

**Chiral Tertiary 2-Furyl Alcohols: Diversified Key Intermediates
to Bioactive Compounds. Their Enantioselective Synthesis via
(2-Furyl)aluminum Additions to Ketones Catalyzed by a
Titanium Catalyst of (*S*)-BINOL**

Supplementary Information

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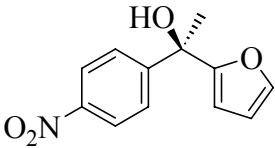
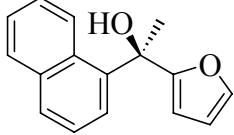
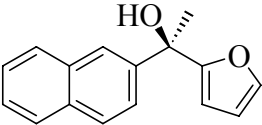
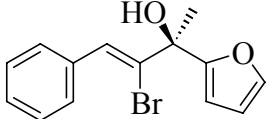
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I. Experimental Section

1. Reagent and General Techniques

Ti(O-*i*-Pr)₄ was freshly distilled prior to use. Ketones were used directly. Solvents were dried by refluxing for at least 24 h over sodium/benzophenone (THF or Hexane) and were freshly distilled prior to use. All syntheses and manipulations were carried out under a dry nitrogen atmosphere.

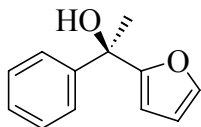
2. Synthesis of (2-Furyl)AlEt₂(THF) (7)



n-Butyl lithium (100 mmol) was added slowly to a solution of furan (36.4 mL, 500 mmol) in dry THF (100 mL) at -78 °C. The mixture was stirred for 1 h at -78 °C and then 30 min at 0 °C. The resulting solution was cooled to -78 °C and then a solution of AlEt₂X (100 mmol, X = Cl or Br) in THF (100 mL) was added. After stirring for 1 h at -78 °C, the mixture was warmed up to room temperature and stirred for 12 h. The solvent was removed under reduced pressures to give an orange oil containing white suspension. The oily material was extracted with dry hexane (3 × 100 mL), and the combined extract was concentrated to furnish an orange oil of **7** which is a mixture of three major species along with trace amounts of unidentified impurities. The reagent **7** is designated as (2-furyl)AlEt₂(THF) for simplification and used directly for the catalytic reactions. ¹H NMR (CDCl₃, 400 MHz): AlEt₃(THF) (25%), δ 0.99 (t, *J* = 8.0 Hz, 9H, CH₃), -0.23 (q, *J* = 8.0 Hz, 6H, CH₂); (2-furyl)AlEt₂(THF) (60%), 7.68 (d, *J* = 1.2 Hz, 1H, CH), 6.61 (d, *J* = 3.2 Hz, 1H, CH), 6.34 (m, 1H, CH), 1.08 (t, *J* = 8.0 Hz, 6H, CH₃), -0.01 (q, *J* = 8.0 Hz, 4H, CH₂); (2-furyl)₂AlEt(THF) (15%), 7.73 (d, *J* = 1.2 Hz, 2H, CH), 6.75 (d, *J* = 2.8 Hz, 2H, CH), 6.37 (m, 2H, CH), 1.16 (t, *J* = 8.0 Hz, 3H, CH₃), 0.19 (t, *J* = 8.0 Hz, 2H, CH₂); 2.04 (m, THF), 4.09 (m, THF) ppm.

II. Characterizations of Tertiary 2-Furyl Alcohols

1-Furan-2-yl-1-phenyl-ethanol (Table 2, entry 1; 93% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 17.736 min, 19.376 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	17.736	19.376	Time	16.972	18.845
Height (mAU)	19.686	17.815	Height (mAU)	0.834	15.575
Area (mAU-s)	627.473	626.455	Area (mAU-s)	18.466	480.948
Area (%)	50.041	49.959	Area (%)	3.697	96.303

Catalytic Reaction Conditions:

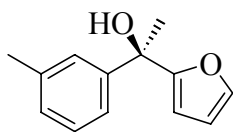
acetophenone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol,
Ti(O-*i*-Pr)₄: 1.15 mmol, 0 °C, THF: 6 mL, 12 h, Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.40-7.26 (m, 6H, *Ph* & OCH=C), 6.33 (dd, *J* = 3.2, 1.6 Hz, 1H, OCH=CH), 6.24 (dd, *J* = 3.2, 0.8 Hz, 1H, CHCH=C), 2.60 (br, 1H, OH), 1.87 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 158.94, 145.80, 142.10, 128.13, 127.27, 125.20, 110.03, 106.20, 72.95, 29.20 ppm.

