New P,N-Ferrocenyl Ligands for the Asymmetric Ir-Catalyzed Hydrogenation of Imines**

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Supporting Information :2

Copies of chiral GC and HPLC data for all chiral compounds

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9,14	n.a.	50,430	15,006	3,95	n.a.	BMB*
2	10,21	n.a.	884,545	365,210	96,05	n.a.	BMB*
Total:			934,975	380,216	100,00	0,000	

92.10 ~ 92.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9,11	n.a.	63,399	18,724	4,04	n.a.	BMB*
2	10,17	n.a.	1047,382	444,435	95,96	n.a.	BMB*
Total:			1110,781	463,159	100,00	0,000	

91.92 ~ 92.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,38	n.a.	218,643	93,717	96,92	n.a.	BMB*
2	12,43	n.a.	6,700	2,983	3,08	n.a.	BMB*
Total:			225,343	96,700	100,00	0,000	

93.84 ~ 94.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,28	n.a.	471,853	169,610	95,85	n.a.	BMB*
2	12,30	n.a.	19,878	7,345	4,15	n.a.	BMB*
Total:			491,731	176,955	100,00	0,000	

91.7 ~ 92.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	57.45	n.a.	441,844	1157,549	99.54	n.a.	BMB*
2	64.91	n.a.	2,554	5,344	0.46	n.a.	BMB*
Total:			444,398	1162,893	100.00	0,000	

99.08 ~ 99.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	57.16	n.a.	716,926	1868,187	99.04	n.a.	BMB*
2	64.74	n.a.	7,719	18,114	0.96	n.a.	BMB*
Total:			724,645	1886,302	100.00	0,000	

98.08 ~ 98.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.52	n.a.	388,554	333,442	95.93	n.a.	BMB*
2	25.27	n.a.	15,035	14,159	4.07	n.a.	BMB*
Total:			403,589	347,601	100.00	0,000	

94.86 ~ 95.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.63	n.a.	234,718	201,990	94.91	n.a.	BMB*
2	25.39	n.a.	10,973	10,822	5.09	n.a.	BMB*
Total:			245,691	212,811	100.00	0,000	

89.82 ~ 90.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.14	n.a.	18,158	7,380	1.11	n.a.	BMB*
2	17.27	n.a.	882,515	659,616	98.89	n.a.	BMB*
Total:			900,673	666,995	100.00	0.000	

97.78: 98.22

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.14	n.a.	16,690	5,969	0.91	n.a.	BMB*
2	17.27	n.a.	877,732	648,047	99.09	n.a.	BMB*
Total:			894,422	654,016	100.00	0.000	

98.18: 98.22

Data File C:\HPCHEM\1\DATA\MURTHY\MCH593R1.D

Sample Name: MCH593-rac1

100 °C(5), 5 °C/min to 160 °C(60), Chiral DEX-CB
racemic amine

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Injection Date : 06.10.06 13:19:50 Location : Vial 1
Sample Name : MCH593-rac1 Inj : 1
Acq. Operator : MURTHY Inj Volume : Manually

Method : C:\HPCHEM\1\METHODS\HELENAB.M
Last changed : 06.10.06 13:17:46 by MURTHY
(modified after loading)

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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Instrument 1 06.10.06 14:46:45 MURTHY

Page 1 of 2

Data File C:\HPCHEM\1\DATA\MURTHY\MCH593R1.D

Sample Name: MCH593-rac1

Signal 1: FID2 B,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.714	MM	0.2647	160.19952	10.08696	49.60671
2	40.682	MM	0.3246	162.73967	8.35537	50.39329

Totals : 322.93919 18.44233

Results obtained with enhanced integrator!

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*** End of Report ***

Data File C:\HPCHEM\1\DATA\MURTHY\MCH595-1.D

Sample Name: MCH595-1

100 °C(5), 5 °C/min to 160 °C(60), Chiral DEX-CB

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Injection Date : 06.10.06 10:00:58
Sample Name    : MCH595-1
Acq. Operator  : MURTHY
Location      : Vial 1
Inj           : 1
Inj Volume    : Manually

Acq. Method    : C:\HPCHEM\1\METHODS\HELENAB.M
Last changed   : 06.10.06 09:57:54 by MURTHY
                (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\HELENAB.M
Last changed   : 06.10.06 11:11:06 by MURTHY
                (modified after loading)

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Instrument 1 06.10.06 11:13:01 MURTHY

Page 1 of 2

Data File C:\HPCHEM\1\DATA\MURTHY\MCH595-1.D

Sample Name: MCH595-1

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Area Percent Report
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Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Sample Amount   : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

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Signal 1: FID2 B,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.658	MM	0.2712	169.54375	10.41825	96.02663
2	41.030	MM	0.2017	7.01534	5.79587e-1	3.97337

Totals : 176.55909 10.99784

Results obtained with enhanced integrator!

*** End of Report ***

5-Phenyl-pyrrolidin-2-one

XX; 92% ee from XXa

92.0533

~92% ee

Data File C:\HPCHEM\1\DATA\MURTHY\MCH596-1.D

Sample Name: MCH596-1

100 °C(5), 5 °C/min to 160 °C(60), Chiral DEX-CB

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Injection Date : 05.10.06 19:16:52
 Sample Name : MCH596-1 Location : Vial 1
 Acq. Operator : MURTHY Inj : 1
 Inj Volume : Manually

Acq. Method : C:\HPCHEM\1\METHODS\HELENAB.M
 Last changed : 05.10.06 19:12:10 by MURTHY
 (modified after loading)

Analysis Method : C:\HPCHEM\1\METHODS\HELENAB.M
 Last changed : 06.10.06 13:17:14 by MURTHY
 (modified after loading)

Instrument 1 06.10.06 13:17:16 MURTHY

Page 1 of 2

Data File C:\HPCHEM\1\DATA\MURTHY\MCH596-1.D

Sample Name: MCH596-1

Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Signal 2: FID2 B,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.690	MM	0.2656	146.64075	9.20036	94.80883
2	41.053	MM	0.2140	8.02918	6.25390e-1	5.19117

Totals : 154.66993 9.82575 → 89.6177

Results obtained with enhanced integrator!

*** End of Report ***

5-Phenyl-pyrrolidin-2-one

XX; 90% ee from XXa

~ 90% ee