Stereoselective Synthesis of 1,4-Bifunctional Compounds by Regioselective Pd-Catalyzed Allylic Substitution Reaction

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Supporting Information

General Procedures for Pd-Catalyzed Allylic Substitution Reaction

(a) with NaCH(CO₂Me)₂ (Synthesis of Compound *syn*-13): NaH (60% in oil, 12.0 mg, 0.300 mmol) was washed *n*-hexane under N₂ and suspended in THF (2 mL). Dimethyl malonate (38 μ L, 0.33 mmol) was added dropwise to the suspension with stirring at 0 °C and the stirring was continued for 10 min at rt. The solution of dimethyl sodiomalonate in THF was added to a mixture of (*E*)-**12** (56.2 mg, 0.15 mmol) and Pd(PPh₃)₄ (17.3 mg, 0.015 mmol) in THF (2 mL) and the whole was stirred at rt for 15 min. The reaction was quenched with water and THF was evaporated. The residue was extracted with AcOEt. The extract was washed with brine prior to drying and solvent evaporation. The residue was chromatographed on silica gel with hexane–AcOEt (4:1) to give *syn*-**13** (56.3 mg, 96%) as a colorless oil.

(b) with Amine (Synthesis of Compound *syn*-14): Benzylamine (33 μ L, 0.30 mmol) was added to a mixture of (*E*)-**12** (56.2 mg, 0.15 mmol) and Pd(PPh₃)₄ (17.3 mg, 0.015 mmol) in THF (3 mL) and the whole was stirred at rt for 30 min. The reaction was quenched with water and THF was evaporated. The residue was extracted with AcOEt. The extract was washed with brine prior to drying and solvent evaporation. The residue was chromatographed on silica gel with hexane–AcOEt (4:1 to 2:1) to give *syn*-**14** (46.5 mg, 84%) as a colorless oil.

Specific Rotations of New Chiral Compounds

<i>anti</i> - 2	$[\alpha]_{\text{D}}^{19} +8.61$ (<i>c</i> 1.13, CHCl ₃)	<i>syn</i> - 2	$[\alpha]_{\text{D}}^{25} +23.2$ (<i>c</i> 1.03, CHCl ₃)
<i>anti</i> - 3	$[\alpha]_{\text{D}}^{22} -31.9$ (<i>c</i> 1.08, CHCl ₃)	<i>anti</i> - 4	$[\alpha]_{\text{D}}^{23} -8.95$ (<i>c</i> 0.90, CHCl ₃)
<i>anti</i> - 5	$[\alpha]_{\text{D}}^{24} -30.0$ (<i>c</i> 0.95, CHCl ₃)	<i>syn</i> - 5	$[\alpha]_{\text{D}}^{25} +33.3$ (<i>c</i> 1.01, CHCl ₃)
<i>anti</i> - 6	$[\alpha]_{\text{D}}^{24} -1.14$ (<i>c</i> 0.54, CHCl ₃)	<i>anti</i> - 7	$[\alpha]_{\text{D}}^{23} +10.8$ (<i>c</i> 0.76, CHCl ₃)
<i>anti</i> - 8	$[\alpha]_{\text{D}}^{25} +21.2$ (<i>c</i> 0.34, CHCl ₃)	<i>syn</i> - 6	$[\alpha]_{\text{D}}^{23} -8.02$ (<i>c</i> 1.03, CHCl ₃)
<i>syn</i> - 7	$[\alpha]_{\text{D}}^{22} -28.1$ (<i>c</i> 0.45, CHCl ₃)	<i>syn</i> - 8	$[\alpha]_{\text{D}}^{25} -42.6$ (<i>c</i> 0.68, CHCl ₃)
<i>syn</i> - 11	$[\alpha]_{\text{D}}^{22} +49.5$ (<i>c</i> 0.66, CHCl ₃)	(<i>E</i>)- 12	$[\alpha]_{\text{D}}^{24} +23.8$ (<i>c</i> 0.82, CHCl ₃)
(<i>Z</i>)- 12	$[\alpha]_{\text{D}}^{25} -18.4$ (<i>c</i> 1.07, CHCl ₃)	<i>syn</i> - 13	$[\alpha]_{\text{D}}^{23} -46.9$ (<i>c</i> 0.76, CHCl ₃)
<i>syn</i> - 14	$[\alpha]_{\text{D}}^{23} -67.1$ (<i>c</i> 0.57, CHCl ₃)	<i>anti</i> - 13	$[\alpha]_{\text{D}}^{24} -31.2$ (<i>c</i> 1.23, CHCl ₃)
<i>anti</i> - 14	$[\alpha]_{\text{D}}^{23} -25.6$ (<i>c</i> 0.71, CHCl ₃)