1-Furan-2-yl-1-*m*-tolyl-ethanol (Table 2, entry 2; 90% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 15.375 min, 18.716 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	15.375	18.716	Time	15.431	18.658
Height (mAU)	24.429	20.061	Height (mAU)	1.330	20.508
Area (mAU-s)	615.271	627.315	Area (mAU-s)	32.835	636.641
Area (%)	49.515	50.485	Area (%)	4.905	95.095

Catalytic Reaction Conditions:

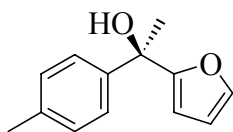
3³-methylacetophenone: 0.50 mmol, (*S*)-BINOL: 20 mol%, AlEt₂(2-furyl)(THF): 1.0 mmol, Ti(O-*i*-Pr)₄: 1.20 mmol, 0 °C, THF: 6 mL, 12 h. Procedure A.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.37-7.08 (m, 5H, *Ar* & OCH=C), 6.33 (dd, *J* = 3.2, 1.6 Hz, 1H, OCH=CH), 6.25 (dd, *J* = 3.6, 1.2 Hz, 1H, CHCH=C), 2.35 (s, 3H, ArCH₃), 1.87 (s, 3H, OCCH₃) ppm.

¹³C {¹H} NMR (100 MHz, CDCl₃): δ 158.98, 145.70, 142.00, 137.66, 127.98, 127.96, 125.78, 122.26, 109.93, 106.05, 72.80, 29.14, 21.50 ppm.

1-Furan-2-yl-1-*p*-tolyl-ethanol (Table 2, entry 3; 93% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99.5/0.5
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 25.305 min, 27.863 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	25.305	27.863	Time	25.597	27.857
Height (mAU)	14.906	13.324	Height (mAU)	0.719	14.528
Area (mAU-s)	643.474	636.980	Area (mAU-s)	27.246	710.070
Area (%)	50.254	49.746	Area (%)	3.695	96.305

Catalytic Reaction Conditions:

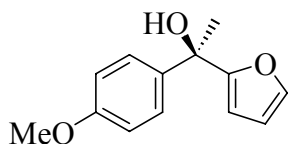
4'-methylacetophenone: 0.50 mmol, (*S*)-BINOL: 20 mol%, AlEt₂(2-furyl)(THF): 1.0 mmol, Ti(O-*i*-Pr)₄: 1.20 mmol, 0 °C, THF: 6 mL, 12 h. Procedure A.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.37-7.03 (m, 5H, *Ar* & OCH=C), 6.34-6.32 (m, 1H, OCH=CH), 6.24-6.23 (m, 1H, CHCH=C), 2.34 (s, 3H, ArCH₃), 1.86 (s, 3H, OCCH₃) ppm.

¹³C {¹H} NMR (100 MHz, CDCl₃): δ 141.78, 136.59, 131.05, 130.62, 128.62, 125.04, 109.82, 105.88, 72.63, 28.97, 20.80 ppm.

1-Furan-2-yl-1-(4-methoxy-phenyl)-ethanol (Table 2, entry 4; 92% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 98/2
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 17.697 min, 20.296 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	17.697	20.296	Time	17.789	20.267
Height (mAU)	45.743	42.534	Height (mAU)	0.898	17.815
Area (mAU-s)	1544.200	1572.293	Area (mAU-s)	26.904	625.325
Area (%)	49.549	50.451	Area (%)	4.125	95.875

Catalytic Reaction Conditions:

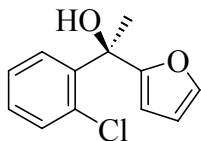
4'-methoxyacetophenone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol, Ti(*O-i-Pr*)₄: 1.15 mmol, 0 °C, THF: 6 mL, 12 h. Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.37-7.26 (m, 3H, *Ar* & OCH=C), 6.88-6.86 (m, 2H, *Ar*), 6.34-6.33 (m, 1H, OCH=CH), 6.23-6.22 (m, 1H, CHCH=C), 3.80 (s, 3H, OCH₃), 2.45 (br, 1H, OH), 1.86 (s, 3H, OCCH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 158.81, 142.07, 138.06, 126.51, 114.77, 113.49, 110.03, 106.05, 72.71, 55.26, 29.26 ppm.

