Synthesis of a Bulky and Electron-rich Derivative of SEGPhos and Its Application in Ru-catalyzed Enantioselective Hydrogenation of β -Ketoesters

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Experimental Section

General: All reactions were carried out under inert atmosphere of dry argon or nitrogen. THF and toluene were freshly distilled from sodium/benzophenone ketyl, while CH_2Cl_2 was distilled from CaH_2 under argon atmosphere. EtOH for catalyst preparation or hydrogenation was distilled from magnesium under atmosphere. The preparation of samples and the setup of high-pressure reactor were either carried out in a glovebox or using standard Schlenk-type techniques. ^1H NMR (300 MHz), ^{13}C NMR (75.4 MHz) and ^{31}P NMR (121MHz) were registered on 300M spectrometers with CDCl_3 as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts are reported in units (ppm) by assigning TMS resonance in the ^1H spectrum as 0.00 ppm and CDCl_3 resonance in the ^{13}C spectrum as 77.0 ppm. All coupling constants (J values) were reported in Hertz (Hz). Column chromatography was performed on silica gel 300-400 mesh. GC, HPLC, MS, HRMS and optical rotations were performed by the State-authorized Analytical Center in Shanghai Institute of Organic Chemistry, Chinese Academy of Science.

3-Hydroxy-3-Phenyl-Propionic acid ethyl ester (6a) ^1H NMR (300MHz, CDCl_3) δ 1.23 (t, $J=6.9\text{Hz}$, 3H), 2.68-2.73 (m, 2H), 3.56 (br, 1H), 4.14 (q, $J=6.9\text{Hz}$, 2H), 5.10 (dd, $J=4.5\text{Hz}$, 8.7Hz , 1H), 7.26-7.34 (m, 5H); ^{13}C NMR (75.4MHz, CDCl_3) δ 13.9, 43.3, 60.7, 70.1, 125.5, 127.6, 128.3, 142.5, 172.2;

3-Hydroxy-3-(4-Methoxyphenyl)-Propionic Acid Ethyl Ester (6b) ^1H NMR (300MHz, CDCl_3) δ 1.26 (t, $J=7.2\text{Hz}$, 3H), 2.64-2.81 (m, 2H), 3.23 (br, 1H), 3.80 (s, 3H), 4.18 (q, $J=7.2\text{Hz}$, 2H), 5.06-5.11 (m, 1H), 6.88 (d, $J=8.4\text{Hz}$, 2H), 7.30(d, $J=8.4\text{Hz}$, 2H); ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 43.3, 55.2, 60.8, 69.9, 113.8, 126.9, 134.9, 159.3, 172.4.

3-Hydroxy-3-(4-Methylphenyl)-Propionic Acid Ethyl Ester (6c) ^1H NMR (300MHz, CDCl_3) δ 1.27 (t, $J=7.2\text{Hz}$, 3H), 2.34 (s, 3H), 2.70-2.75 (m, 2H), 3.25 (br, 1H), 4.14 (q, $J=7.2\text{Hz}$, 2H), 5.08-5.13 (m, 1H), 7.17 (d, $J=8.1\text{Hz}$, 2H), 7.27 (d, $J=8.1\text{Hz}$, 2H) ; ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 21.1, 43.3, 60.8, 70.1, 125.6, 129.2, 137.5, 139.5, 172.4.

3-Hydroxy-3-(4-Bromophenyl)-Propionic Acid Ethyl Ester (6d) ^1H NMR (300MHz, CDCl_3) δ 1.25 (t, $J=7.2\text{Hz}$, 3H), 2.64-2.70 (m, 2H), 3.47 (br, 1H), 4.16 (q, $J=7.2\text{Hz}$, 2H), 5.08(m, 1H), 7.24 (d, $J=7.8\text{Hz}$, 2H), 7.46 (d, $J=7.8\text{Hz}$, 2H); ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 43.1, 61.0, 69.6, 121.5, 127.4, 131.6, 141.4, 172.2.

3-Hydroxy-3-(4-Chlorophenyl)-Propionic Acid Ethyl Ester (6e) ^1H NMR (300MHz, CDCl_3) δ 1.27 (t, $J=7.2\text{Hz}$, 3H), 2.64-2.75 (m, 2H), 3.45 (br, 1H), 4.18 (q, $J=7.2\text{Hz}$, 2H), 5.08-5.13 (m, 1H), 7.26-7.32 (m, 4H); ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 43.1, 61.0, 69.6, 127.0, 128.6, 133.4, 140.9, 172.3.