Date : Fri Mar 28 16:08:29 2003

```

Filename      : Loading-ID.nmdata
Channel       : 1H-13C

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Sicehistory

ה

POINT : 16384 points

SAFETY	10.04 points
FREQU	10000.0 Hz
TIME	5000 Hz

FLIGHT	5000 Hz
DELAY	40.0 usec

```

DEAD: 28.7 usec
INTL: 100.0 usec

```

1 TIMES	:	16 times
DUMMY	:	1 times

```
PL          : 5.3616 sec
ACQIM      : 1638.3999 msec
```

```

.PREDL      : 0.01000 msec
INIT        : 1000.0000 msec

```

RESOL	0.61 HZ
PM1	2.63 USEC

```
DBNUC      : 1H
DBFBRG      : 500.00 MHz
```

OBSET	:	162167.63 HZ
RGAIN	:	23

16 times

SI UNIT : .

SPINNING	13 HZ
TEMP	25.5 C

20.05

8

1000000

 $\bar{\text{C}}\text{H}(\text{CO}_2\text{Me})$ CC(C)=CC[n+](c1ccccc1)CC1=CC=CC=C1

OTRS

anti-6

1. *Journal of the American Medical Association*, 2000; 283: 2686-2692.

10

[illegible]

 

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DFILE      F:\YH-231 BCM.ALS
COMNT
DATIM      Wed Mar 05 16:49:3
OBNUC      13C
EXMOD      BCM
OBFRO      67.80 MHz
OBSET      135.00 KHz
OBFIN      5200.0 Hz
POINT      32768
FREQU      18315.0 Hz
SCANS      700
ACQTM      1.789 sec
PD          1.211 sec
PWL        4.0 us
IRNUC      1H
CTEMP      21.3 c
SLVNT      CDCL3
EXREF      77.00 ppm
BF          0.12 Hz
RGAIN      26

```

DFILE F:\YH-233 BCM.ALS
 COMNT Wed Mar 05 17:33:0
 DATIM 13C
 OBNUC 13C
 EXMOD BCM
 OBFRO 67.80 MHz
 OBSET 135.00 KHz
 OBFIN 5200.0 Hz
 POINT 32768
 FREQU 18315.0 Hz
 SCANS 700
 ACQTM 1.789 sec
 PD 1.211 sec
 PW1 4.0 us
 IRNUC 1H
 CTEMP 21.5 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 26

```

Filename      : LoadingFID.mdata
Comment       : 1H Line
SjiceHistory  :
EXMODE        : non

```

POINT	16384	points
SAMPLE	16384	points
FREQU	10000	0 Hz
FILTR	5000	Hz
DELAY	40	0 usec
DEAT	57	2 usec
INTVL	100	0 usec
TIMES	16	times
PD	1	times
CLIMY	5	3515 sec
ACQTM	1638	3399 msec
PREDL	0	01000 msec
INITM	1000	0000 msec
RESOL	0	61 Hz
PMT	5	50 usec
DBNAC	1H	
DBFPG	500	00 MHz
DBEST	162167	63 Hz
RGAIN	25	
SCANS	16	times
SLVNT	CDCL3	
SPINNING	11	Hz
TEMP	24.0	C

DFILE F:\yh-344 bcm.als
 COMNT Wed Dec 10 10:56:08 2003
 DATIM 13C
 OBNUC 13C
 EXMOD BCM
 OBFRO 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.00 Hz
 POINT 32768
 FREQU 20408.10 Hz
 SCANS 500
 ACQTM 1.6056 sec
 PD 1.3940 sec
 PW1 4.30 usec
 IRNUC 1H
 CTEMP 24.0 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24

Date : Wed Jan 14 10:54:17 2004

Filename	: Loading1D.mdata
Comment	: 1H Line
SliceHistory	:
EXMODE	: non
POINT	: 16384 points
SAMPD	: 16384 points
FREQD	: 10000.0 Hz
FILTR	: 5000 Hz
DELT	: 40.0 usec
DEADT	: 57.2 usec
INVTL	: 100.0 usec
TIMES	: 16 times
DUMMY	: 1 times
PD	: 5.3616 sec
ACQTM	: 1638.399 msec
PRECL	: 0.01000 msec
INIKT	: 1000.0000 msec
RESOL	: 0.61 Hz
PA1	: 5.50 usec
ORNUC	: 1H
ORFRQ	: 500.00 MHz
ORSET	: 162167.63 Hz
RGAIN	: 25
SCANS	: 16 times
SLVNT	: CDCL3
SPINNING	: 13 Hz
TEMP	: 23.6 C

