Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Mechanistic investigations of the asymmetric hydrosilylation of ketimines with trichlorosilane reveals a dual activation model and an organocatalyst with enhanced efficiency

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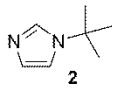
XL5–91
PRO CDCl3 {C:\08au2011} ch3sj 44



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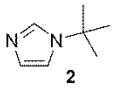

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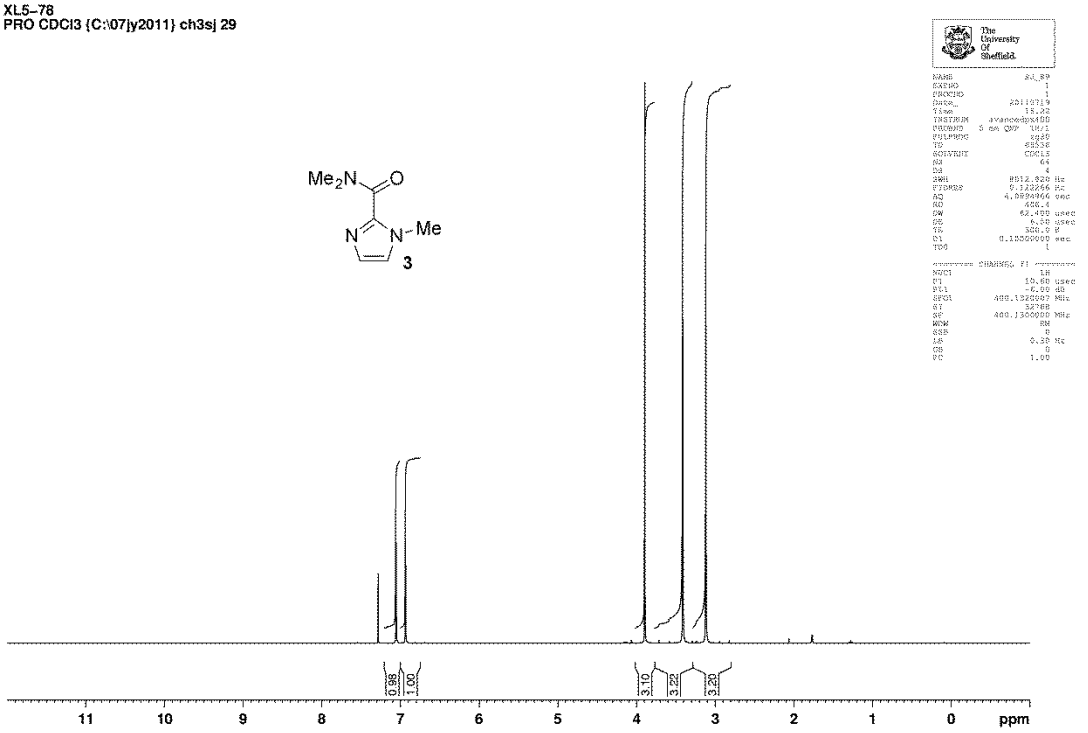

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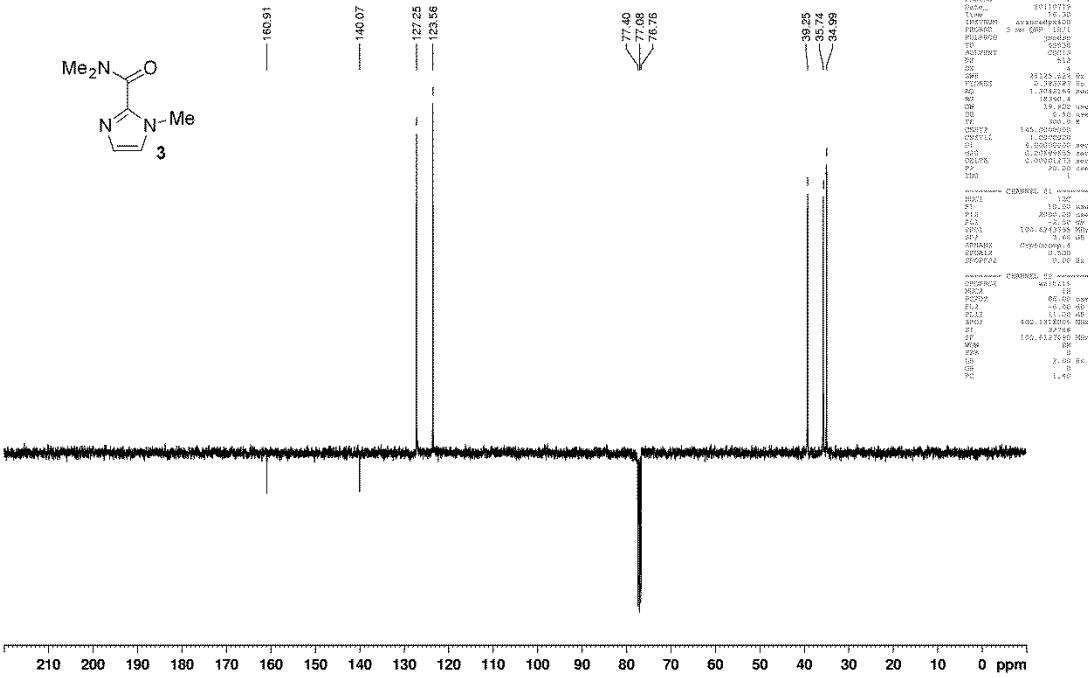

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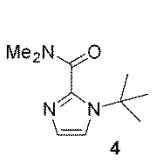

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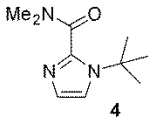

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xl018 after column
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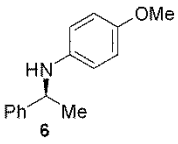

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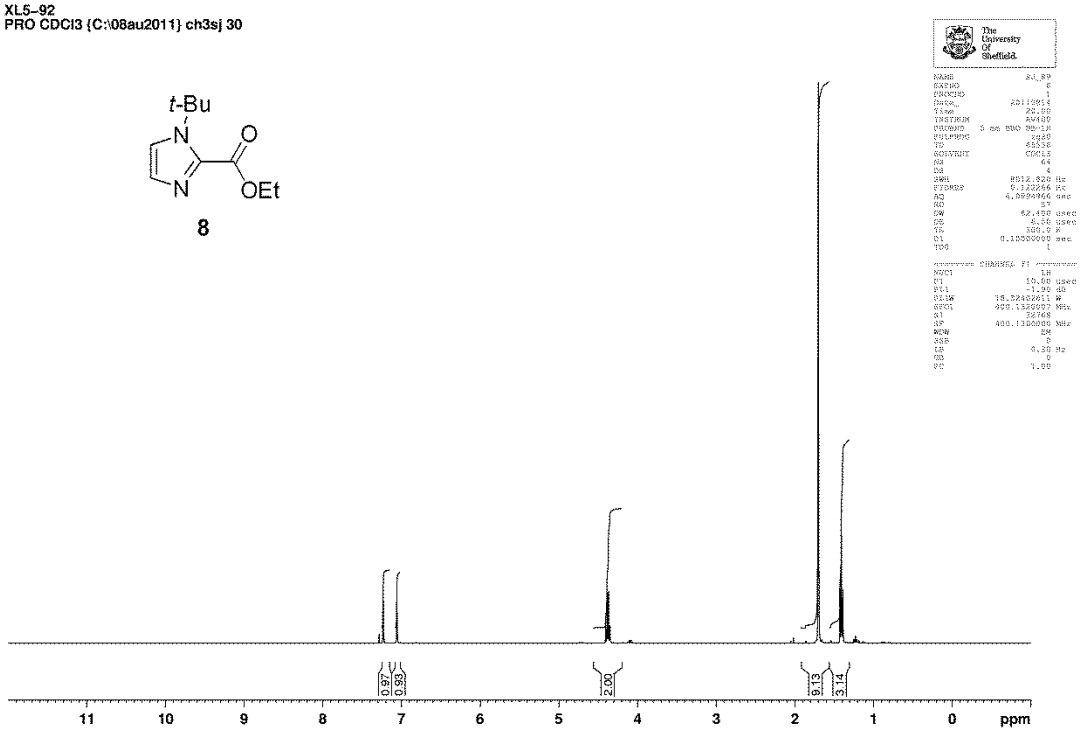