3-Hydroxy-3-(4-Fluorophenyl)-Propionic Acid Ethyl Ester (6f) ^1H NMR (300MHz, CDCl_3) δ 1.26 (t, $J=7.2\text{Hz}$, 3H), 2.64-2.77 (m, 2H), 3.45 (br, 1H), 4.17 (q, $J=7.2\text{Hz}$, 2H), 5.08-5.13 (m, 1H), 7.00-7.06 (m, 2H), 7.32-7.37 (m, 2H); ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 43.3, 60.9, 69.6, 115.2, 115.5, 127.3, 128.4, 138.2, 163.8, 172.3;

3-Hydroxy-3-(3-Methylphenyl)-Propionic Acid Ethyl Ester (6g) ^1H NMR (300MHz, CDCl_3) δ 1.26 (t, $J=7.2\text{Hz}$, 3H), 2.35 (s, 3H), 2.68-2.77 (m, 2H), 3.27 (br, 1H), 4.18 (q, $J=7.2\text{Hz}$, 2H), 5.08-5.11(m, 1H), 7.08-7.26 (m, 4H); ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 21.4, 43.3, 60.8, 70.3, 122.7, 126.3, 128.4, 128.5, 138.2, 142.4, 172.4.

3-Hydroxy-3-(3-Chlorophenyl)-Propionic Acid Ethyl Ester (6h) ^1H NMR (300MHz, CDCl_3) δ 1.26 (t, $J=7.2\text{Hz}$, 3H), 2.68-2.70 (m, 2H), 3.46 (br, 1H), 4.18 (q, $J=7.2\text{Hz}$, 2H), 5.09(m, 1H), 7.22-7.28 (m, 3H), 7.38 (s, 1H); ^{13}C NMR (75.4MHz, CDCl_3) δ 14.1, 43.2, 61.0, 69.6, 123.8, 125.9, 127.8, 129.8, 134.4, 144.5, 172.2.

3-Hydroxy-3-(2-Methylphenyl)-Propionic Acid Ethyl Ester (6i) ^1H NMR (300 MHz, CDCl_3): δ 1.29 (t, $J = 7.2$ Hz, 3H), 2.35 (s, 3H), 2.62-2.75 (m, 2H), 3.27 (br, 1H), 4.20 (q, $J = 7.2$ Hz, 2 H), 5.34-5.38 (m, 1H), 7.13-7.26 (m, 3H), 7.49-7.52 (m, 1H). ^{13}C NMR (75.4 MHz, CDCl_3): δ 14.1, 18.9, 42.1, 60.9, 68.9, 125.2, 126.3, 127.5, 130.4, 134.2, 140.4, 172.6.

3-Hydroxy-Butyric Acid Ethyl Ester (8a) ^1H NMR (300 MHz, CDCl_3): δ 1.24 (d, $J = 6.6$ Hz, 3H), 1.29 (t, $J = 7.2$ Hz, 3H), 2.43-2.53 (m, 2H), 3.07 (br, 1H), 4.19 (q, $J = 7.2$ Hz, 2H). ^{13}C NMR (75.4 MHz, CDCl_3): δ 14.1, 22.4, 42.7, 60.6, 64.2, 172.9.

3-Hydroxy-Butyric Acid Isopropyl Ester (8b) ^1H NMR (300 MHz, CDCl_3): δ 1.23 (d, $J = 6.3$ Hz, 3 H), 1.26 (d, $J = 6.3$ Hz, 6H), 2.31-2.46 (m, 2H), 3.28 (br, 1H), 4.12-4.18 (m, 1H), 4.97-5.05 (m, 1H). ^{13}C NMR (75.4 MHz, CDCl_3): δ 21.6, 22.2, 42.9, 64.1, 68.0, 172.3.

3-Hydroxy-Butyric Acid Tert-butyl Ester (8c) ^1H NMR (300 MHz, CDCl_3): δ 1.19 (d, $J = 6.3$ Hz, 3H), 1.45 (s, 9H), 2.32-2.38 (m, 2H), 3.23 (br, 1H), 4.08-4.20 (m, 1H). ^{13}C NMR (75.4 MHz, CDCl_3): δ 22.2, 28.1, 43.7, 64.3, 81.2, 171.4.