1-(2-Chloro-phenyl)-1-furan-2-yl-ethanol (Table 2, entry 5; 92% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 15.147 min, 18.421 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	15.147	18.421	Time	15.411	18.873
Height (mAU)	26.869	22.465	Height (mAU)	0.941	16.331
Area (mAU-s)	706.315	709.475	Area (mAU-s)	23.003	518.525
Area (%)	49.888	50.112	Area (%)	4.248	95.752

Catalytic Reaction Conditions:

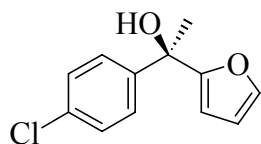
2'-chloroacetophenone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol, Ti(O-*i*-Pr)₄: 1.15 mmol, 0 °C, THF: 6 mL, 24 h. Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.79-7.22 (m, 5H, *Ar* & OCH=C), 6.36-6.35 (dd, *J* = 4.8, 1.6 Hz, 1H, OCH=CH), 6.27-6.25 (dd, *J* = 3.6, 0.8 Hz, 1H, CHCH=C) 2.17 (br, 1H, OH) 2.01 (s, 3H, CH₃) ppm.

¹³C {¹H} NMR (100 MHz, CDCl₃): δ 147.37, 146.50, 132.64, 128.23, 128.15, 127.28, 127.14, 125.72, 75.80, 30.68 ppm.

1-(4-Chloro-phenyl)-1-furan-2-yl-ethanol (Table 2, entry 6; 91% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 16.809 min, 20.932 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	16.809	20.932	Time	16.544	20.388
Height (mAU)	11.623	9.244	Height (mAU)	7.534	130.962
Area (mAU-s)	319.714	314.718	Area (mAU-s)	425.605	8755.197
Area (%)	50.394	49.606	Area (%)	4.636	95.364

Catalytic Reaction Conditions:

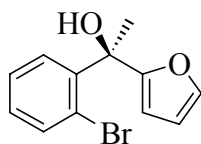
4'-chloroacetophenone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol, Ti(O-*i*-Pr)₄: 1.15 mmol, 0 °C, THF: 6 mL, 12 h. Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.39-7.28 (m, 5H, *Ar* & OCH=C), 6.35-6.33 (dd, J = 3.6, 2.0 Hz, 1H, OCH=CH), 6.25-6.24 (dd, J = 3.6, 1.2 Hz, 1H, CHCH=C), 2.52 (br, 1H, OH), 1.85 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 158.43, 144.34, 142.31, 133.15, 128.27, 126.79, 110.14, 106.38, 72.62, 29.26 ppm.

1-(2-Bromo-phenyl)-1-furan-2-yl-ethanol (Table 2, entry 7; 93% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 15.568 min, 19.159 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	15.568	19.159	Time	15.472	18.992
Height (mAU)	2.374	2.019	Height (mAU)	0.203	4.271
Area (mAU-s)	69.833	66.135	Area (mAU-s)	5.132	134.797
Area (%)	51.360	48.640	Area (%)	3.667	96.333

Catalytic Reaction Conditions:

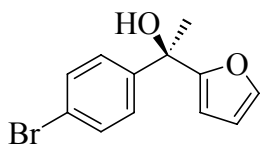
2'-bromoacetophenone: 0.50 mmol, (*S*)-BINOL: 20 mol%, AlEt₂(2-furyl)(THF): 1.15 mmol, Ti(O-*i*-Pr)₄: 1.2 mmol, 0 °C, THF: 6 mL, 24 h. Procedure A.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.82-7.14 (m, 5H, *Ar* & OCH=C), 6.37-6.36 (dd, *J* = 3.2, 1.6 Hz, 1H, OCH=CH), 6.26-6.25 (dd, *J* = 3.2, 0.8 Hz, 1H, CHCH=C) 2.02(s, 3H, CH₃)ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 141.61, 134.67, 129.06, 129.02, 128.21, 127.86, 127.40, 125.29, 110.47, 107.07, 26.56, 21.42 ppm.

