Supporting Information**Synthesis of 1,4-benzodiazepine-3,5-diones**

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S2 ^1H -NMR for compound **3a**

S3 ^{13}C -NMR for compound **3a**

S4 ^1H -NMR for compound **3b**

S5 ^{13}C -NMR for compound **3b**

S6 ^1H -NMR for compound **21**

S7 ^{13}C -NMR for compound **21**

S8 ^1H -NMR for compound **22**

S9 ^{13}C -NMR for compound **22**

S10 ^1H -NMR for compound **23**

S11 ^{13}C -NMR for compound **23**

S2

Current Data Parameters

NAME pw8901

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20031020

Time 14.10

INSTRUM DPX300

PROBHD 5 mm BBO BB-1

PULPROG zg

TD 28900

SOLVENT DMSO-d₆

NS 8

DS 2

SWH 4816.956 Hz

FIDRES 0.16677 Hz

AQ 2.9998701 sec

RG 101.6

DW 103.800 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

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

NUC1 1H

P1 7.50 usec

PL1 -6.00 dB

SFO1 300.1322510 MHz

F2 - Processing parameters

SI 32768

SF 300.1300063 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 8.350 ppm

F1 2506.04 Hz

F2P 1.138 ppm

F2 341.52 Hz

PPMCM 0.36060 ppm/cm

HZCM 108.22612 Hz/cm

S3

Current Data Parameters

NAME	pw8901
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20031020
Time	14.00
INSTRUM	DPX300
PROBHD	5 mm BBO BB-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	121
DS	2
SWH	16556.291 Hz
FIDRES	0.252629 Hz
AQ	1.9792372 sec
RG	16384
DW	30.200 usec
DE	6.00 usec
TE	300.0 K
D1	4.00000000 sec
D11	0.03000000 sec
D12	0.0002000 sec

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

NUC1	13C
P1	7.50 usec
PL1	-6.00 dB
SFO1	75.4760204 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-6.00 dB
PL12	20.00 dB
PL13	20.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	65536
SF	75.4677395 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1p	170.613 ppm
F1	12875.78 Hz
F2p	11.332 ppm
F2	855.19 Hz
PPMCM	7.36406 ppm/cm
HZCM	601.02966 Hz/cm

ppm

8.22156
8.21660
8.19395
8.18899
7.45397
7.44830
7.43397
7.42908
7.40734
7.40179
7.38392
7.37712
7.37274
7.25999
7.19986
7.19479
7.17692
7.17180
7.16872
6.94734
6.81048
6.80825
6.78312
6.78081

¹H-NMR compound 3b

Current Data Parameters

NAME 9204
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040407
Time 8.13

INSTRUM dpx300
PROBHD 5 mm BB0 BB-1
PULPROG zg30

TD 32768
SOLVENT DMSO
NS 16

DS 2
SMH 6172.839 Hz
FIDRES 0.188380 Hz

AQ 2.6542580 sec
RG 362

DW 81.000 usec
DE 6.00 usec
TE 300.0 K

D1 1.00000000 sec

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

NUC1 ¹H
P1 6.90 usec
PL1 -6.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters

SI 16384
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.321 ppm
F1 2497.29 Hz
F2P 3.956 ppm
F2 1187.24 Hz
PPMCM 0.21825 ppm/cm
HZCM 65.50227 Hz/cm

Current Data Parameters

NAME B602

EXPNO 3

PROCNO 1

F2 - Acquisition Parameters

Date_ 20031002

Time 13.02

INSTRUM dpx300

PROBHD 5 mm BBO BB-1

PULPROG zg30

TD 32768

SOLVENT DMSO

NS 1

DS 2

SWH 6172.839 Hz

FIDRES 0.188380 Hz

AG 2.6542580 sec

RG 362

DW 81.000 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

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

NUC1 1H

P1 6.90 usec

PL1 -6.00 dB

SFO1 300.1318534 MHz

F2 - Processing Parameters

SI 16384

SF 300.1300007 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 8.531 ppm

F1 2560.52 Hz

F2P 1.154 ppm

F2 346.28 Hz

PPMCM 0.36888 ppm/cm

HZCM 110.71220 Hz/cm

S7

B1968602 17mg DMSO

81969201 22mg

Current Data Parameters

NAME	EXPNO	PROCNO
9201	1	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DW	DE	TE	D1
20040406	17.32	dp3300	5 mm BB0 BB-1	zg30	32768	DMSO	1	2	6172.839 Hz	0.188380 Hz	2.6542580 sec	362	81.000 usec	6.00 usec	300.0 K	1.00000000 sec

Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
16384	300.130011 MHz	EM	0	0.30 Hz	0	1.00

1D NMR plot parameters

CK	F1P	F1	F2P	F2	PPMCM	HZCM
20.00 cm	10.269 ppm	3082.09 Hz	3.763 ppm	1129.48 Hz	0.32529 ppm/cm	97.63035 Hz/cm

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

NUC1	P1	PL1	SFO1
1H	6.90 usec	-6.00 dB	300.1318534 MHz

S9

81969201 22mg

Current Data Parameters
NAME 9201
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040406
Time 17.41
INSTRUM dpx300
PROBHD 5 mm BBO BB-1
PULPROG pendant.mo
TD 65536
SOLVENT DMSO
NS 123
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 16384
DM 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
D4 0.00150000 sec
D12 0.00020000 sec
D15 0.00470000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.50 usec
P2 11.00 usec
PL1 -6.00 dB
SF01 75.4760204 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 6.90 usec
P4 13.80 usec
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 18.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677858 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 23.00 cm
F1P 169.435 ppm
F1 12786.86 Hz
F2P 43.837 ppm
F2 3308.31 Hz
PPMCM 5.46075 ppm/
HZCM 412.1111 Hz/C

12.63
1H

S10

81969202 22mg

ppm
10.3507

¹H-NMR compound
23

ppm
10
9
8
7
6
5

Integral
0.9987

0.9855
2.0755
3.1249
1.0636
2.0390

2.0929

7.8420
7.8363
7.8224
7.8148
7.8097
7.6516
7.6249
7.4042
7.3989
7.3759
7.3525
7.3471
7.3330
7.3073
7.2805
7.0716
7.0470
7.0226
6.6219
6.6032
6.5923
6.5795

4.0919

Current Data Parameters
NAME 9202
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040408
Time 13.04

INSTRUM dpx300
PROBHD 5 mm BBO BB-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 1
DS 2

SWH 6172.839 Hz
FIDRES 0.189380 Hz
AQ 2.6542580 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.90 usec
PL1 -6.00 dB
SF01 300.1318534 MHz

F2 - Processing Parameters
SI 16384
SF 300.1300015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F4P 10.481 ppm
F1 3145.54 Hz
F2P 3.954 ppm
F2 1186.75 Hz
PPMCM 0.32632 ppm/cm
HZCM 97.93963 Hz/cm