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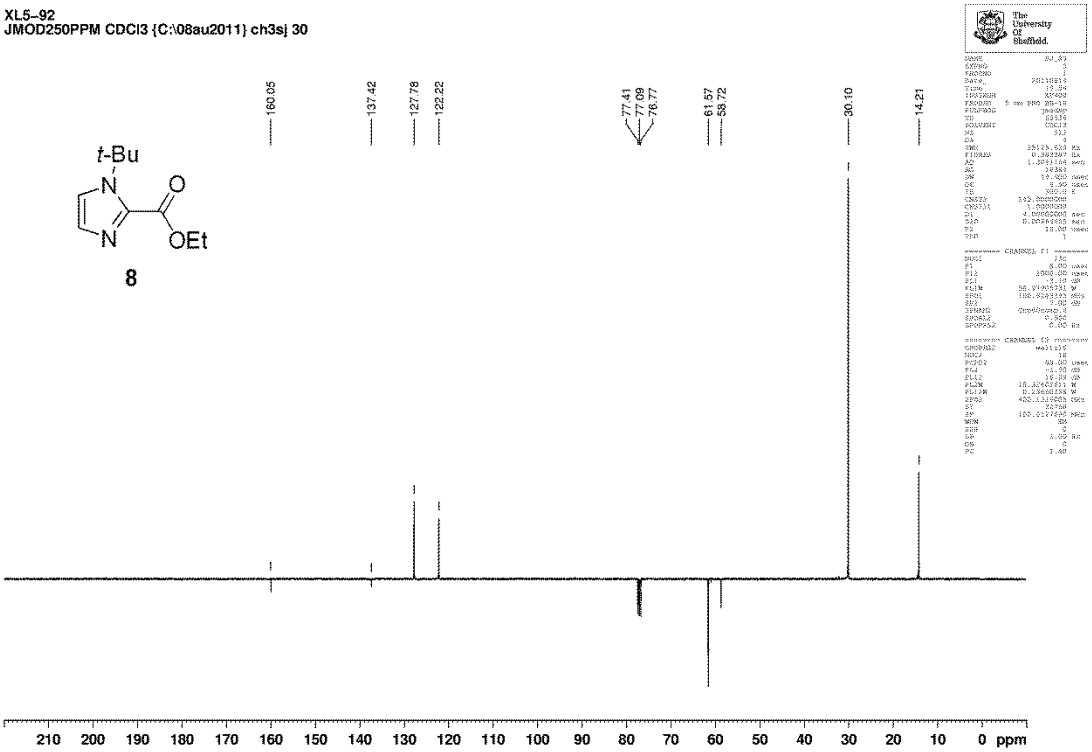

XL5–82
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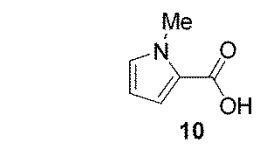

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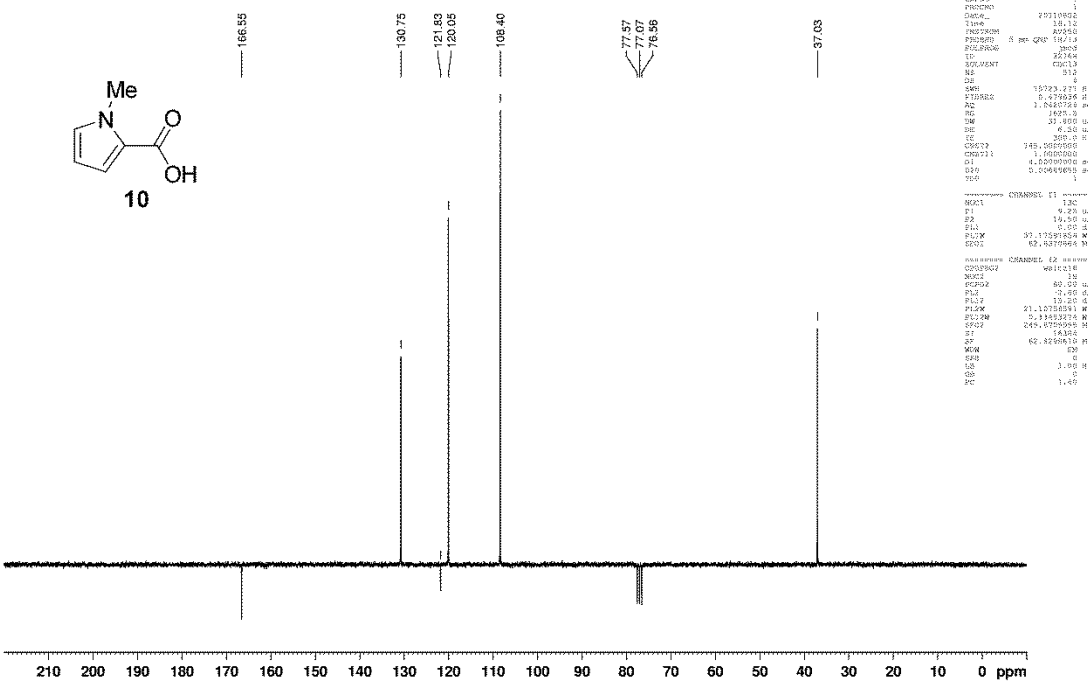

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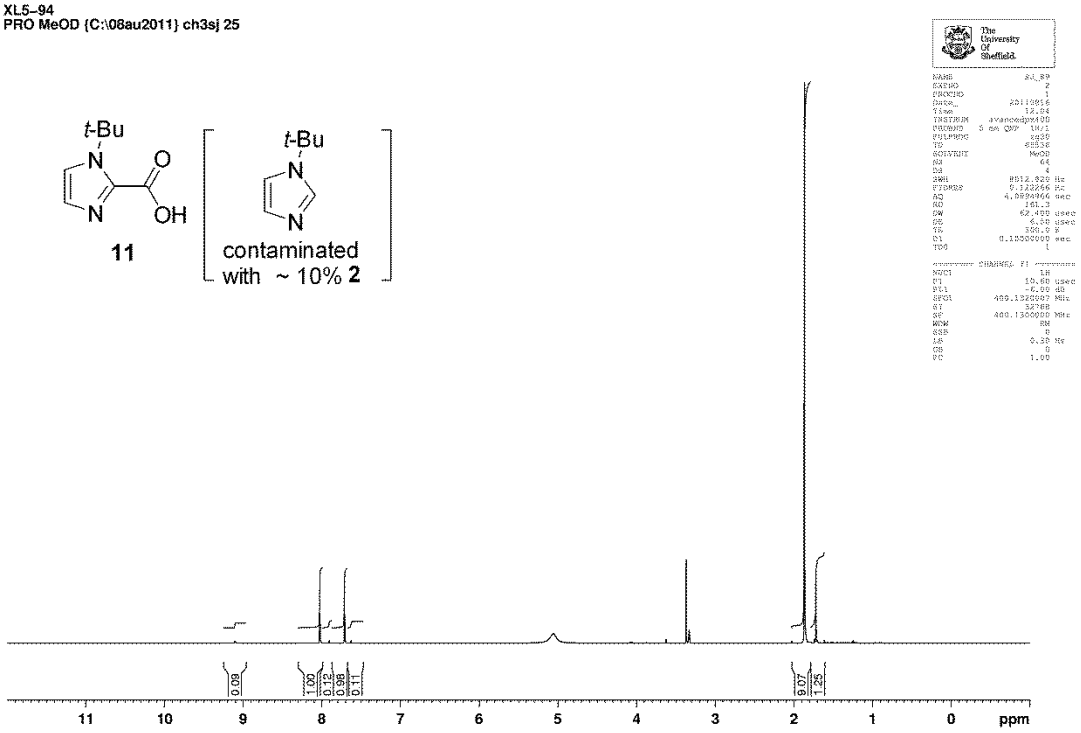
PRO MeOD {C:\08au2011} ch3sj 25