1-(4-Bromo-phenyl)-1-furan-2-yl-ethanol (Table 2, entry 8; 90% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 16.509 min, 20.951 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	16.509	20.951	Time	16.231	20.264
Height (mAU)	39.547	33.083	Height (mAU)	1.595	21.707
Area (mAU-s)	1388.805	1379.962	Area (mAU-s)	40.175	729.544
Area (%)	50.159	49.841	Area (%)	5.219	94.781

Catalytic Reaction Conditions:

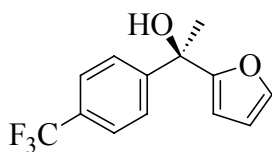
4'-bromoacetophenone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol, Ti(O-*i*-Pr)₄: 1.15 mmol, 0 °C, THF: 6 mL, 12 h. Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.47-7.26 (m, 5H, *Ar* & OCH=C), 6.35-6.26 (m, 1H, OCH=CH), 6.26-6.25 (m, 1H, CHCH=C), 2.47 (br, 1H, OH), 1.85 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 144.87, 142.34, 131.25, 127.15, 121.32, 110.15, 106.41, 72.67, 29.23 ppm.

1-Furan-2-yl-1-(4-trifluoromethyl-phenyl)-ethanol (Table 2, entry 9; 91% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 97/3
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 8.869 min, 11.177 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	8.869	11.177	Time	8.577	10.622
Height (mAU)	114.889	91.139	Height (mAU)	5.891	87.993
Area (mAU-s)	1738.978	1738.751	Area (mAU-s)	76.590	1559.355
Area (%)	50.003	49.997	Area (%)	4.682	95.318

Catalytic Reaction Conditions:

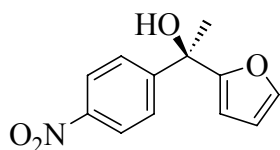
4'-trifluoromethylacetophenone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol, Ti(*O-i*-Pr)₄: 1.15 mmol, 0 °C, THF: 6 mL, 12 h. Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.61-7.26 (m, 5H, *Ar* & OCH=C), 6.37-6.38 (m, 1H, OCH=CH), 6.36-6.28 (m, 1H, CHCH=C), 2.55 (br, 1H, OH), 1.88 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 158.11, 149.71, 142.47, 125.70, 125.18, 125.14, 114.79, 110.22, 106.57, 72.77, 29.28 ppm.

1-Furan-2-yl-1-(4-nitro-phenyl)-ethanol (Table 2, entry 10; 92% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 95/5
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 14.180 min, 17.799 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	14.180	17.799	Time	13.824	17.173
Height (mAU)	54.963	43.583	Height (mAU)	18.794	333.794
Area (mAU-s)	1355.074	1355.172	Area (mAU-s)	445.455	10220.3
Area (%)	49.999	50.001	Area (%)	4.176	95.824

Catalytic Reaction Conditions:

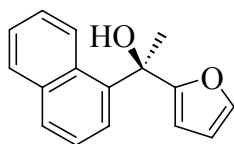
4'-nitroacetophenone: 0.50 mmol, (*S*)-BINOL: 20 mol%, AlEt₂(2-furyl)(THF): 1.0 mmol, Ti(O-*i*-Pr)₄: 1.2 mmol, 0 °C, THF: 6 mL, 12 h. Procedure A.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 8.20-8.18 (dd, *J* = 6.8, 2.0 Hz, 1H, OCH=C), 7.61-7.16 (m, 4H, *Ar*), 6.38-6.37 (m, 1H, OCH=CH), 6.32-6.31 (dd, *J* = 3.2, 0.8 Hz, 1H, CHCH=C), 2.36 (br, 1H, OH), 1.90 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 142.64, 128.99, 128.18, 126.31, 125.25, 123.40, 110.28, 106.77, 72.66, 29.20 ppm.

