Supporting Information

Indium(III) Trifluoromethanesulfonate as an Efficient Catalyst for the Deprotection of Acetals and Ketals

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Experimental

General Procedures. All solvents and reagents were obtained from commercial sources and used without further purification. Reactions were monitored by LCMS data and were recorded on a single quadrupole mass-spectrometer (AUC 254 nm and 210 nm) using a 5 μ m C8 column (100 x 4.60 mm). Two mobile phases (A: 99.98% water, 0.02% TFA; B: 99.98% acetonitrile, 0.02% TFA) were used as a gradient 5% B to 95% B over 6.0 min and 5% B for 2.0 min with a flow rate of 2.0 mL/min. ^1H NMR spectra were recorded in 5 mm tubes on a 300 MHz NMR in CDCl_3 . Chemical shifts are reported in δ units (ppm) downfield from TMS as an internal standard. All microwave-heated reaction mixtures were conducted in a Personal Chemistry, Emrys Creator microwave reactor fitted with an IR sensor for continuous monitoring of reaction temperature.

All known compounds were identified based on their reported ^1H and ^{13}C NMR spectroscopic data as compared to authentic samples. Identity was verified by comparison with authentic samples of commercially available materials. The following commercially available reagents were used to identify reaction products: **2**, 100-52-7; **4**, 28785-06-0; **6**, 6630-33-7; **8**, 98-86-2; **10**, 134-81-6; **12**, 1074-12-0; **18**, 3920-50-1; **20**, 347-93-3; **22**, 104-87-0; **24**, 3132-99-8; **26**, 122-78-1; **30**, 555-16-8; **32**, 24964-64-5; **34**, 447-61-0; **36**, 123-11-5; **38**, 5398-77-6; **40**, 179321-49-4.

General Procedure for the Room Temperature Deprotection of Acetals and Ketals with Acetone and Indium(III) Trifluoromethanesulfonate: To a 50 mL round-bottomed flask was added the appropriate acetal or ketal (2.0 mmol) and acetone (20 mL) to which was added indium(III) trifluoromethanesulfonate (0.8 mol %). Reactions were carried out at room temperature and monitored by both HPLC and TLC analysis. Upon

completion of the reaction the solvent was removed under reduced pressure and the resulting crude material was typically pure enough to be used directly. Alternatively, the crude product was purified by column chromatography on silica gel (40 g) using hexanes/ethyl acetate (20:1 to 5:1 gradient) as the eluent.

General Procedure for the Microwave Assisted Deprotection of Acetals and Ketals with Acetone and Indium(III) Trifluoromethanesulfonate: To a 30 mL glass microwave reactor vessel was added the appropriate acetal or ketal (2.0 mmol) and acetone (20 mL) to which was added indium(III) trifluoromethanesulfonate (0.8 mol %) followed by sealing the vessel and heating to 100 °C for 300 sec in a microwave reactor (Personal Chemistry, Emrys Creator). The reaction temperature increased from 25 to 100 °C in 35 sec and was maintained at 100 °C for the duration. The resulting reaction progress was monitored by both HPLC and TLC analysis. Upon completion of the reaction the volatile organics were removed under reduced pressure and the resulting crude material was typically pure enough to be used directly. Alternatively, the crude product was purified by column chromatography on silica gel (40 g) using hexanes/ethyl acetate (10:1 to 4:1 gradient) as the eluent.

Deprotection of 2-Benzyl-1,3-dioxolane (25) - (entry 13, Table 1): To a 30 mL glass microwave reactor vessel was added 2-benzyl-1,3-dioxolane (**25**, 0.328 g, 2.0 mmol) and acetone (20 mL) to which was added indium(III) trifluoromethanesulfonate (0.8 mol %), followed by sealing the vessel and heating to 100 °C for 300 sec in a microwave reactor (Personal Chemistry, Emrys Creator). The reaction temperature increased from 25 to 100

°C in 35 sec and was maintained at 100 °C for the duration. The reaction was monitored by both ¹H NMR and TLC analysis for completion. The volatile organics were removed under vacuum and the residue was redissolved in fresh acetone (20 mL). The reactions were subjected to additional microwave heating for 200 sec at 100 °C after which time the reaction was determined to be complete. The reaction was then concentrated to remove the volatile organics under reduced pressure and the resulting crude product was purified by column chromatography on silica gel (40 g) using hexanes/ethyl acetate (10:1 to 4:1 gradient) as the eluent giving 200 mg of 2-phenylacetaldehyde (1.67 mmol, 84% yield) as a colorless liquid.

