHz) δ: 25.5 , 26.2, 28.5, 31.2, 54.6, 78.8, 155.3.; MS (APCI) *m/z*: 181 (M⁺-100); Anal. calcd. for C₁₇H₃₁NO₂ C, 72.55; H, 11.10; N, 4.98. Found: C, 72.45; H, 10.95; N, 4.95.

(2,2-Dimethoxy-ethyl)-carbamic acid *tert*-butyl ester¹ (Table 1, Entry 26): Colorless oil, yield 95 %; IR (Neat) v: 1682 cm⁻¹. ¹H NMR (CDCl₃, 300 MHz) δ : 1.44 (s, 9H), 3.25 (t, *J* = 5.27, 2H), 3.38 (s, 6H), 4.37 (t, *J* = 5.54, 1H), 4.76 (bs, 1H); ¹³C NMR (CDCl₃, 75 MHz) δ : 28.1, 41.8, 53.8, 78.9, 102.7, 155.7.; MS (EI): *m/z* 205(M⁺).

(S)-(1-Phenyl-ethyl)-carbamic acid *tert*-butyl ester⁸ (Table 1, Entry 27): White solid, yield 96 %; IR (KBr) v: 1690 cm⁻¹. ¹H NMR (CDCl₃, 300 MHz) δ : 1.41 (bs, 12H), 4.78

⁷ Sharma, G. V. S.; Reddy, J. J.; Lakshmi, P. S.; Krishna, P. R. *Tetrahedron Lett.* **2004**, 45, 6963.

⁸ Heydari, A.; Hosseini, E. S. *Adv. Synth. Catal.* **2005**, 37, 1929.

(bs, 1H), 4.92 (bs, 1H), 7.22-7.33 (m, 5H). ^{13}C NMR (CDCl_3 , 75 MHz) δ : 22.3, 29.3, 49.8, 79.0, 125.5, 126.7, 128.2, 143.7, 154.8. MS (EI): m/z 221 (M^+).

(S)- *tert*-Butoxycarbonylamino-phenyl-acetic acid methyl ester⁸ (Table 1, Entry 28):

White solid, yield 91 %; Mp: 110-111°C; ^1H NMR (300 MHz, CDCl_3) d: 1.43 (s, 9H), 3.71 (s, 3H), 5.32 (d, $J = 7.15$, 1H), 5.54 (bs, 1H), 7.33-7.35 (m, 5H). $[\alpha]_{\text{D}}^{20} + 135.7^\circ$, ($c = 0.8$ in CHCl_3); Found: $[\alpha]_{\text{D}}^{25} + 134.1^\circ$, ($c = 0.8$ in CHCl_3).

(S)- 2-*tert*-Butoxycarbonylamino-3-phenyl-propionic acid methyl ester² (Table 1,

Entry 29): Yellow solid, yield 90 %; Mp: 37-38°C. ^1H NMR (300 MHz, CDCl_3) d: 1.41 (s, 9H), 3.04-3.12 (m, 2H), 3.70 (s, 3H), 4.57-4.59 (m, 1H), 5.00-5.03 (m, 1H), 7.11-7.25 (m, 2H), 7.28-7.31 (m, 3H). Optical rotation Reported: $[\alpha]_{\text{D}}^{20} -4.0^\circ$, ($c = 2$ in CH_3OH); Found: $[\alpha]_{\text{D}}^{25} -4.1^\circ$, ($c = 2$ in CH_3OH).

(S)- 2-*tert*-Butoxycarbonylamino-3-(4-hydroxy-phenyl)-propionic acid methyl ester⁴

(Table 1, Entry 30): White solid yield 90 %; Mp: 102°C. ^1H NMR (300 MHz, CDCl_3) d: 1.42 (s, 9H), 2.99-3.01 (m, 2H), 3.71 (s, 3H), 4.54-4.55 (m, 1H), 5.05-5.07 (m, 1H), 6.73 (d, $J = 7.14$ Hz, 2H), 6.95 (d, $J = 7.72$ Hz, 2H). Optical rotation Reported: $[\alpha]_{\text{D}}^{22} + 51.0^\circ$, ($c = 1$ in CHCl_3); Found: $[\alpha]_{\text{D}}^{25} -50.0^\circ$, ($c = 1$ in CHCl_3).