1-Furan-2-yl-1-naphthalen-1-yl-ethanol (Table 2, entry 11; 87% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 99/1
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 21.915 min, 29.874 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	21.915	29.874	Time	22.726	30.154
Height (mAU)	29.783	21.850	Height (mAU)	3.943	38.495
Area (mAU-s)	1198.058	1191.555	Area (mAU-s)	145.197	2010.523
Area (%)	50.136	49.864	Area (%)	6.735	93.265

Catalytic Reaction Conditions:

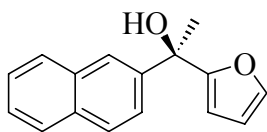
1'-acetonaphthone: 0.50 mmol, (*S*)-BINOL: 20 mol%, AlEt₂(2-furyl)(THF): 1.15 mmol, Ti(O-*i*-Pr)₄: 1.20 mmol, 0 °C, THF: 6 mL, 24 h. Procedure A.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 8.10-7.25 (m, 8H, *Ar* & OCH=C), 6.37-6.36 (m, 1H, OCH=CH), 6.29-6.28 (m, 1H, CHCH=C), 2.63 (br, 1H, OH), 2.12 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.40, 141.85, 140.63, 134.58, 129.08, 129.00, 128.93, 125.89, 125.46, 125.10, 124.92, 123.74, 110.38, 106.43, 73.43, 28.37 ppm.

1-Furan-2-yl-1-naphthalen-2-yl-ethanol (Table 2, entry 12; 90% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 95/5
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 10.363 min, 13.683 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	10.363	13.683	Time	9.910	12.824
Height (mAU)	407.983	307.500	Height (mAU)	54.639	717.753
Area (mAU-s)	7537.483	7574.478	Area (mAU-s)	885.479	16161.7
Area (%)	49.878	50.122	Area (%)	5.194	94.806

Catalytic Reaction Conditions:

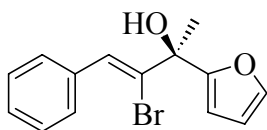
2'-acetonaphthone: 0.50 mmol, (*S*)-BINOL: 10 mol%, AlEt₂(2-furyl)(THF): 1.1 mmol, Ti(O-*i*-Pr)₄: 1.15 mmol, 0 °C, THF: 6 mL, 12 h. Procedure B.

Spectrum Data:

¹H NMR (400 MHz, CDCl₃): δ 7.91-7.25 (m, 8H, *Ar* & OCH=C), 6.36-6.35 (m, 1H, OCH=CH), 6.29-6.28 (m, 1H, CHCH=C), 2.63 (br, 1H, OH), 1.96 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 158.89, 143.14, 142.23, 133.10, 132.65, 128.28, 127.88, 127.51, 126.11, 125.98, 123.94, 123.62, 110.13, 106.40, 73.11, 29.13 ppm.

3-Bromo-2-furan-2-yl-4-phenyl-but-3-en-2-ol (Table 2, entry 13; 88% ee):



Column: Chiralcel OD
Eluent: Hexane/IPA = 95/5
Flow rate: 1 mL/min
Detector: UV, 254 nm
Retention time: 9.384 min, 11.564 min

Racemic standard			Catalytic Reaction Product		
Peak No.	1	2	Peak No.	1	2
Time	9.384	11.564	Time	9.856	12.100
Height (mAU)	944.953	775.362	Height (mAU)	119.521	1481.022
Area (mAU-s)	16097.6	16454.0	Area (mAU-s)	2025.7	31384.7
Area (%)	49.453	50.547	Area (%)	6.063	93.937

Catalytic Reaction Conditions:

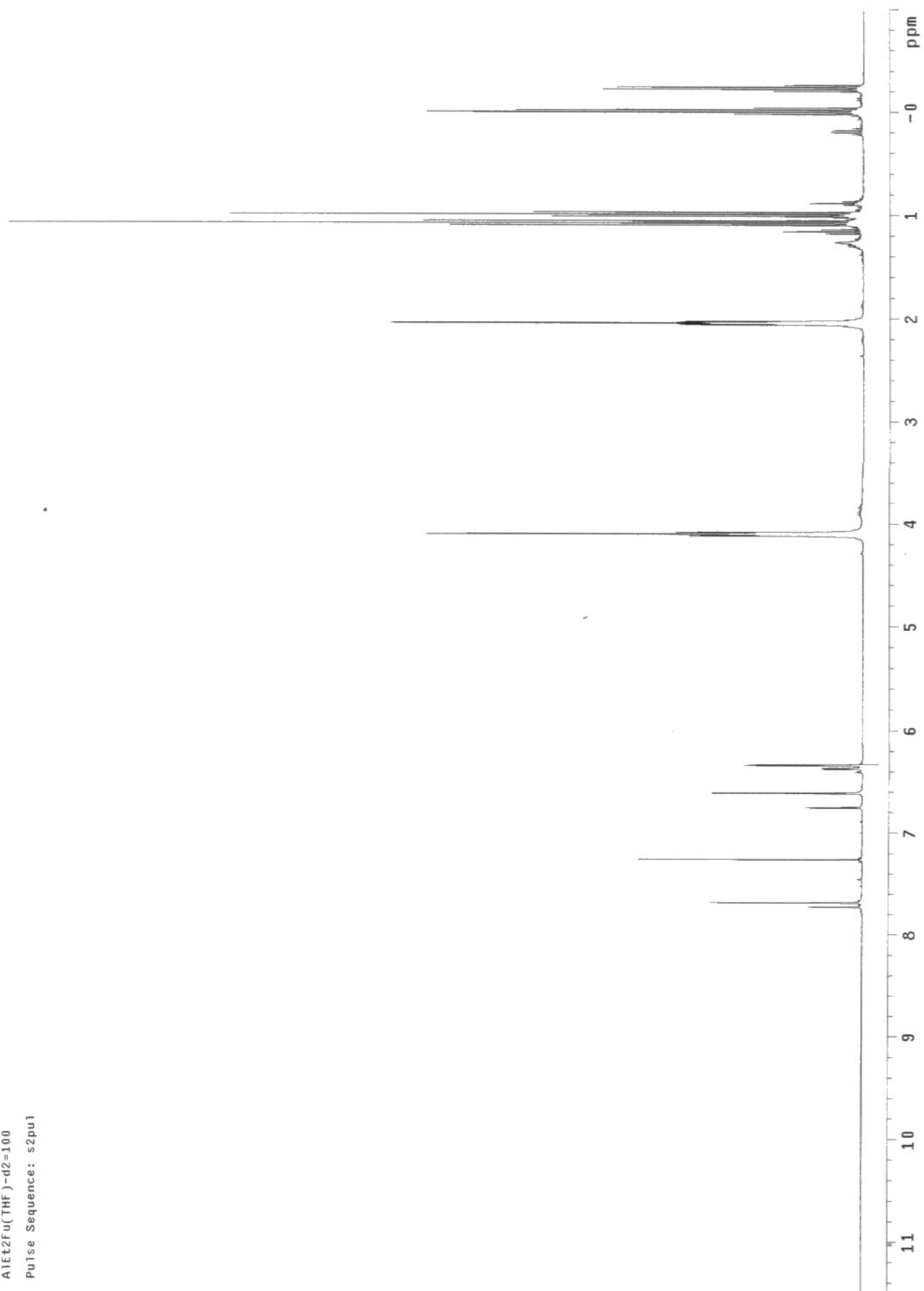
(*Z*)-3-bromo-4-phenylbut-3-en-2-one 0.50 mmol, (*S*)-BINOL: 20 mol%,
AlEt₂(2-furyl)(THF): 1.0 mmol, Ti(O-*i*-Pr)₄: 1.2 mmol, 0 °C, THF: 6 mL, 12 h. Procedure A.