***N*-(3,3-diethoxypropyl)-4-methylbenzamide (13):** ¹H NMR (300 MHz, CDCl₃) δ ppm 7.66 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.04 (br s, 1H), 4.63 (t, *J* = 4.9 Hz, 1H), 3.71 (pent, *J* = 7.1 Hz, 4H), 3.55 (m, *J* = 6.4 Hz, 4H), 2.38 (s, 3H), 1.93 (q, *J* = 6.4 Hz), 1.23 (t, *J* = 6.9 Hz); ¹³C NMR (125 MHz, CDCl₃) δ ppm 167.0, 141.5, 131.9, 129.1, 126.8, 103.0, 62.1, 35.9, 32.8, 21.4, 15.4; HREI-MS *m/z*: found 265.1666 (C₁₅H₂₃NO₃ requires 265.1678)

4-Methyl-*N*-(3-oxopropyl)benzamide (14): ¹H NMR (300 MHz, CDCl₃) δ ppm 9.83 (s, 1H); 7.64 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.82 (br s, 1H); 3.71 (q, *J* = 5.9 Hz, 2H), 2.826 (t, *J* = 5.6 Hz, 2H), 2.38 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ ppm 201.7, 167.5, 141.9, 131.4, 129.2, 126.9, 43.8, 33.4, 21.4; HREI-MS *m/z*: found 191.0937 (C₁₁H₁₃NO₂ requires 191.0946)

***tert*-Butyl-1-(3,3-diethoxypropylamino)-1-oxo-3-phenylpropan-2-ylcarbamate (15):**

NMR (300 MHz, CDCl₃) δ ppm 7.24-7.31 (m, 2H), 7.18-7.23 (m, 3H), 6.35 (br s, 1H), 5.04 (br d, 1H), 4.43 (t, *J* = 5.2 Hz, 1H), 4.27 (br q, 1H), 3.59 (pent, *J* = 5.1 Hz, 2H), 3.42 (m, 2H), 3.28 (q, *J* = 5.1 Hz), 3.04 (d, *J* = 6.7 Hz, 2H), 1.69 (pent, *J* = 5.0 Hz, 2H), 1.39 (s, 9H), 1.16 (t, *J* = 7.1 Hz); ¹³C NMR (125 MHz, CDCl₃) δ ppm 170.7, 155.2, 136.8, 129.3, 128.6, 126.8, 102.2, 80.0, 61.9, 61.7, 56.0, 38.9, 35.4, 32.7, 28.3, 15.3. ; HREI-MS *m/z*: found 394.2458 (C₂₁H₃₄N₂O₅ requires 394.2468)

***tert*-Butyl-1-oxo-1-(3-oxopropylamino)-3-phenylpropan-2-ylcarbamate (16):**

NMR (300 MHz, CDCl₃) δ ppm 9.64 (s, 1H), 7.16-7.31 (m, 5H), 6.22 (br s, 1H), 5.06 (br s, 1H), 4.25 (br m, 1H), 3.44 (br m, 2H), 3.03 (m, 2H), 2.58 (m, 2H), 1.41 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ ppm 200.8, 171.2, 156.2, 136.7, 129.3, 128.7, 127.0, 80.2, 56.0, 43.5, 38.7, 32.7, 28.3. ; HREI-MS *m/z*: found 320.1723 (C₁₇H₂₄N₂O₄ requires 320.1736)

8-(Tetrahydro-2*H*-pyran-2-yloxy)-1,4-dioxaspiro[4.5]decane (27):