3-Hydroxy-4,4-Dimethyl-Pentanoic Acid Ethyl Ester (8d) ^1H NMR (300MHz, CDCl_3): δ 0.93 (s, 9H), 1.29 (t, $J = 7.2$ Hz, 3H), 2.31-2.56 (m, 2H), 2.92 (d, $J = 3.6$ Hz, 3H), 3.71 (m, 1H), 4.18 (q, $J = 7.2$ Hz, 2H). ^{13}C NMR (75.4 MHz, CDCl_3): δ 14.1, 25.5, 34.3, 36.5, 60.7, 75.4, 173.9.

4-Chloro-3-Hydroxy-Butyric Acid Ethyl Ester (8e) ^1H NMR (300 MHz, CDCl_3): δ 1.28 (t, $J = 7.2$ Hz, 3H), 2.55-2.59 (m, 2H), 3.47 (br, 1H), 3.55 (d, $J = 5.1$ Hz, 2H), 4.12 (q, $J = 7.2$ Hz, 2H), 4.22-4.31 (m, 1H). ^{13}C NMR (75.4 MHz, CDCl_3): δ 13.9, 38.4, 48.0, 60.8, 67.7, 171.6.

3

Ar=

¹H NMR in 300MHz

Ar=

³¹P NMR in 300MHz

Ar=

1H NMR spectrum of 1,3-bis(4-methoxyphenyl)propan-2-one. The spectrum shows peaks at 7.68, 7.08, 6.99, 6.00, 5.60, 3.91, and 3.16 ppm. Integration values are 1.00, 1.00, 1.00, 1.00, 1.00, 1.00, and 1.00. The x-axis is labeled PPM and ranges from 1 to 10.

¹H NMR in 300MHz

¹³CNMR in
300MHz

6c

¹HNMR in
300MHz

¹³CNMR in
300MHz

6d

¹H NMR in 300MHz

¹³C NMR in 300MHz

6e

¹H NMR in
300MHz

¹H NMR in 300MHz

^{13}C NMR in
300MHz

6g

¹H NMR in 300MHz

¹³C NMR in 300MHz

¹H NMR in 300MHz

¹³C NMR in 300MHz

6i

¹H NMR in 300MHz

¹³C NMR in 300MHz

8a

¹H NMR in 300MHz

¹³C NMR in 300MHz

8b

¹H NMR in
300MHz

¹³C NMR in
300MHz

8c

¹H NMR in 300MHz

¹³C NMR in 300MHz

8d

¹H NMR in 300MHz

¹³C NMR in 300MHz

8e

¹H NMR in
300 MHz

¹³C NMR in
300 MHz

8a racemate

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

Signal 1: FID1 A,

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Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	25.670	PV	0.1572	416.29910	36.45700	50.04906
2	26.219	VB	0.1743	415.48294	31.01268	49.95094
Totals :				831.78204	67.46968	

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Results obtained with enhanced integrator!
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                        *** End of Report ***
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Table1 entry1

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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.)

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|-----|
1 25.491 PB 0.1677 457.09436 37.12185 99.58801
2 26.320 BP 0.1179 1.89099 2.00804e-1 0.41199

Totals : 458.98535 37.32266

Results obtained with enhanced integrator!
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*** End of Report ***

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Table entry2

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	25.282	PB	0.2217	1318.87524	74.07607	99.60706
2	26.258	MM	0.2967	5.20289	2.92303e-1	0.39294

Totals : 1324.07813 74.36838

Results obtained with enhanced integrator!

*** End of Report ***

8b racemate

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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.)

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|
1 27.950 VV 0.2214 2284.10986 128.51309 50.01782
2 28.866 VB 0.2871 2282.48193 98.24083 49.98218

Totals :                4566.59180 226.75392

Results obtained with enhanced integrator!
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                        *** End of Report ***
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Table entry3

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                        Area Percent Report
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Sample Amount  :      1.00000 [ng/ul]  (not used in calc.)
  
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Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	27.916	PB	0.2693	3353.64575	150.88533	99.77046
2	29.534	PP	0.1695	7.71579	5.50421e-1	0.22954

Totals : 3361.36154 151.43575

Results obtained with enhanced integrator!

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                        *** End of Report ***
  
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8c racemate

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

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|
1 34.182 BB 0.2111 793.70892 50.58587 50.00264
2 35.196 BB 0.2298 793.62524 44.14273 49.99736

Totals : 1587.33417 94.72860

Results obtained with enhanced integrator!
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*** End of Report ***

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Table1 entry4

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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.)

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|
1 33.750 PB 0.3324 3113.55371 113.36675 99.63541
2 35.519 PP 0.2081 11.39327 6.64338e-1 0.36459

Totals :                3124.94698 114.03109

Results obtained with enhanced integrator!
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                        *** End of Report ***

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8d racemate

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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.)