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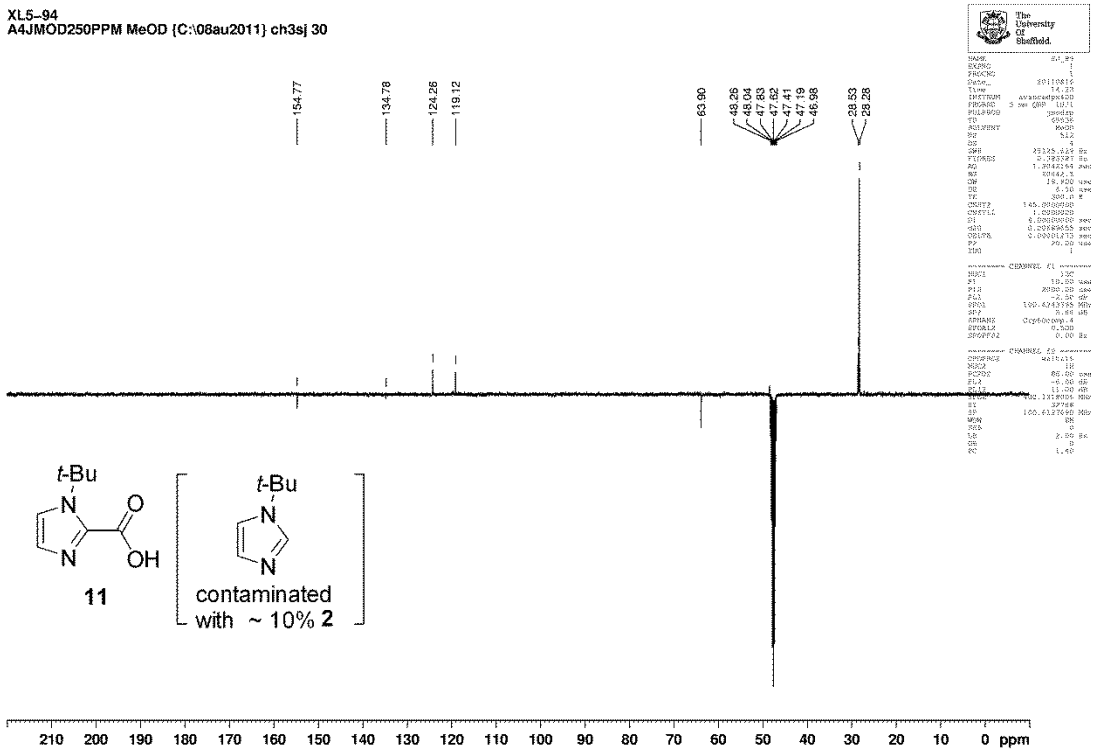
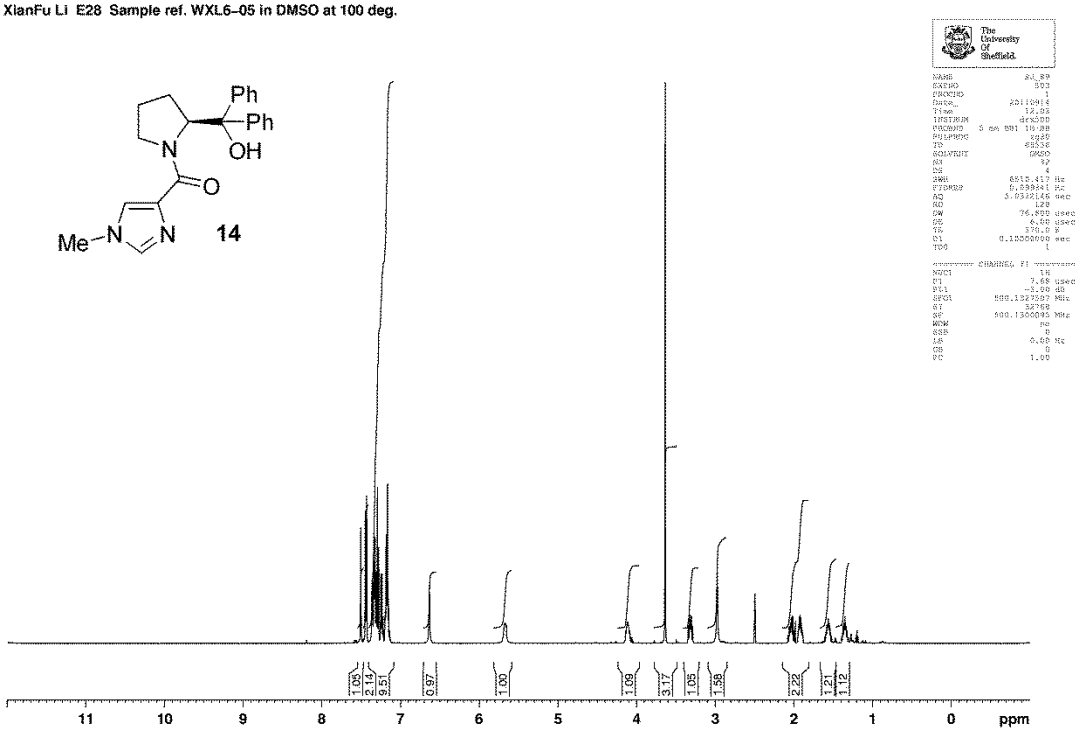
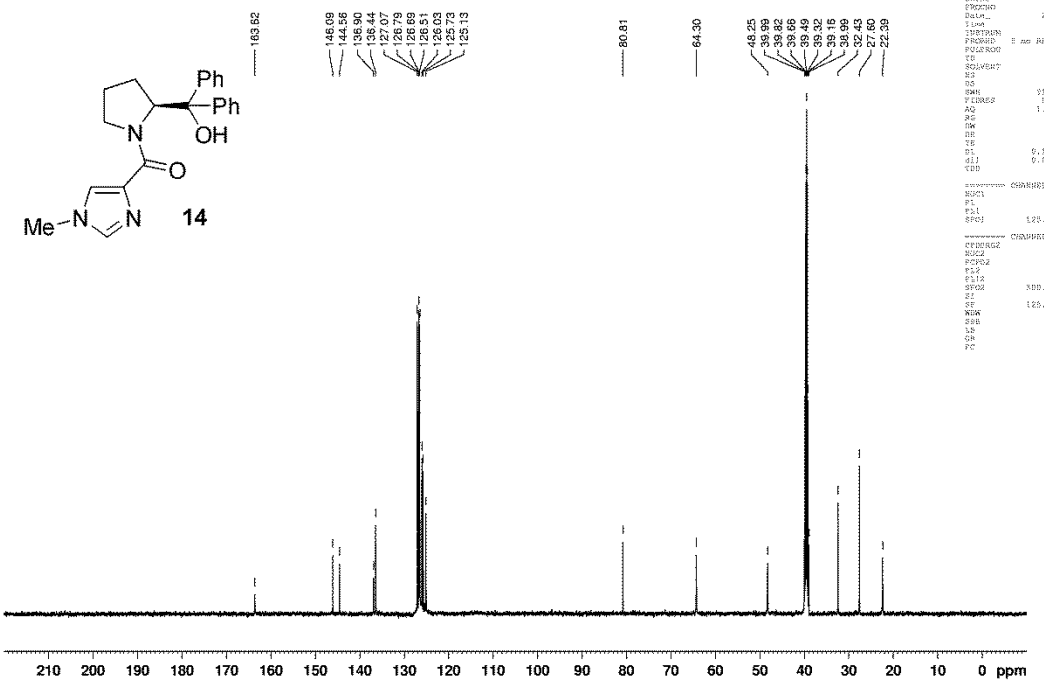


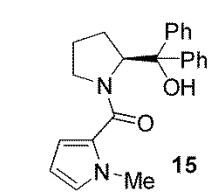
XianFu Li E28 Sample ref. WXL6-05 in DMSO at 100 deg.



XianFu Li E28 Sample ref. WXL6-05 in DMSO at 100 deg.
Backwards linear prediction parameters: NCOEF = 2048 TDOFF = 32



XL5–89
PRO CDCl3 {C:\08au2011} ch3sj 52



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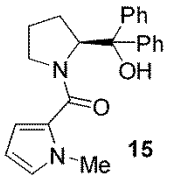

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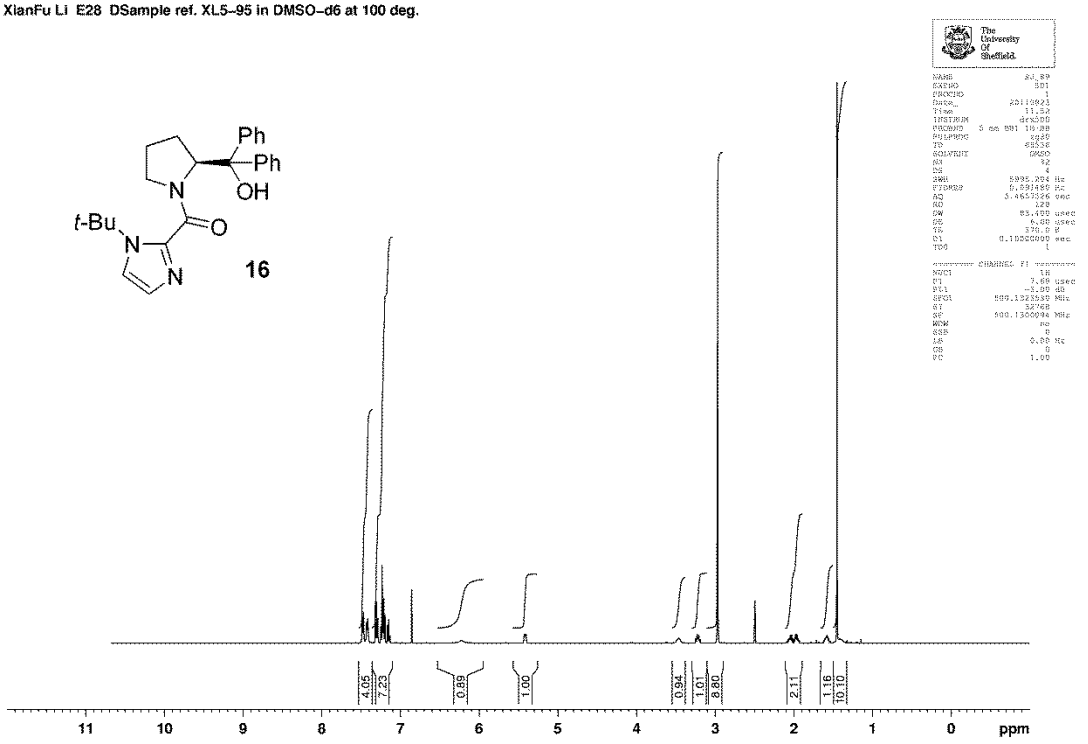
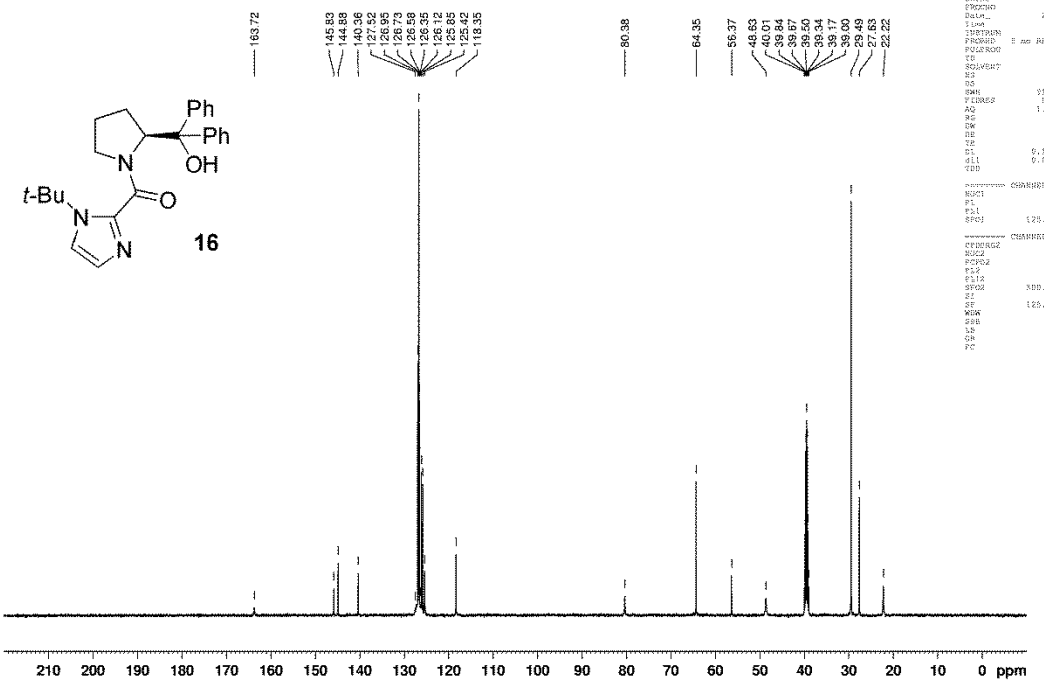
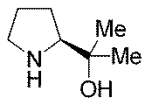
XianFu Li E28 DSample ref. XL5–95 in DMSO–d6 at 100 deg.