(S)- (1-Hydroxymethyl-2-phenyl-ethyl)-carbamic acid *tert*-butyl ester⁷ (Table 1,

Entry 31): White solid yield 92 %; Mp: 95°C. ^1H NMR (300 MHz, CDCl_3) d: 1.40 (s, 9H), 2.72 (bs, 1H), 2.83 (d, $J = 7.17$ Hz, 2H), 3.51-3.57 (m, 1H), 3.63-3.68 (m, 1H), 3.81 (bs, 1H), 4.82 (bs, 1H), 7.19-7.32 (m, 5H). Optical rotation Reported: $[\alpha]_{\text{D}}^{25} -27.0^\circ$, ($c = 1$ in CHCl_3); Found: $[\alpha]_{\text{D}}^{25} -26.9^\circ$, ($c = 1$ in CHCl_3).

Experimental procedure for *N-tert*-butoxycarbonylation of amines during intermolecular competition studies:

Scheme 2. Aniline Vs Benzylamine: To a magnetically stirred mixture of aniline (0.093 g, 1 mmol) and benzylamine (0.107g, 1 mmol) in water (1 mL) was added $(\text{Boc})_2\text{O}$ (0.218 g, 1 mmol, 1.0 equiv) at rt (30-35°C). After 5 min, the reaction mixture was diluted with EtOAc (5 mL), the EtOAc layer was separated and the aqueous part extracted with EtOAc (2 $\times$ 5 mL). The combined EtOAc extracts were washed with water (2 $\times$ 5 mL), dried (Na_2SO_4) and evaporated to yield a liquid product which on submission

to GCMS analyses revealed to contain *N*-*t*-Boc aniline and *N*-*t*-Boc benzylamine in a ratio of 30:70.

Scheme 2. (S)-(a)-Methylbenzylamine Vs (S)-Phenylglycinemethyl ester: To a magnetically stirred mixture of (S)-a-Methylbenzylamine (0.121 g, 1 mmol) and (S)-Phenylglycinemethyl ester (0.165g, 1 mmol) in water (1 mL) was treated with (Boc)₂O (0.218 g, 1 mmol, 1.0 equiv) under magnetic stirring at room temperature (30-35°C). After 10 min (a solid mass was formed), the supernatant water was decanted off, the solid residue washed with water (2 × 10 mL), and dried under vacuum to afford a white solid (0.198 g, 90 %). This product was analyzed without any further purification by ¹H NMR (300 MHz, CDCl₃)δ : 1.42 (bs, 12H), 4.81 (bs, 2H), 7.20-7.30 (m, 5H); MS (EI): *m/z* 221 (M⁺), which confirmed the formation of (S)-(1-Phenyl-ethyl)-carbamic acid *tert*-butyl ester as the sole product.

Scheme 2. (S)-(a)-Methylbenzylamine Vs (S)- Phenylalaninol: To a magnetically stirred mixture of (S)-a-Methylbenzylamine (0.121 g, 1 mmol) and (S)- Phenylalaninol (0.151g, 1 mmol) in water (1 mL) was added (Boc)₂O (0.218 g, 1 mmol, 1.0 equiv) at rt (30-35°C). After 10 min (a solid mass was formed), the supernatant water was decanted off, the solid residue washed with water (2 × 10 mL), and dried under vacuum to afford a white solid (0.203 g, 92 %). This product was analyzed without any further purification by ¹H NMR (300 MHz, CDCl₃)δ : 1.42 (bs, 12H), 4.81 (bs, 2H), 7.20-7.33 (m, 5H); MS (EI): *m/z* 221 (M⁺), which confirmed the formation of (S)-(1-Phenyl-ethyl)-carbamic acid *tert*-butyl ester as the sole product.

Scheme 2. Cyclohexylamine Vs Dicyclohexylamine : To a magnetically stirred mixture of Cyclohexylamine (0.099 g, 1 mmol) and Dicyclohexylamine (0.181g, 1 mmol) in water (1 mL) was added (Boc)₂O (0.218 g, 1 mmol, 1.0 equiv) at rt (30-35°C). After 1h (a solid mass was formed), the supernatant water was decanted off, the solid residue washed with water (3 × 10 mL), and dried under vacuum to afford a white solid (0.172 g, 95 %). This product was analyzed without any further purification by ¹H NMR (300 MHz, CDCl₃)δ : 1.06-1.11 (m, 3H), 1.15-1.34 (m, 2H), 1.47 (s, 9H), 1.61-1.72 (m, 4H), 1.89-1.93 (m, 2H), 3.40 (bs, 1H), 4.42 (bs, 1H); IR (CCl₄): 3365, 2972, 2934, 2854, 1680, 1523, 1448, 1412, 1365, 1251, 1233, 1667 1048, 1026 cm⁻¹, which confirmed the formation of cyclohexylcarbamic acid *tert*-butyl ester as the sole product.