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	33.286	BV	0.2093	364.46973	23.19306	49.91851
2	34.073	VB	0.2429	365.65967	20.22982	50.08149

Totals : 730.12939 43.42289

Results obtained with enhanced integrator!

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*** End of Report ***

Table1 entry5

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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.)

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|
1 27.210 BB 1.2111 356.75183 3.44791 23.73979
2 33.398 BV 0.1839 29.16174 2.39744 1.94055
3 33.753 VB 0.3084 1116.84546 46.47160 74.31966

Totals : 1502.75903 52.31695

Results obtained with enhanced integrator!
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*** End of Report ***

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Table1 entry6

Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 02-12-10 10:54:30 下午
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Area %	Name
1	2.021		0.0000	0.00000	0.00000	
2	2.131		0.0000	0.00000	0.00000	
3	2.271		0.0000	0.00000	0.00000	
4	2.353		0.0000	0.00000	0.00000	
5	2.513		0.0000	0.00000	0.00000	
6	2.626		0.0000	0.00000	0.00000	
7	2.698		0.0000	0.00000	0.00000	
8	3.026		0.0000	0.00000	0.00000	
9	27.199	MM	1.7886	378.69730	24.69345	?
10	33.398	MM	0.2063	30.10651	1.96313	?
11	33.756	MM	0.3992	1124.79028	73.34342	?

Table1 entry7

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	33.427	BV	0.1672	10.88686	9.12545e-1	0.91576
2	33.747	VB	0.3095	1177.94897	48.14172	99.08424

Totals : 1188.83583 49.05426

Results obtained with enhanced integrator!

*** End of Report ***

Table1 entry8

Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 02-12-10 10:54:30 下午
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Area %	Name
1	2.021		0.0000	0.00000	0.00000	
2	2.131		0.0000	0.00000	0.00000	
3	2.271		0.0000	0.00000	0.00000	
4	2.353		0.0000	0.00000	0.00000	
5	2.513		0.0000	0.00000	0.00000	
6	2.626		0.0000	0.00000	0.00000	
7	2.698		0.0000	0.00000	0.00000	
8	3.026		0.0000	0.00000	0.00000	
9	33.379	MM	0.2025	7.82195	0.67303	?
10	33.731	VB	0.3300	1154.38428	99.32697	?

8e racemate

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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.)

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|
1 31.171 BV 0.3347 3722.75757 143.47624 49.97392
2 32.379 VP 0.2612 3726.64307 191.33293 50.02608

Totals : 7449.40063 334.80917

Results obtained with enhanced integrator!
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                        *** End of Report ***
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Table1 entry9

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	31.471	BV	0.4121	8087.93115	245.64191	96.63807
2	32.268	VB	0.1936	281.36978	22.85906	3.36193

Totals : 8369.30093 268.50097

Results obtained with enhanced integrator!

*** End of Report ***

Table1 entry10

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	30.902	BP	0.2430	1674.33789	96.21351	96.81602
2	32.031	BP	0.2029	55.06378	4.14743	3.18398

Totals : 1729.40167 100.36093

Results obtained with enhanced integrator!

*** End of Report ***

Table1 entry11

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Area Percent Report
=====

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	30.932	BP	0.2481	1828.78442	102.55066	98.33941
2	32.048	BP	0.1996	30.88146	2.34546	1.66059

Totals : 1859.66589 104.89612

Results obtained with enhanced integrator!

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*** End of Report ***

Table1 entry12

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	30.931	MM	0.2979	1830.47534	102.42465	98.20065
2	32.041	MM	0.2304	33.54008	2.42598	1.79935

Totals : 1864.01543 104.85063

Results obtained with enhanced integrator!

*** End of Report ***

6a racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	28.008	25960885	50.06	275343	65.41
2	33.901	25898248	49.94	145635	34.59

Table2 entry1

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	29.475	594306	1.55	12269	6.15
2	32.910	37812844	98.45	187069	93.85

6a racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	15.465	2292624	50.08	83228	61.82
2	18.785	2284903	49.92	51399	38.18

Table2 entry2

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	15.448	52115	1.72	1933	4.03
2	Peak2	18.618	2970837	98.28	46013	95.97

6b racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	15.038	30383063	49.92	502168	70.93
2	20.478	30482282	50.08	205832	29.07

Table2 entry3

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	14.785	61645442	96.60	840586	97.37
2	23.195	2170327	3.40	22691	2.63

