Supporting Information

Chiral Diols: A New Class of Additives for Direct Aldol Reaction

Catalyzed by L-proline

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NMR spectra and HPLC analysis

S2-S25

zhouy051228-3
 Archive directory: /export/home/ncj/vnmr/sys/data
 Sample directory:
 File: PROTON
 Pulse Sequence: s2pu1

zhouy20060105-3
 Archive directory: /export/home/ncj01/vnmr/sys/data
 Sample directory:
 File: PROTON
 Pulse Sequence: s2pu1

Zhou12.27-C
 Archive directory: /export/home/vu/vmr/sys/data
 Sample directory:
 File: CH000
 Pulse Sequence: szpul
 Solvent: CDCl3
 Ambient temperature
 Mercury-300MS "mercury300"
 Relax delay 1.000 sec
 Pulse 20.1 degrees
 Acq. time 0.485 sec
 Width 17899.1 Hz
 4576 repetitions
 OBSERVE C13 75.4552576 MHz
 DECOUPLE H1 300.0815582 MHz
 Power 35 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 4.0 Hz
 FT size 32768
 Total time 3 hr, 39 min, 55 sec

5 zhouyan4

AS-H

Sample Name:	zhouyan4	Injection Volume:	20.0
Vial Number:	RA4	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	220
Control Program:	220-280-10-90-30min	Bandwidth:	1
Quantif. Method:	13	Dilution Factor:	1.0000
Recording Time:	2006-3-28 13:07	Sample Weight:	1.0000
Run Time (min):	30.00	Sample Amount:	1.0000

No.	Ret. Time min	Peak Name	Height mAU	Area mAU*min	Rel. Area %	Amount	Type
1	11.68	n.a.	1219.498	359.893	50.92	n.a.	BMB*
2	14.16	n.a.	823.941	346.913	49.08	n.a.	BMB*
Total:			2043.438	706.806	100.00	0.000

7 zhouyan6

AS-H

Sample Name:	zhouyan6	Injection Volume:	20.0
Vial Number:	RA6	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	220
Control Program:	220-280-10-90-30min	Bandwidth:	1
Quantif. Method:	13	Dilution Factor:	1.0000
Recording Time:	2006-3-28 14:12	Sample Weight:	1.0000
Run Time (min):	30.00	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.24	n.a.	1683.655	529.346	91.60	n.a.	BMB*
2	15.02	n.a.	135.679	48.512	8.40	n.a.	BMB*
Total:			1819.334	577.858	100.00	0.000

default/Integration

Chromeleon (c) Dionex 1996-2001
Version 6.70 Build 1820

ZhouY11.17-C
 Archive directory: /export/home/wu/vnmrsys/data
 Sample directory:
 File: CARBON
 Pulse Sequence: szpul
 Solvent: CDCl3
 Ambient temperature
 Mercury-300BB "mercury300"
 Relax. delay 1.000 sec
 Pulse 28.1 degrees
 Acq. time 0.355 sec
 Width 37565.9 Hz
 4098 repetitions
 OBSERVE C13, 75.4552576 MHz
 DECOUPLE H1, 300.0814762 MHz
 Power 33 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 4.0 Hz
 FT 140.32766
 Total time 1 hr, 47 min, 22 sec

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	whdx-10	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	12/20/05 4:44:32 PM
Vial:	1	Acq. Method:	100A262
Injection #:	4	Date Processed:	12/20/05 5:07:32 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:

	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	7.306	41371	0.49	4048	0.83
2	10.639	8244656	97.91	480370	98.04
3	13.334	134211	1.59	5537	1.13

Report Method: Untitled

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Page: 1 of 1

BrC1=CC=C(C=C1)C(C)(O)CC(=O)C R
A-77 96.8% ee

zhouy051209-4
Archive directory: /export/home/wu/vnmr/sys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pu1

ZhouY12.12-C
 Archive directory: /export/home/wu/vnmr/sys/data
 Sample directory:
 Pulse Sequence: v2pul
 Solvent: CDCl3
 Ambient temperature
 File: ZhouY12.12-C
 Mercury-300MHz "mercury300"
 Relax. delay 1.000 sec
 Pulse 20.1 degrees
 Acq. time 0.500 sec
 Width 17543.9 Hz
 3272 repetitions
 nucleus C13, 75.4852576 MHz
 DECOUPLE H1, 399.8818578 MHz
 Power 33 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 4.0 Hz
 FT size 32768
 Total time 1 hr, 20 min, 26 sec

ulas

Project Name: Defaults
Reported by User: System

Br222

SAMPLE INFORMATION

Sample Name:	whdx-4	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1/22/06 10:22:58 AM
Vial:	1	Acq. Method:	100A
Injection #:	3	Date Processed:	1/22/06 10:45:01 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	14.412	15905192	97.52	401607	96.85 ✓
2	18.086	404379	2.48	13047	3.15 ✓