DFILE F:\yh-347-b bcm2.als
 COMNT
 DATIM Wed Jan 14 11:45:30 2004
 OBNUC 13C
 EXMOD BCM
 OBFRQ 67.80 MHz
 OBSET 135.00 KHz
 OBFIN 5200.00 Hz
 POINT 32768
 FREOU 18315.00 Hz
 SCANS 521
 ACQTM 1.7891 sec
 PD 1.2110 sec
 PW1 4.00 usec
 IRNUC 1H
 CTEMP 18.2 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 26

Date : Wed Jun 18 15:06:06 2003

Filename : LoadingFID.mdata

Comment : 1H Line

Slcchistory :

EXMODE : non

POINT	16384 points
SAMPD	16384 points
FREQU	10000.0 Hz
FILTR	5000 Hz
DELT	40.0 usec
DEADT	58.7 usec
INVL	100.0 usec
TIMES	16 times
DUMWY	1 times
PD	5.3616 sec
ACQIM	1638.3999 msec
PREDL	0.01000 msec
ININT	1000.0000 msec
RESOL	0.61 Hz
PMI	2.63 usec
ORNUC	1H
ORFHO	500.00 MHz
ORSET	162167.63 Hz
RGAIN	25
SCANS	16 times
SLVNT	CDCl3
SPINNING	14 Hz
TEMP	30.8 C

DFILE F:\yh-277 bcm.als
 COMNT
 DATIM Mon Jun 09 18:15:16 2003
 OBNUC 13C
 EXMOD BCM
 OBFRO 67.80 MHz
 OBSET 135.00 KHz
 OBFIN 5200.00 Hz
 POINT 32768
 FREQU 18315.00 Hz
 SCANS 700
 ACQTM 1.7891 sec
 PD 1.2110 sec
 PW1 4.00 usec
 IRNUC 1H
 CTEMP 24.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 27

yh-281-b

DFILE E:\yh-281-b bcm.als
 COMNT yh-281-b
 DATIM Mon Jan 12 17:16:13 2004
 OBNUC 13C
 EXMOD BCM
 OBFRO 67.80 MHz
 OBSET 135.00 KHz
 OBFIN 5200.0 Hz
 POINT 32768
 FREQU 18315.0 Hz
 SCANS 485
 ACQTM 1.789 sec
 PD 1.211 sec
 PW1 4.0 us
 IRNUC 1H
 CTEMP 19.4 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 26

1H Line

Date : Wed Dec 3 15:27:01 2003
 Filename : seizure_data
 Comment : 1H Line
 SliceHistory : non
 EXMODE : non
 POINT : 16384 points
 SAMPD : 16384 points
 FREQ : 10000.0 Hz
 F1LIR : 5000 Hz
 DELAY : 40.0 usec
 DEADT : 57.2 usec
 INVT : 100.0 usec
 TIMES : 16 times
 DUMY : 1 times
 PD : 5.3616 sec
 ACQTM : 1638.389 msec
 PREUL : 0.01000 msec
 INVT : 1000.0000 msec
 RESOL : 0.61 Hz
 PUL : 5.50 usec
 DBNLC : 1H
 DBFRG : 500.00 MHz
 DBSET : 162167.63 Hz
 REAIN : 24
 SCANS : 16 times
 SLVNT : CDCl3
 SPTNNG : 10 Hz
 TEMP : 24.4 C

FILE F:\yh-342 bcm.als
 COMNT
 DATIM Wed Dec 03 14:10:23 2003
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.00 Hz
 POINT 32768
 FREQU 20408.10 Hz
 SCANS 600
 ACQTM 1.6056 sec
 PD 1.3940 sec
 PW1 4.30 usec
 IRNUC 1H
 CTEMP 24.2 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24