¹H NMR (300 MHz, CDCl₃) δ ppm 4.70-4.68 (m, 1H), 3.97-3.93 (m, 5H), 3.91-3.89 (m, 1H), 3.77-3.48 (m, 1H), 1.88-1.48 (m, 14H); ¹³C NMR (125 MHz, CDCl₃) δ ppm 108.5, 96.7, 71.6, 64.3, 62.6, 31.6, 31.4, 31.3, 30.2, 27.9, 25.6, 19.8; HREI-MS *m/z*: found 265.1411 (C₁₃H₂₂O₄+Na requires 265.1416)

4-(Tetrahydro-2*H*-pyran-2-yloxy)cyclohexanone (28):

¹H NMR (300 MHz, CDCl₃) δ ppm 4.77 (t, *J* = 2.8 Hz, 1H), 4.12-4.06 (m, 1H), 3.96-3.88 (m, 1H), 3.57-3.50 (m, 1H), 2.70-2.51 (m, 2H), 2.36-2.23 (m, 2H), 2.15-1.72 (m, 6H), 1.70-1.51 (m, 4H); ¹³C NMR

(125 MHz, CDCl₃) δ ppm 211.3, 97.1, 69.9, 62.8, 37.6, 37.3, 32.3, 31.2, 30.1, 25.5, 19.8;
HREI-MS m/z : found 199.1333 (C₁₁H₁₈O₃ requires 199.1334)

***tert*-Butyl-1,4-dioxaspiro[4.5]decan-8-ylcarbamate (39):** ¹H NMR (300 MHz, CDCl₃) δ ppm 4.46 (br m, 1H), 3.93 (s, 4H), 3.51 (br m, 1H), 1.94 (m, 2H), 1.47-1.89 (m, 7H), 1.44 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ ppm 155.3, 108.0, 79.2, 64.3, 64.2, 48.1, 33.1, 30.2, 28.4; HREI-MS m/z : found 257.1625 (C₁₃H₂₃NO₄ requires 257.1627)

***tert*-Butyldimethyl(2-(2-methyl-1,3-dioxolan-2-yl)ethoxy)silane (41):** ¹H NMR (500 MHz, CDCl₃) δ ppm 3.94-3.90 (m, 4H), 3.73 (t, J = 7.3 Hz, 2H), 1.91 (t, J = 7.25, 2H), 1.34 (s, 3H), 0.89 (s, 9H), 0.09-0.05 (m, 6H); ¹³C NMR (125 MHz, Acetone-*d*₆) δ ppm 107.9, 63.6, 58.5, 41.4, 24.8, 23.3, 17.3, -6.6; HREI-MS m/z : found 247.1732 (C₁₂H₂₆O₃Si requires 247.1729)

4-(*tert*-Butyldimethylsilyloxy)butan-2-one (42): ¹H NMR (300 MHz, CDCl₃) δ ppm 3.83 (t, J = 6.4, 2H), 2.56 (t, J = 6.2 Hz, 2H), 2.13 (s, 3H), 0.83 (s, 9H), 0.01 (s, 6H); ¹³C NMR (125 MHz, CDCl₃) δ ppm 207.7, 58.8, 46.5, 30.7, 25.9, 18.2, -2.8; HREI-MS m/z : found 203.1474 (C₁₀H₂₂O₂Si requires 203.1467)

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME BTG-1-6
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060919
Time_ 8.52
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
DW 83.400 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
MCKEY 0.00000000 sec
MCMRK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 10.12 usec
PL1 -2.00 dB
SFO1 300.2621018 MHz
F2 - Processing Parameters
SI 32768
SF 300.260023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMBI 30 Corporate Circle AVANCE 300
location: 4

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location; 4

14

Name _____
Date _____
NB# _____

Current Data Parameters
NAME BTG-XYZ-43
EXPNO 19
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061027
Time_ 18.24
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
RW 85.400 usec
LW 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWPRK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 10.12 usec
PL1 220.000000 MHz
SFO1 300.262108 MHz
F2 - Processing parameters
SI 32768
SF 300.2600014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI; 30 Corporate Circle
location; 13