XianFu Li E28 Sample ref. XL5–95 in DMSO at 100 deg. C
Backwards linear prediction parameters: NCOEF = 2048 TDOFF = 32



XL3–76 400MHz
PRO CDCl3 {C:\04ap2010} ch3sj 22



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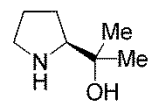
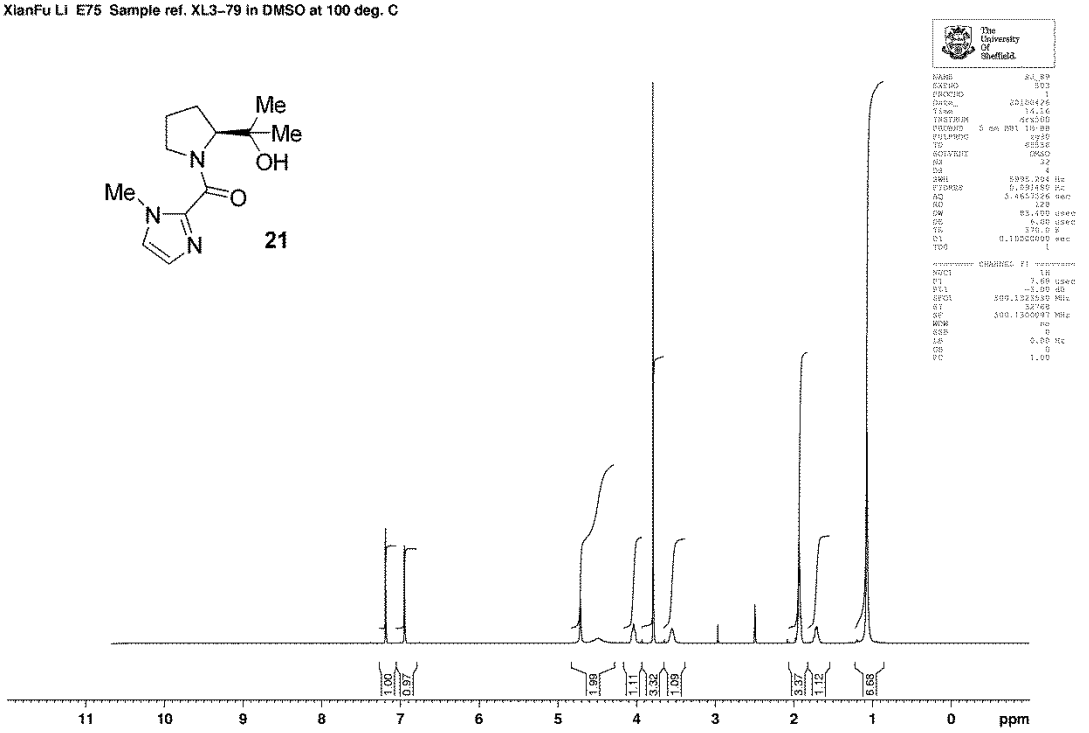
XL3–76 400MHz
JMOD250PPM CDCl3 {C:\04ap2010} ch3sj 22



19

XianFu Li E75 Sample ref. XL3-79 in DMSO at 100 deg. C



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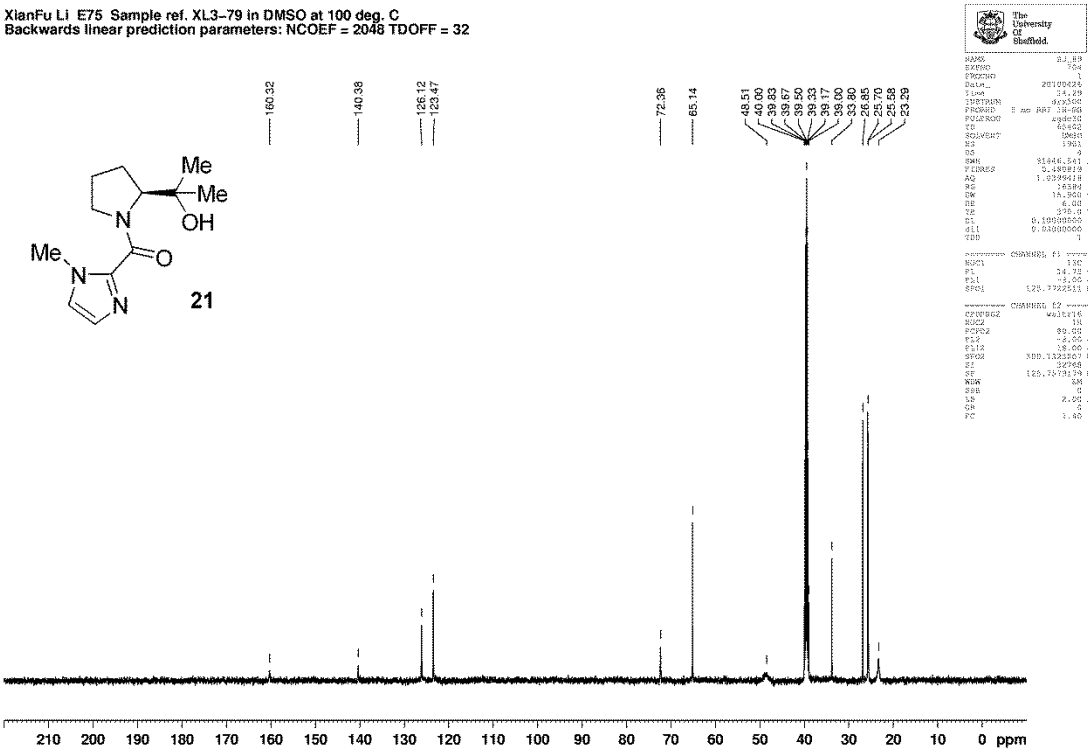
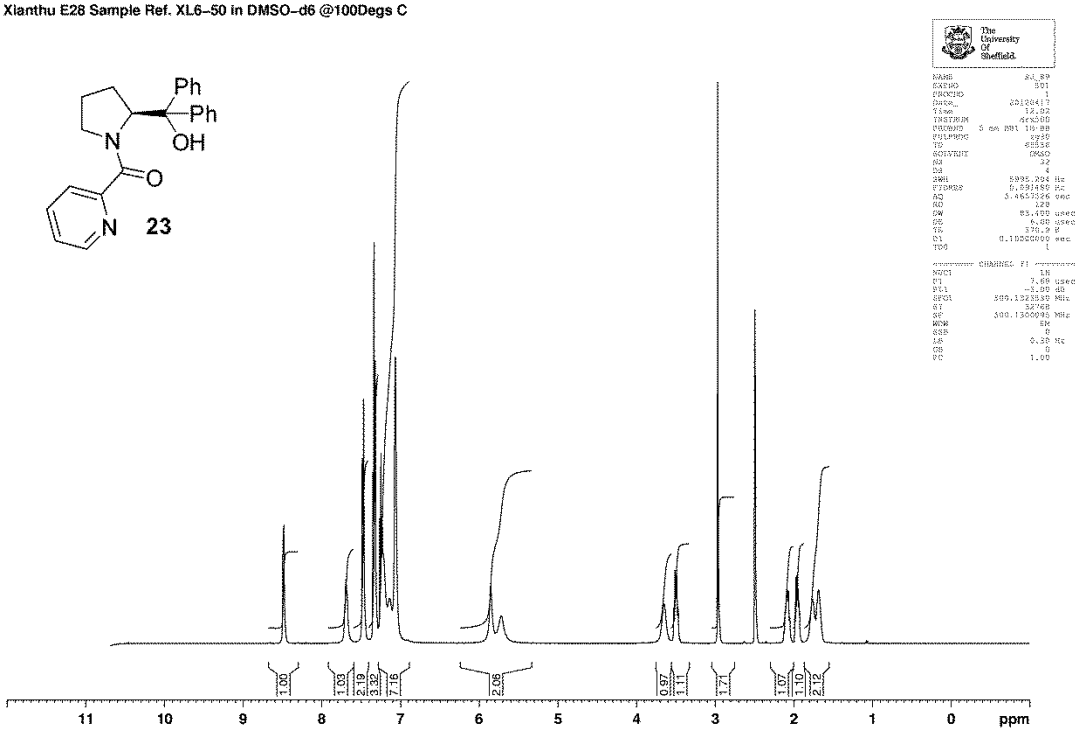
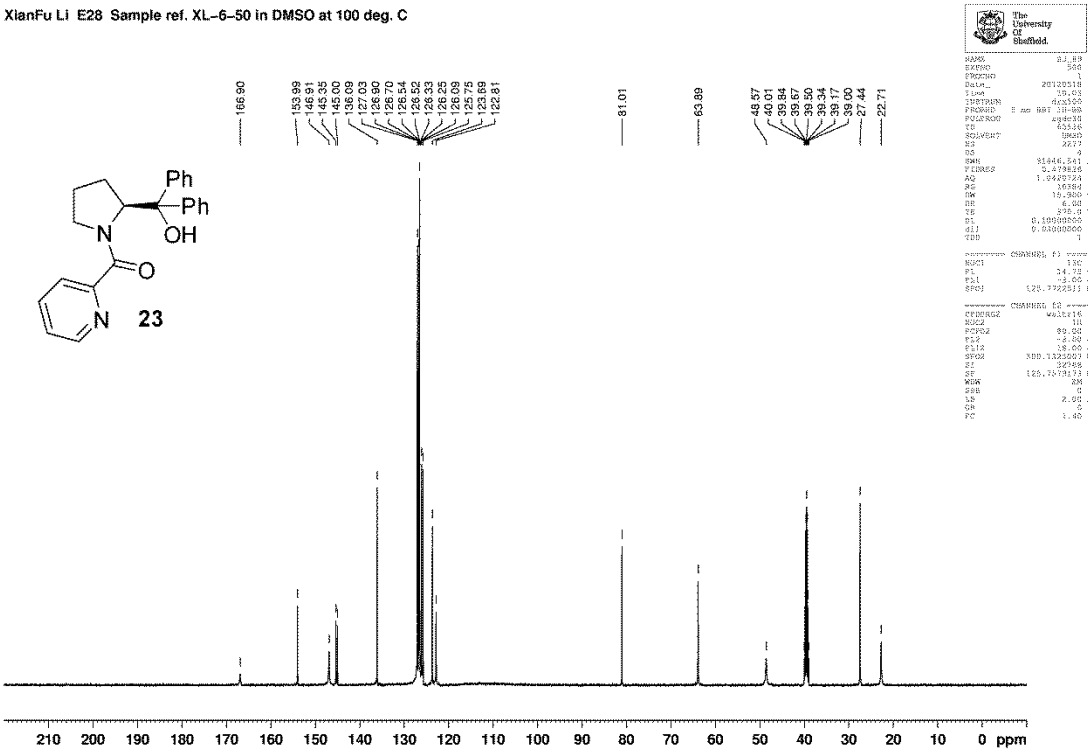
Backwards linear prediction parameters: NCOEF = 2048 TDOFF = 32