Table2 entry4

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	14.785	61740066	96.51	841195	97.35
2	23.195	2234144	3.49	22937	2.65

6c racemate

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	19.403	9679061	50.83	177889	57.73
2	Peak2	21.557	9363522	49.17	130267	42.27

Table2 entry5

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	18.135	140385	1.92	7031	3.80
2	Peak2	19.368	7176776	98.08	178144	96.20

6d racemate

Table2 entry6

6e racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	21.890	17598901	49.91	615913	56.35
2	24.295	17661107	50.09	477178	43.65

Table2 entry7

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	21.430	206465	1.67	9182	2.04
2	Peak2	22.978	12127017	98.33	441705	97.96

6f racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	26.108	11872930	50.07	220477	54.50
2	28.572	11841500	49.93	184087	45.50

Table2 entry8

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	26.604	236552	1.44	5811	2.43
2	Peak2	28.247	16181372	98.56	233634	97.57

6g racemate

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	28.517	5083019	50.00	113418	55.37
2	Peak2	30.449	5083729	50.00	91423	44.63

Table2 entry9

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	27.589	10919821	98.11	186978	97.46
2	Peak2	30.547	210367	1.89	4879	2.54

6h racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	17.305	6493335	49.92	267029	48.28
2	18.807	6513362	50.08	286105	51.72

Table2 entry10

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	17.242	20679577	97.66	672347	96.92
2	19.076	495050	2.34	21367	3.08

6i racemate

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	18.706	4386991	50.03	199690	52.28
2	21.220	4381945	49.97	182275	47.72

Table2 entry11

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	17.920	39946395	98.37	1028579	97.61
2	Peak2	21.085	660944	1.63	25231	2.39

Table3 entry1

=====
Area Percent Report
=====

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	23.819	BV	2.0619	823.38721	4.67708	64.07090
2	25.452	VV	0.1693	452.69266	35.37795	35.22574
3	26.175	VP	0.1670	9.03897	6.98604e-1	0.70336

Totals : 1285.11883 40.75364

Results obtained with enhanced integrator!

=====
*** End of Report ***

Table3 entry2

Area Percent Report

Sorted By : Signal
 Calib. Data Modified : 02-12-10 10:54:30 下午
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Area %	Name
1	2.021		0.0000	0.00000	0.00000	
2	2.131		0.0000	0.00000	0.00000	
3	2.271		0.0000	0.00000	0.00000	
4	2.353		0.0000	0.00000	0.00000	
5	2.513		0.0000	0.00000	0.00000	
6	2.626		0.0000	0.00000	0.00000	
7	2.698		0.0000	0.00000	0.00000	
8	3.026		0.0000	0.00000	0.00000	
9	23.870	MM	2.9755	822.28564	64.27015	?
10	25.458	MM	0.2129	449.47134	35.13084	?
11	26.173	MM	0.2245	7.66383	0.59901	?

Table3 entry3

```

=====
                        Area Percent Report
=====

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

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
----|-----|-----|-----|-----|-----|
1 23.918 BV 1.2927 621.53094 5.62667 43.12925
2 25.789 VV 0.1868 785.51544 53.66879 54.50845
3 26.640 VB 0.1706 34.04292 2.99452 2.36230

Totals : 1441.08931 62.28998

Results obtained with enhanced integrator!
=====
*** End of Report ***

```

Table3 entry4

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	23.605	MM	1.7876	453.33228	4.22663	37.49927
2	25.466	VB	0.1799	711.70294	50.66411	58.87148
3	26.268	BB	0.1756	43.87442	3.72063	3.62926

Totals : 1208.90964 58.61137

Results obtained with enhanced integrator!

*** End of Report ***

Table3 entry5

```

=====
                        Area Percent Report
=====

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

Signal 1: FID1 A,

Peak RetTime Type Width Area Height Area
# [min] [min] [pA*s] [pA] %
-----|-----|-----|-----|-----|
1 25.585 PB 0.1428 242.47488 23.41097 98.42145
2 26.301 PP 0.1341 3.88898 4.04707e-1 1.57855

Totals :                246.36386 23.81568

Results obtained with enhanced integrator!
=====
                        *** End of Report ***

```

Table3 entry6

Area Percent Report

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

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	25.297	MM	0.3085	1482.42261	80.07620	98.76524
2	26.286	MM	0.2283	18.53320	1.35308	1.23476

Totals : 1500.95581 81.42928

Results obtained with enhanced integrator!

*** End of Report ***