Current Data Parameters
NAME ETO-X12-43
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061027
Time 19:49
INSTRUM spect
PROBHD 5 mm PABBO-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.024 Hz
FIDRES 0.456222 Hz
AQ 1.0912410 sec
RG 2048
DW 16.650 usec
DE 6.00 usec
TE 300.2 K
D1 0.5000000 sec
d11 0.0300000 sec
DELTA 0.4000001 sec
MCREST 0.0000000 sec
MCNRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 16.00 usec
PL1 -5.00 dB
SFO1 125.7929971 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 500.2220009 MHz

F2 - Processing parameters
SI 32768
SF 125.7804171 MHz
WDW EM
SSB 0
GB 0
PC 1.40

AMR 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME 15
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060919
Time 8.44
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TOLPROG 6536
SOLVENT CDCl3
NS 16
DS 5985.20 Hz
SMA 0.091480 Hz
FIDRES 5.4657526 sec
AQ 71.8
RG 83.400 usec
DM 0.000000 sec
TE 300.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCRRK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 13
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PL1 2.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SI 32768
SF 300.2600023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME BTG-XYZ-43
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061027
Time 13.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.465756 sec
RG 327.68
DM 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.0000000 sec
d11 0.0500000 sec
SFO1 300.2621018 MHz
NMRK1 0.01500000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 10.12 usec
PL1 -2.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SF 300.2600039 MHz
WDW EM
SSB 0
LB 0.0 Hz
GB 0
PC 1.00

AVRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-43
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070323
Time 5:23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.465726 sec
RG 327.22
IN 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1
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NUC1 1H
P1 10.09 usec
PL1 0.00 dB
SFO1 300.262018 MHz
F2 - Processing parameters
SI 32768
SF 300.260000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location, 4

Name _____

Date _____

NB# _____

Current Data Parameters
 NAME ETO-XYZ-F58
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20070323
 Time 11.33
 INSTRUM 5 mm QNP HX
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.1057420 Hz
 AQ 5.4657420 sec
 RG 326
 DW 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 10.09 usec
 PL1 -3.00 dB
 SFO1 300.2621018 MHz
 F2 - Processing Parameters
 SI 32768
 SF 300.2650032 MHz
 KW EM
 SSB 0
 GB 0
 LB 0.30 Hz
 PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location: 4

Name _____
Date _____
NB # _____

39

Current Data Parameters
NAME BTG-XY2-33
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060706
Time 15.02
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 4
SS 16
AQ 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.465556 sec
RG 655.36
DE 83.400 usec
TE 300.2 K
PC 0.000000 sec
MCREST 0.0000000 sec
MCRESK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 10.12 usec
PL1 -2.00 dB
SFO1 300.2621018 MHz
F2 - Processing Parameters
SI 32768
SF 300.2600010 MHz
RG 655.36
DE 83.400 usec
TE 300.2 K
PC 0.000000 sec
MCREST 0.0000000 sec
MCRESK 0.01500000 sec

Current Data Parameters
NAME: 39
EXPNO: 21
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060706
Time: 14:09
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 256
DS: 4
SWH: 18832.393 Hz
FIDRES: 0.574719 Hz
AQ: 0.870464 sec
RG: 186.250
DM: 26.550 usec
DE: 6.00 usec
TE: 0.0 K
D1: 0.5000000 sec
D11: 0.5000000 sec
DELTA: 0.4000001 sec
ACQRES: 0.0000000 sec
MCREST: 0.0000000 sec
MCRMK: 0.0150000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.50 usec
PL1: -2.00 dB
SFO1: 75.5079872 MHz

===== CHANNEL f2 =====
CPRPG2: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: -2.00 dB
PL12: 16.00 dB
PL13: 12.00 dB
SFO2: 300.2612010 MHz

F2 - Processing parameters
SI: 16384
SF: 75.5004370 MHz
WDW: EM
SSB: 0
LB: 2.00 Hz
GB: 0
PC: 1.40