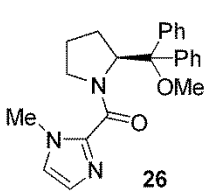
Xianthu E28 Sample Ref. XL6-50 in DMSO-d6 @100Degs C



XianFu Li E28 Sample ref. XL-6-50 in DMSO at 100 deg. C



XL5–75
PRO CDCl3 {C:\08au2011} ch3sj 47



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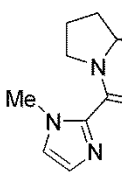
XL5–75
JMOD250PPM CDCl3 {C:\08au2011} ch3sj 47



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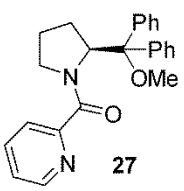
XL6–66
PRO CDCl3 {C:\04Apr2012} ch3sj 17



XL6–66
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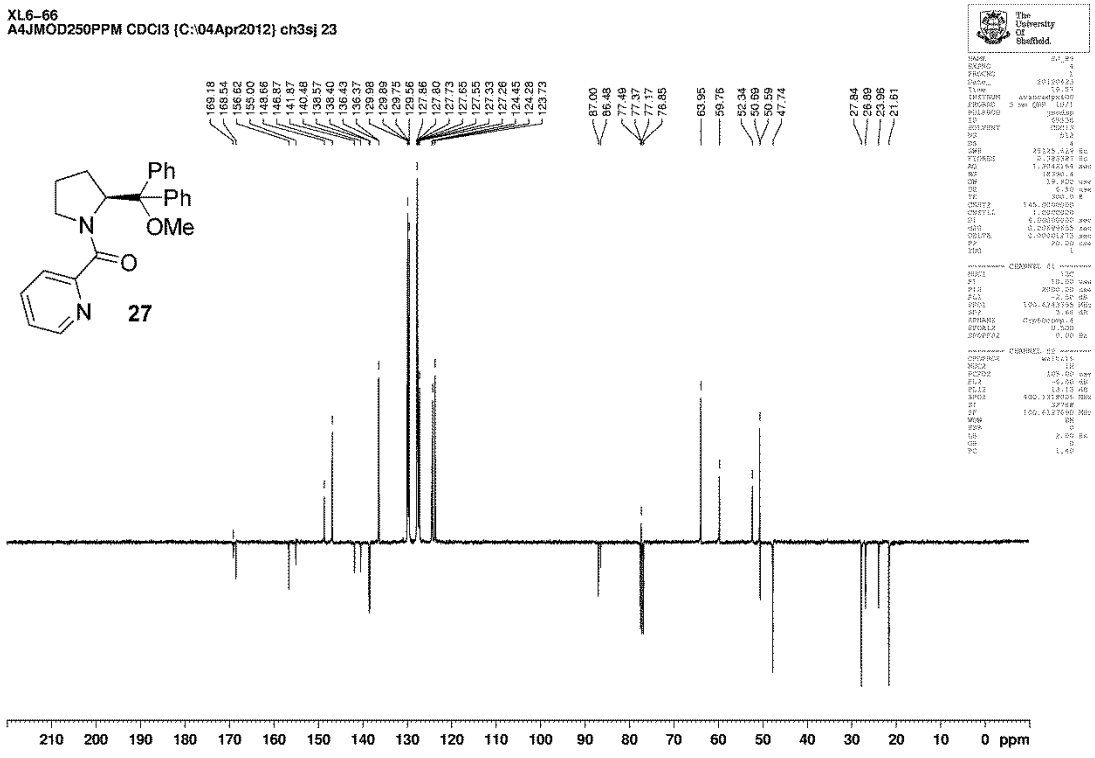
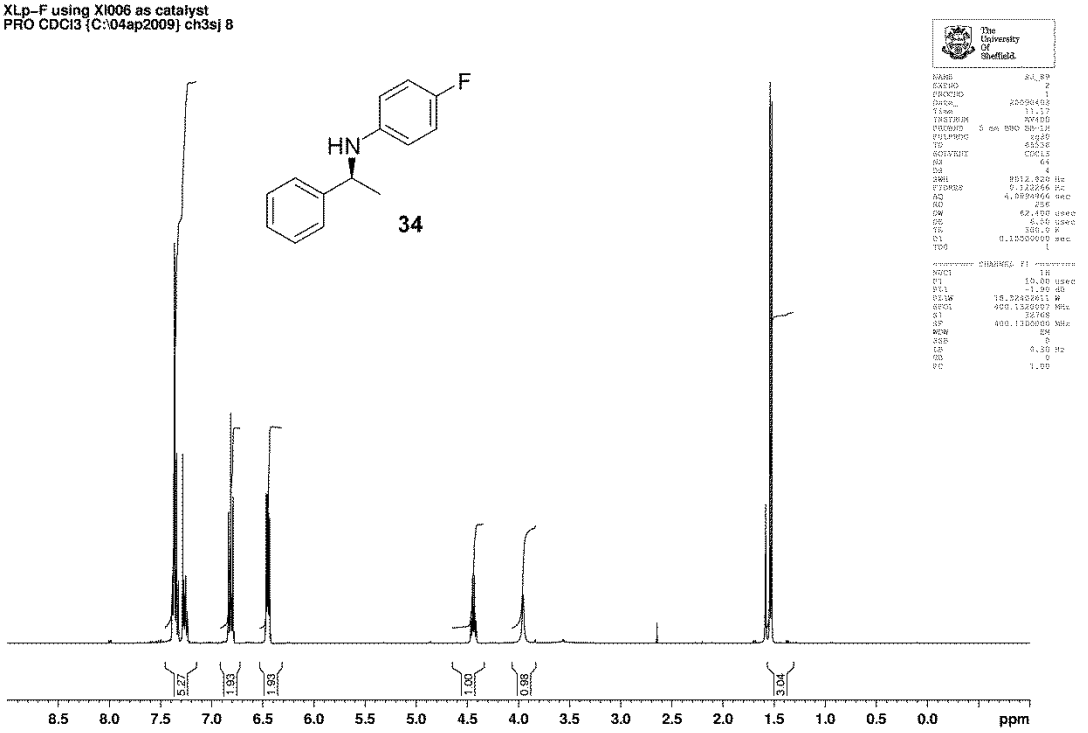
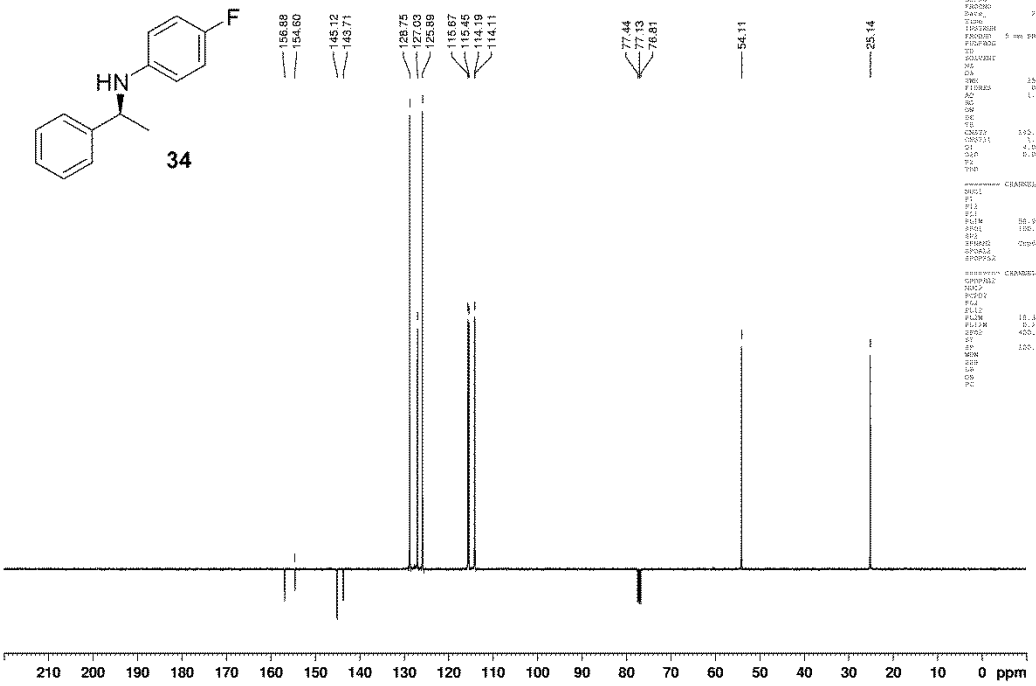