¹H Line

Date : Fri Nov 21 14:24:49 2003
 Filename : LoadingFID.mdata
 Comment : 1H Line
 SliceHistory :
 EXMODE : non
 POINT : 16384 points
 SAMPD : 16384 points
 FREQD : 10000.0 Hz
 F1FID : 5000 Hz
 DELTA : 40.0 usec
 DELT2 : 57.2 usec
 DECT : 100.0 usec
 INVT : 16 times
 TIMES : 16 times
 DUMMY :
 PD : 5.3614 sec
 ACQTM : 1638.3999 msec
 PREDT : 0.01000 msec
 INVT : 1000.0000 msec
 RESOL : 0.61 Hz
 PM1 : 5.50 usec
 ORNLC :
 ORFTG : 500.00 MHz
 ORSET : 162167.63 Hz
 RGA1N : 17
 SCANS : 16 times
 SLVNT : CDCL₃
 SPINNING : 13 Hz
 TEMP : 13.1 C

DFILE F:\yh-333 bcm.als
 COMNT
 DATIM Fri Nov 21 13:56:21 2003
 OBNDU 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.00 Hz
 POINT 32768
 FREQU 20408.10 Hz
 SCANS 400
 ACQTM 1.6056 sec
 PD 1.3940 sec
 PW1 4.30 usec
 IRNUC 1H
 CTEMP 13.3 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 25

Date : Fri Dec 5 15: 01: 16 2003

FileName	: LoadingID.nmdata
Comment	: 1H Line

```
Sjcehistory : non
EXMODE : non
```

non

POINT	16384	points
SAMPD	16384	points

16384 points

```

FREQU      10000.0 HZ
FILTR      5000 HZ
RELAX      3.000

```

5000 Hz
4000 Hz

DEADT	57.2 usec
INTVL	100.0 usec

57.2 usec
100.0 usec

TIME	100.0 usec
16 times	
1 times	

1 times

PD	5.3616 sec
ACQIM	1638.3999 msec
PCOM	0.0000

1638.3999 msec
0.01000 msec

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PHELE      0.01000 msec
INIWT      1000.0000 msec
RESOL      0.51 Hz

```

1000.0000 msec
0.61 Hz

PM1	PM10	PM2.5	PM10-2.5	PM2.5-1.0	PM10-1.0	PM2.5-0.425	PM10-0.425	PM2.5-0.15	PM10-0.15	PM2.5-0.075	PM10-0.075	PM2.5-0.0425	PM10-0.0425	PM2.5-0.015	PM10-0.015	PM2.5-0.0075	PM10-0.0075	PM2.5-0.00425	PM10-0.00425	PM2.5-0.0015	PM10-0.0015	PM2.5-0.00075	PM10-0.00075	PM2.5-0.000425	PM10-0.000425	PM2.5-0.00015	PM10-0.00015	PM2.5-0.000075	PM10-0.000075	PM2.5-0.0000425	PM10-0.0000425	PM2.5-0.000015	PM10-0.000015	PM2.5-0.0000075	PM10-0.0000075	PM2.5-0.00000425	PM10-0.00000425	PM2.5-0.0000015	PM10-0.0000015	PM2.5-0.00000075	PM10-0.00000075	PM2.5-0.000000425	PM10-0.000000425	PM2.5-0.00000015	PM10-0.00000015	PM2.5-0.000000075	PM10-0.000000075	PM2.5-0.0000000425	PM10-0.0000000425	PM2.5-0.000000015	PM10-0.000000015	PM2.5-0.0000000075	PM10-0.0000000075	PM2.5-0.00000000425	PM10-0.00000000425	PM2.5-0.0000000015	PM10-0.0000000015	PM2.5-0.00000000075	PM10-0.00000000075	PM2.5-0.000000000425	PM10-0.000000000425	PM2.5-0.00000000015	PM10-0.00000000015	PM2.5-0.000000000075	PM10-0.000000000075	PM2.5-0.0000000000425	PM10-0.0000000000425	PM2.5-0.000000000015	PM10-0.000000000015	PM2.5-0.0000000000075	PM10-0.0000000000075	PM2.5-0.00000000000425	PM10-0.00000000000425	PM2.5-0.0000000000015	PM10-0.0000000000015	PM2.5-0.00000000000075	PM10-0.00000000000075	PM2.5-0.000000000000425	PM10-0.000000000000425	PM2.5-0.00000000000015	PM10-0.00000000000015	PM2.5-0.000000000000075	PM10-0.000000000000075	PM2.5-0.0000000000000425	PM10-0.0000000000000425	PM2.5-0.000000000000015	PM10-0.000000000000015	PM2.5-0.0000000000000075	PM10-0.0000000000000075	PM2.5-0.00000000000000425	PM10-0.00000000000000425	PM2.5-0.0000000000000015	PM10-0.0000000000000015	PM2.5-0.00000000000000075	PM10-0.00000000000000075	PM2.5-0.000000000000000425	PM10-0.000000000000000425	PM2.5-0.00000000000000015	PM10-0.00000000000000015	PM2.5-0.000000000000000075	PM10-0.000000000000000075	PM2.5-0.0000000000000000425	PM10-0.0000000000000000425	PM2.5-0.000000000000000015	PM10-0.000000000000000015	PM2.5-0.0000000000000000075	PM10-0.0000000000000000075	PM2.5-0.00000000000000000425	PM10-0.00000000000000000425	PM2.5-0.0000000000000000015	PM10-0.0000000000000000015	PM2.5-0.00000000000000000075	PM10-0.00000000000000000075	PM2.5-0.000000000000000000425	PM10-0.000000000000000000425	PM2.5-0.00000000000000000015	PM10-0.00000000000000000015	PM2.5-0.000000000000000000075	PM10-0.000000000000000000075	PM2.5-0.0000000000000000000425	PM10-0.0000000000000000000425	PM2.5-0.000000000000000000015	PM10-0.000000000000000000015	PM2.5-0.0000000000000000000075	PM10-0.0000000000000000000075	PM2.5-0.00000000000000000000425	PM10-0.00000000000000000000425	PM2.5-0.0000000000000000000015	PM10-0.0000000000000000000015	PM2.5-0.00000000000000000000075	PM10-0.00000000000000000000075	PM2.5-0.000000000000000000000425	PM10-0.000000000000000000000425	PM2.5-0.00000000000000000000015	PM10-0.00000000000000000000015	PM2.5-0.000000000000000000000075	PM10-0.000000000000000000000075	PM2.5-0.0000000000000000000000425	PM10-0.0000000000000000000000425	PM2.5-0.000000000000000000000015	PM10-0.000000000000000000000015	PM2.5-0.0000000000000000000000075	PM10-0.0000000000000000000000075	PM2.5-0.00000000000000000000000425	PM10-0.00000000000000000000000425	PM2.5-0.0000000000000000000000015	PM10-0.0000000000000000000000015	PM2.5-0.00000000000000000000000075	PM10-0.00000000000000000000000075	PM2.5-0.000000000000000000000000425	PM10-0.000000000000000000000000425	PM2.5-0.00000000000000000000000015	PM10-0.00000000000000000000000015	PM2.5-0.000000000000
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1H
END OF FILE

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OBFRQ      : 500.00 MHz
OBSET      : 162167.63 Hz
GCATN      : 47