AMRI, 30 Corporate Circle
location, 13

Name _____
Date _____
NB # _____

Current Data Parameters
NAME jfq-m-28.2
EXPRO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070212
Time_ 14:22
INSTRUM spect
PROBHD 5 mm PABBI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 327.68
WDW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
ACQPRG 0.01500000 sec
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NUC1 1H
P1 7.34 usec
PL1 -2.50 dB
SFO1 500.220091 MHz
F2 - Processing Parameters
SI 32768
SF 500.220093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB# _____

Current Data Parameters
NAME 20070327
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070327
Time 23:20
INSTRUM 5 mm QNP 1H/13
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.1021490 Hz
AQ 5.4657828 sec
RG 71.8
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1
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NUC1 1H
P1 10.09 usec
PL1 -3.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SI 32768
SF 300.2600122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

O=Cc1ccccc1

Name _____
Date _____
NB # _____

[illegible]

AMRI 30 Corporate Circle AVANCE 300
location; 4

4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-80-3
EXNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070516
Time_ 9.36
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 1024
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.09 usec
PL1 -3.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2600066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME BTG-XYZ-22B
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20060413
Time 10.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 101.6
DM 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2600069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

8

Name _____
Date _____
NB # _____

Current Data Parameters
NAME BTG-XYZ-22C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060413
Time_ 10.19
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 114
DN 83.400 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNKK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2600071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB# _____

Current Data Parameters
NAME BTG-XYZ-22-2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060413
Time_ 15:49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
DN 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRX 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2600072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI; 30 Corporate Circle
location; 8

Name _____
Date _____
NB# _____

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Current Data Parameters
NAME 17-s
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070523
Time 11.20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 812.7
DW 104.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.80 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1299999 MHz
WDW EN
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME BTG-XY2-22P
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060414
Time_ 8.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
DW 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2600068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

22

Name _____
Date _____
NB # _____

Current Data Parameters
NAME BTG-XYZ-22-G2
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060414
Time_ 8.31
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
DM 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNPK 0.01500000 sec
----- CHANNEL f1 -----
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SI 32768
SF 300.2600070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI; 30 Corporate Circle
location; 8

24

Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-78
EXPNO 20
PROCNO 1
P2 - Acquisition Parameters
Date_ 20070510
Time 14.06
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SHE 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 203.2
DM 104.400 usec
DE 1.000000 sec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 8.80 usec
PL1 0.00 dB
SFO1 300.1319506 MHz
P2 - Processing Parameters
SI 16384
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.5 Hz
GB 0
PC 1.00

AMRI; 30 Corporate Circle
location; 8

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Name _____
Date _____
NB # _____

Current Data Parameters
NAME 25-9
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070522
Time_ 9.44
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 362
DW 104.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 8.80 usec
PL1 0.00 dB
SFO1 300.1319508 MHz
F2 - Processing parameters
SI 16384
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-79-1
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070511
Time_ 13.09
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091000 Hz
AQ 5.465756 sec
RG 1149.4
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SI 32768
SF 300.2600000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-79-2
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070516
Time_ 10.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 1149.4
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.09 usec
PLA -3.00 dB
SFO1 300.2621018 MHz

F2 - Processing Parameters
SI 32768
SF 300.2600068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

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Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-79-3
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070515
Time_ 13.58
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 574.7
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.09 usec
PL1 -3.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2600059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME KCG-XYZ-79-4
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date 20070510
Time 9.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.187456 Hz
AQ 5.746752 sec
RG 456.1
DN 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1
===== CHANNEL f1 =====
NUC1 1H
P1 10.09 usec
PL 0.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SI 32768
SF 300.2600051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME RCG-XYZ-79-5
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070514
Time 10.24
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 574.7
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.09 usec
PL1 -3.00 dB
SFO1 300.2621018 MHz
F2 - Processing parameters
SI 32768
SF 300.260047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AMRI 30 Corporate Circle AVANCE 300
location; 4

Name _____
Date _____
NB # _____

Current Data Parameters
NAME HTG-LJS-F-134
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date 20060705
Time 17.19
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 71.8
DW 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.12 usec
PL1 -2.00 dB
SFO1 300.2621018 MHz

F2 - Processing parameters
SI 32768
SF 300.2599934 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00