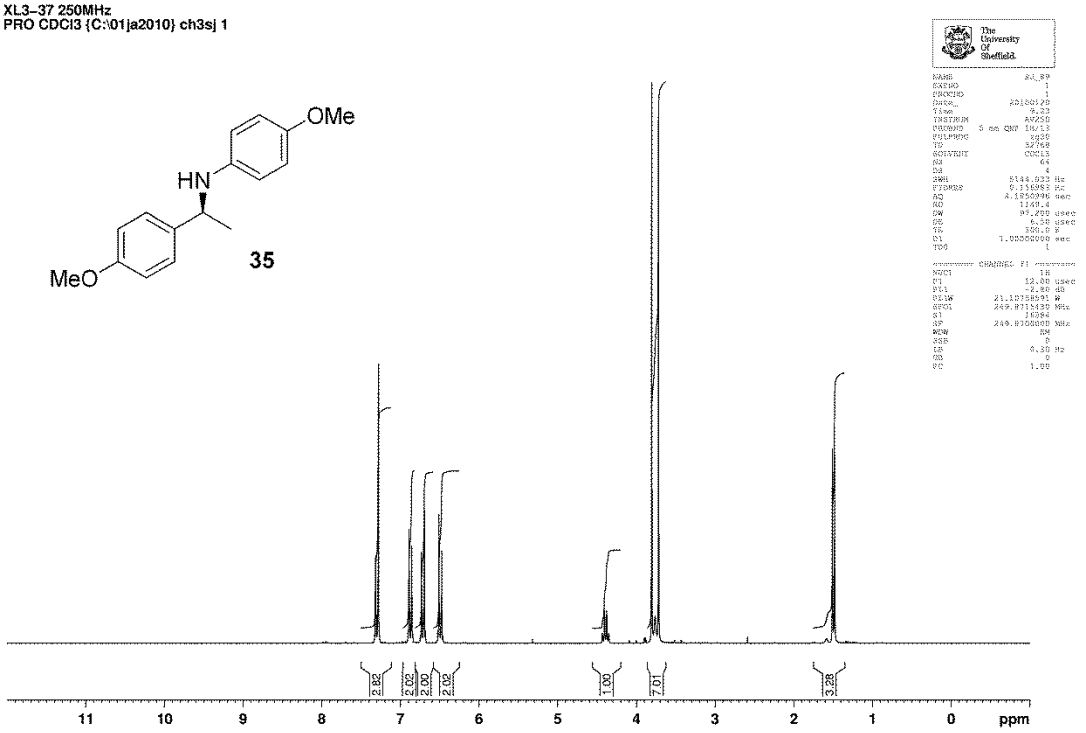
XLp–F using XI006 as catalyst
PRO CDCl3 {C:\04ap2009} ch3sj 8



XL078 400MHz
JMOD250PPM CDCl3 {C:\04ap2009} ch3sj 53



XL3-37 250MHz
PRO CDCl3 {C:\01ja2010} ch3sj 1



XL3-39 250MHz
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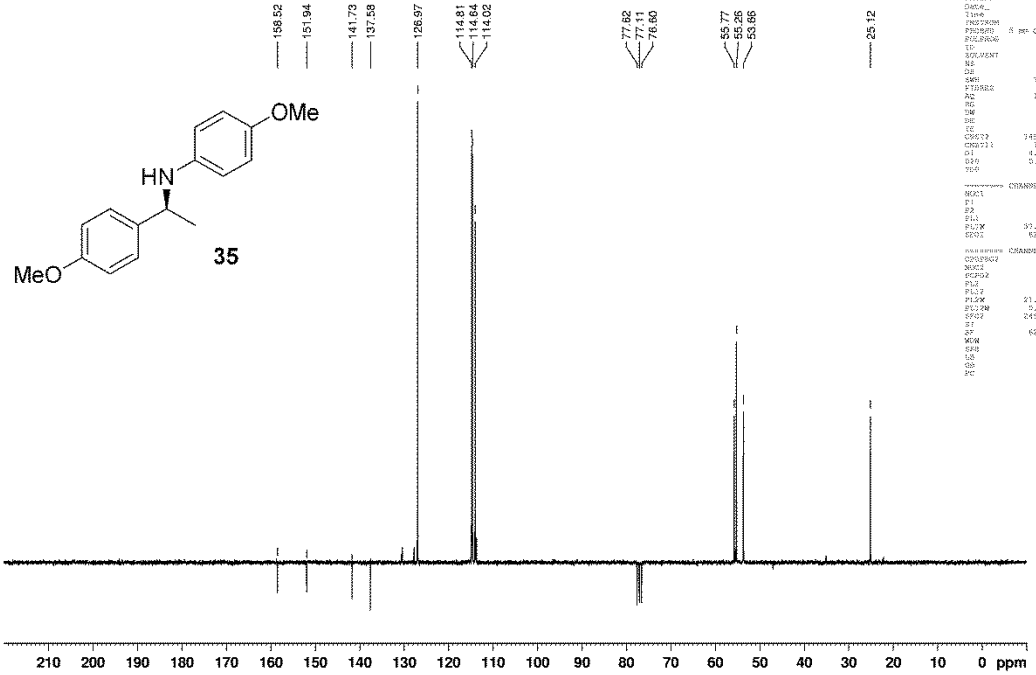

XL3–34 400MHz
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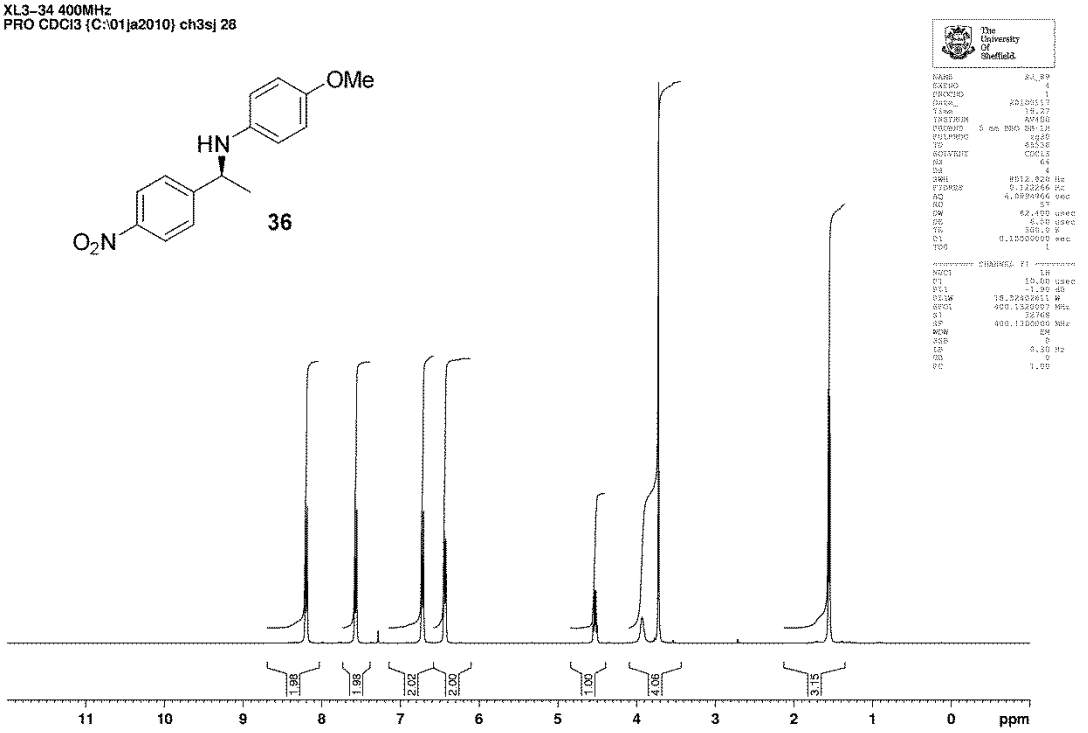