Spectrum Data:

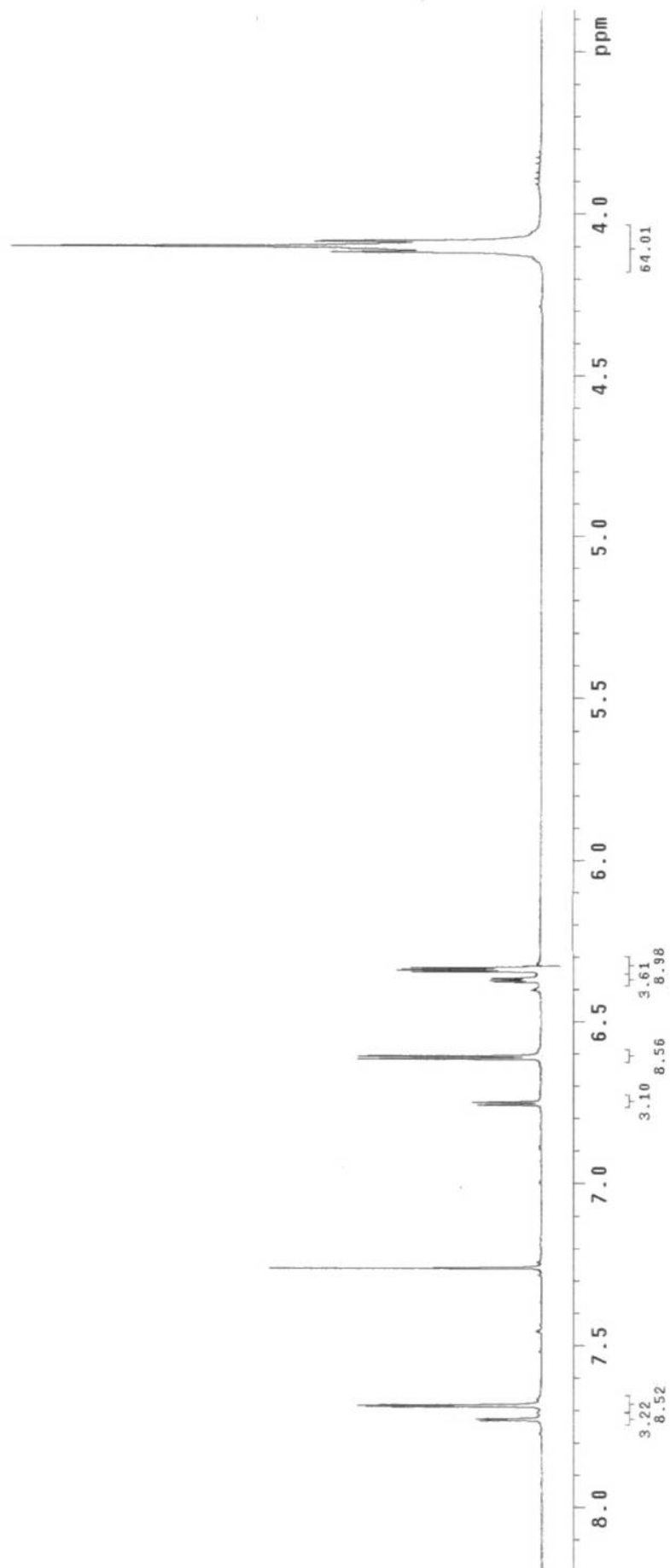
¹H NMR (400 MHz, CDCl₃): δ 7.48-7.16 (m, 7H, *Ph* & PhCH & OCH=C), 6.47-6.45 (m, 1H, OCH=CH), 6.36-6.35 (m, 1H, CHCH=C), 2.36 (br, 1H, OH), 1.94 (s, 3H, CH₃) ppm.

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 142.40, 131.71, 128.96, 128.53, 128.21, 128.16, 125.23, 122.22, 110.18, 105.78, 90.23, 83.85, 65.23, 28.62 ppm.

A1Et2Fu(THF)-d2=100
Pulse Sequence: s2pu1



A1Et2Fu(THF)-d2=100
Pulse Sequence: s2pu1



A1E12Fu(THF)-d2=100
Pulse Sequence: s2pu1