```

162167.63 Hz
17

FDALIN	:	17
SCANS	:	16 times

16 times

SLVNT : CDCL3

CDCL3
13 Hz

SPINNING	13 Hz
TEMP	24.3 C

24.3.C

yh-343-c

DFILE E:\yh-343-c bcm.als
 COMNT yh-343-c
 DATIM Fri Dec 05 14:00:03 2003
 OBNUC 13C
 EXMOD BCM
 OBPRO 67.80 MHz
 OBSET 135.00 KHz
 OBFIN 5200.0 Hz
 POINT 32768
 FREOU 18315.0 Hz
 SCANS 450
 ACQTM 1.789 sec
 PD 1.211 sec
 PW1 4.0 us
 IRNUC 1H
 CTEMP 21.5 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 26

¹H Line

Date : Fri Nov 21 14:00:58 2003

Filename : LoadingID.mdata

Comment : ¹H Line

Slc:history

EXMODE : non

POINT : 16384 points

SAMPD : 16384 points

FREQD : 100000.0 Hz

FILTR : 5000 Hz

DELTA : 40.0 usec

DEADT : 57.2 usec

INVT : 100.0 usec

TIMES : 16 times

DUMY : 1 times

PD : 5.3616 sec

ACQTM : 1638.3999 msec

PREDL : 0.01000 msec

INVT : 1000.0000 msec

RESOL : 0.61 Hz

PM1 : 5.50 usec

ORNUC : ¹H

ORFRO : 500.00 MHz

ORSET : 162167.63 Hz

RGAIN : 17

SCANS : 16 times

SLVNT : CDCL3

SPINNING : 13 Hz

TEMP : 13.1 C

DFILE F:\yh-334-b bcm.als
 COMNT
 DATIM Fri Nov 21 14:21:47 2003
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.00 Hz
 POINT 32768
 FREQU 20408.10 Hz
 SCANS 400
 ACQTM 1.6056 sec
 PD 1.3940 sec
 PM1 4.30 usec
 IRNUC 1H
 CTEMP 13.6 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24