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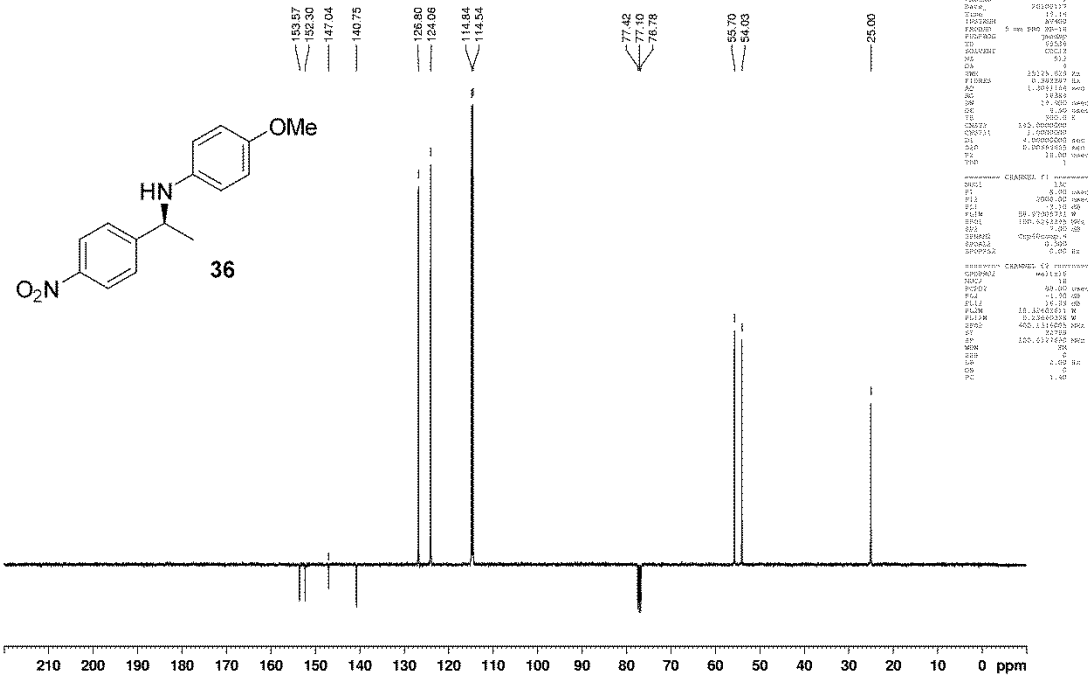

XL3–66 250MHz
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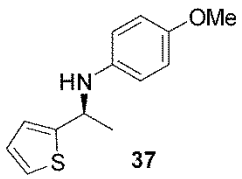

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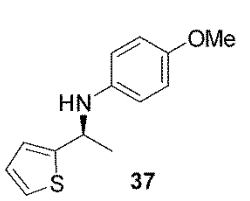

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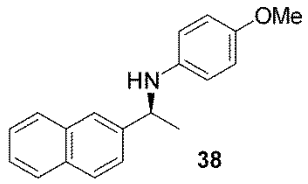

XL3–43 250MHz
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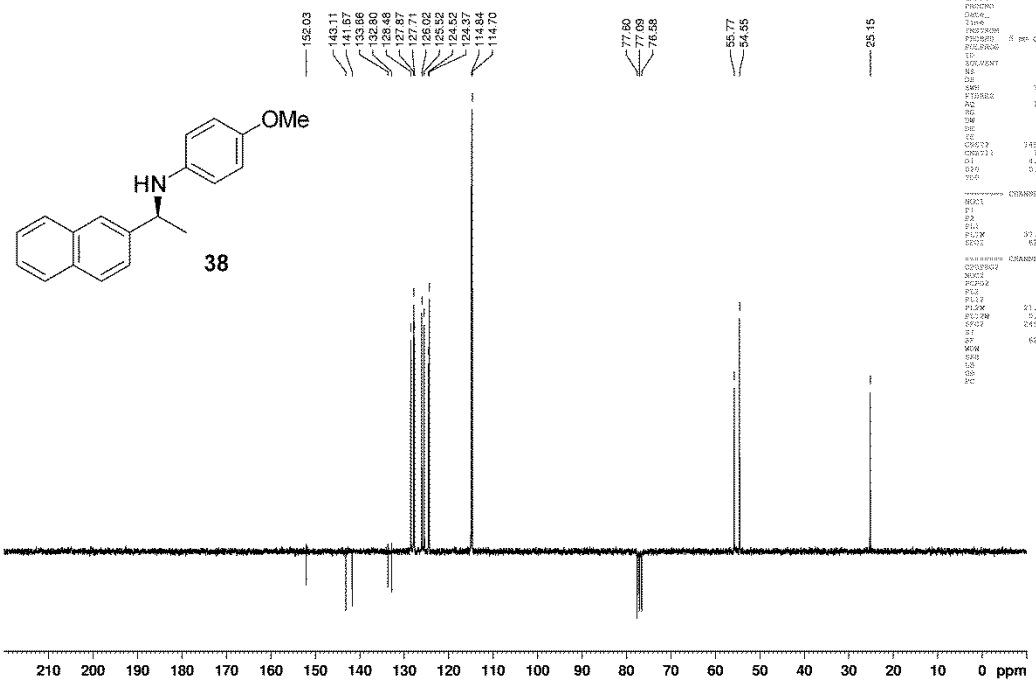

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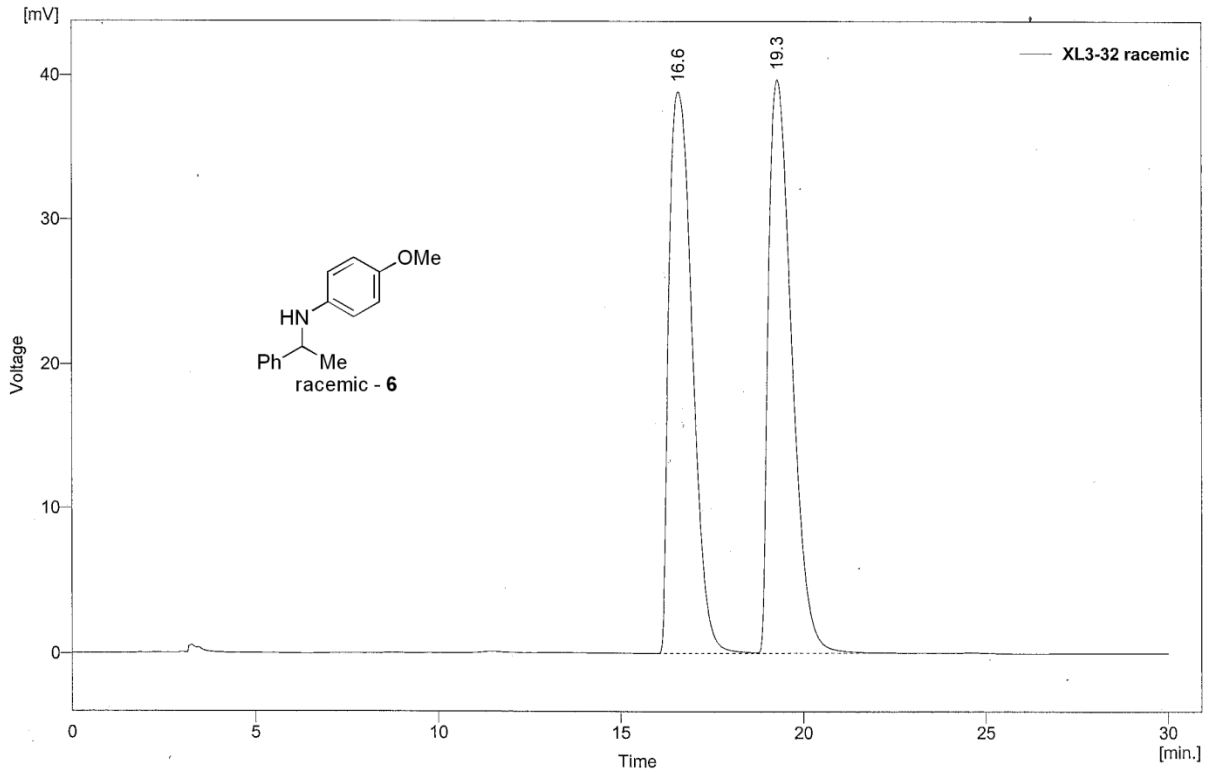
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-32	Sample	: XL3-32
Calibration	: XL3-32 racemic	Chromatogram	: DATA\XL3-32 racemic

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 10/01/2010 16:00
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 2% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 30.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