Report Method: Untitled

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Page: 1 of 1

CC(=O)O[C@H](c1ccc(Br)cc1)c2ccccc2 A-68

ZhouY12.14-C
 Archive directory: /export/home/du/vnmr/sys/data
 Sample directory:
 File: CARBON
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 Mercury-300BB "mercury300"
 Relax. delay 1.000 sec
 Pulse 20.1 degrees
 Acq. time 0.500 sec
 Width 17545.9 Hz
 2048 repetitions
 OBSERVE G13, 75.4552570 MHz
 DECOUPLE H1, 300.0816570 MHz
 Power 35 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 4.0 Hz
 FT size 32768
 Total time 55 min, 0 sec

A-68

20 zhouyan19

AS-H

Sample Name:	zhouyan19	Injection Volume:	20.0
Vial Number:	RB6	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	220
Control Program:	220-280-30-70-30min	Bandwidth:	1
Quantif. Method:	13	Dilution Factor:	1.0000
Recording Time:	2006-3-28 21:14	Sample Weight:	1.0000
Run Time (min):	30.00	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.13	n.a.	1539.746	182.733	47.32	n.a.	BMb*
2	5.59	n.a.	1411.323	203.466	52.68	n.a.	bMB*
Total:			2951.069	386.199	100.00	0.000

22 zhouyan21

AS-H

Sample Name:	zhouyan21	Injection Volume:	20.0
Vial Number:	RB8	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	220
Control Program:	220-280-30-70-30min	Bandwidth:	1
Quantif. Method:	13	Dilution Factor:	1.0000
Recording Time:	2006-3-28 22:19	Sample Weight:	1.0000
Run Time (min):	30.00	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.14	n.a.	71.922	7.842	1.92	n.a.	BMB*
2	5.57	n.a.	2324.902	399.666	98.08	n.a.	BMB*
Total:			2396.824	407.508	100.00	0.000	

→ R A-6
96.16% ee

ZhouY-11.6-2-c
Archive directory: /export/home/vu/vmrsys/data
Sample directory:
File: OMR09
Pulse Sequence: s2pu1

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	whdx-12	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	12/20/05 5:28:08 PM
Vial:	1	Acq. Method:	100A257
Injection #:	7	Date Processed:	12/20/05 5:41:31 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:

	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	6.930	22072	0.23	2362	0.34
2	8.966	9362486	98.76	680411	98.88
3	10.182	95251	1.00	5316	0.77

Report Method: Untitled

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Page: 1 of 1

R

98.0% ee

zhouy20051206-2
Archive directory: /export/home/vuxj/vmr/sys/data
Sample directory:
F110 PHOTON
Pulse Sequence: s2pul

ZhouY12.6-C
Archive directory: /export/home/nu/vnmrSYS/data
Sample directory:
File: C0000
Pulse Sequence: s2pu1

38 zhouyan34**AS-H**

Sample Name:	zhouyan34	Injection Volume:	20.0
Vial Number:	RA10	Channel:	UV_VIS_3
Sample Type:	unknown	Wavelength:	260
Control Program:	220-280-3-97-50min	Bandwidth:	1
Quantif. Method:	13	Dilution Factor:	1.0000
Recording Time:	2006-4-1 20:18	Sample Weight:	1.0000
Run Time (min):	50.00	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	39.31	n.a.	200.927	295.392	49.61	n.a.	BM *
2	42.10	n.a.	200.916	300.002	50.39	n.a.	MB *
Total:			401.843	595.394	100.00	0.000	

40 zhouyan36**AS-H**

Sample Name:	zhouyan36	Injection Volume:	20.0
Vial Number:	RA12	Channel:	UV_VIS_3
Sample Type:	unknown	Wavelength:	260
Control Program:	220-280-3-97-50min	Bandwidth:	1
Quantif. Method:	13	Dilution Factor:	1.0000
Recording Time:	2006-4-1 22:03	Sample Weight:	1.0000
Run Time (min):	50.00	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	38.39	n.a.	466.935	851.573	93.53	n.a.	BM *
2	42.11	n.a.	44.796	58.897	6.47	n.a.	MB*
Total:			511.731	910.470	100.00	0.000

ZhouY6.27-C

Solvent: CDCl₃
 Ambient temperature
 Mercury-300WB "mercury300"
 Relax. delay 1.000 sec
 Pulse 43.0 degrees
 Acq. time 0.500 sec
 Width 13367.9 Hz
 SFO 5120 repetitions
 OBSERVE C13 75.4552576 MHz
 DECOUPLE H1 300.0014604 MHz
 Power 33 db
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 4.0 Hz
 FT size 32768
 Total time 2 hr, 17 min, 49 sec