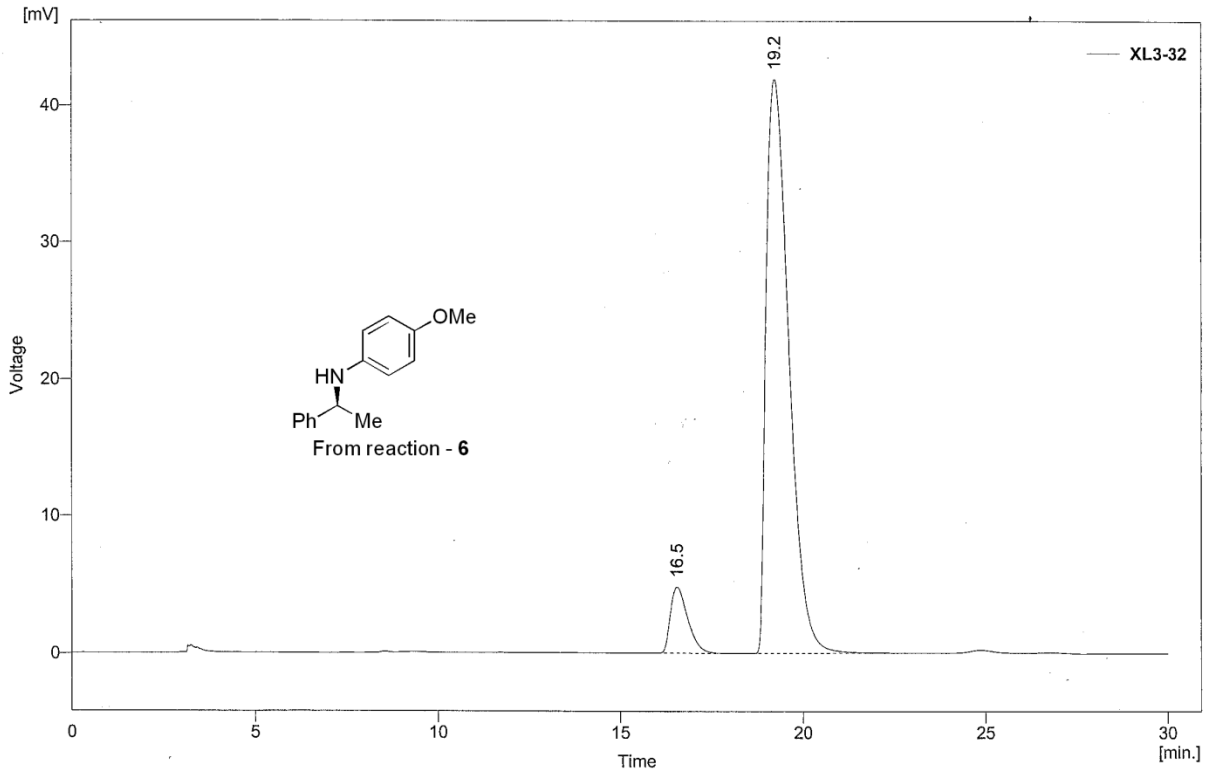
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	16.590	17196.929	388.580	49.7	49.5	0.72
2	19.300	17434.270	396.850	50.3	50.5	0.70
	Total	34631.199	785.431	100.0	100.0	

Created	: 10/01/2010 12:34:15	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-32	Sample	: XL3-32
Calibration	: XL3-32	Chromatogram	: DATA\XL3-32

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 10/01/2010 15:21
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 2% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 30.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



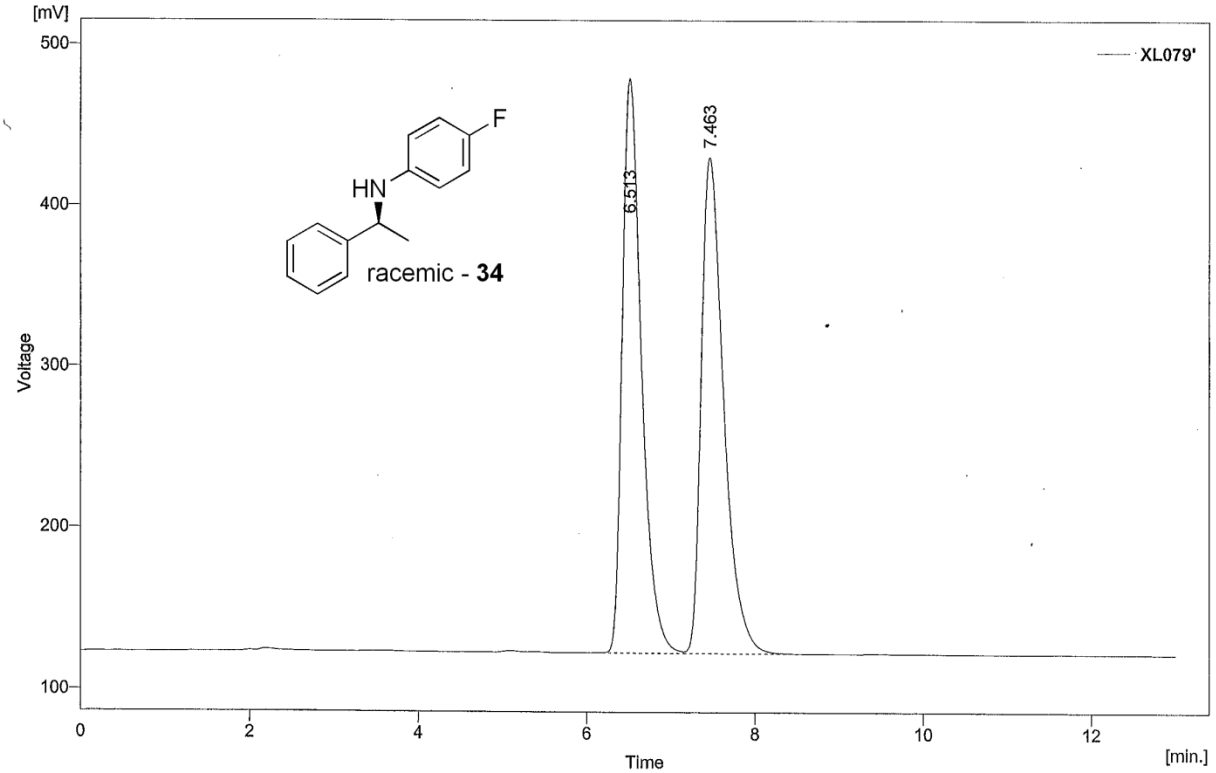
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	16.547	1589.334	48.278	8.1	10.3	0.51
2	19.233	17979.914	419.226	91.9	89.7	0.68
	Total	19569.247	467.504	100.0	100.0	

Created	: 04/04/2009 19:02:19	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL078	Sample	: XL078
Calibration	: XL079'	Chromatogram	: DATA\XL079'

Method	: Cellucoat	By	: Clarity
Description	: Kromasil OD		
Created	: 24/08/2004 16:25	Modified	: 04/04/2009 19:02
Column	: Kromasil 3-Cellucoat OD	Detection	: UV@254nm
Mobile Phase	: 1% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 13.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



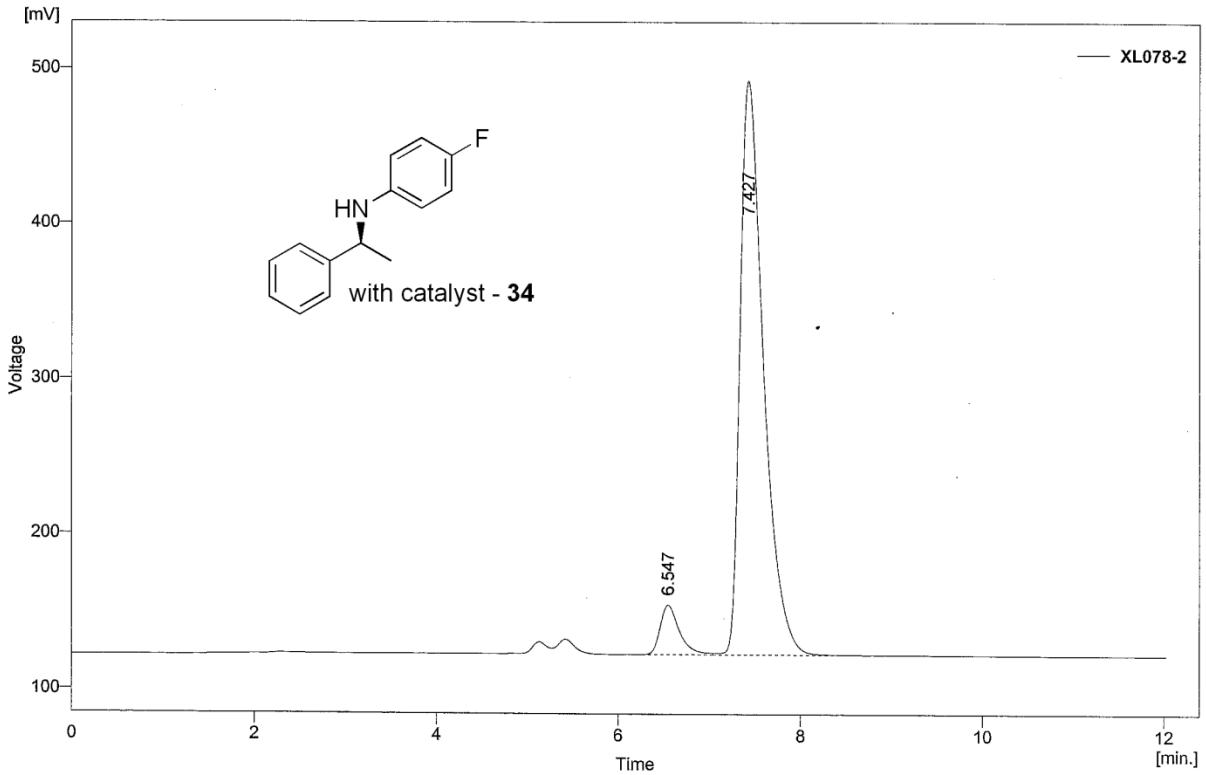
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.513	5684.755	356.335	49.9	53.7	0.24
2	7.463	5696.551	307.619	50.1	46.3	0.28
	Total	11381.306	663.954	100.0	100.0	

Created	: 04/04/2009 19:48:47	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL078	Sample	: XL078
Calibration	: XL078-2	Chromatogram	: DATA\XL078-2

Method	: Cellucoat	By	: Clarity
Description	: Kromasil OD		
Created	: 24/08/2004 16:25	Modified	: 04/04/2009 19:48
Column	: Kromasil 3-Cellucoat OD	Detection	: UV@254nm
Mobile Phase	: 1% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 13.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



Result Table - Calculation Method Uncal

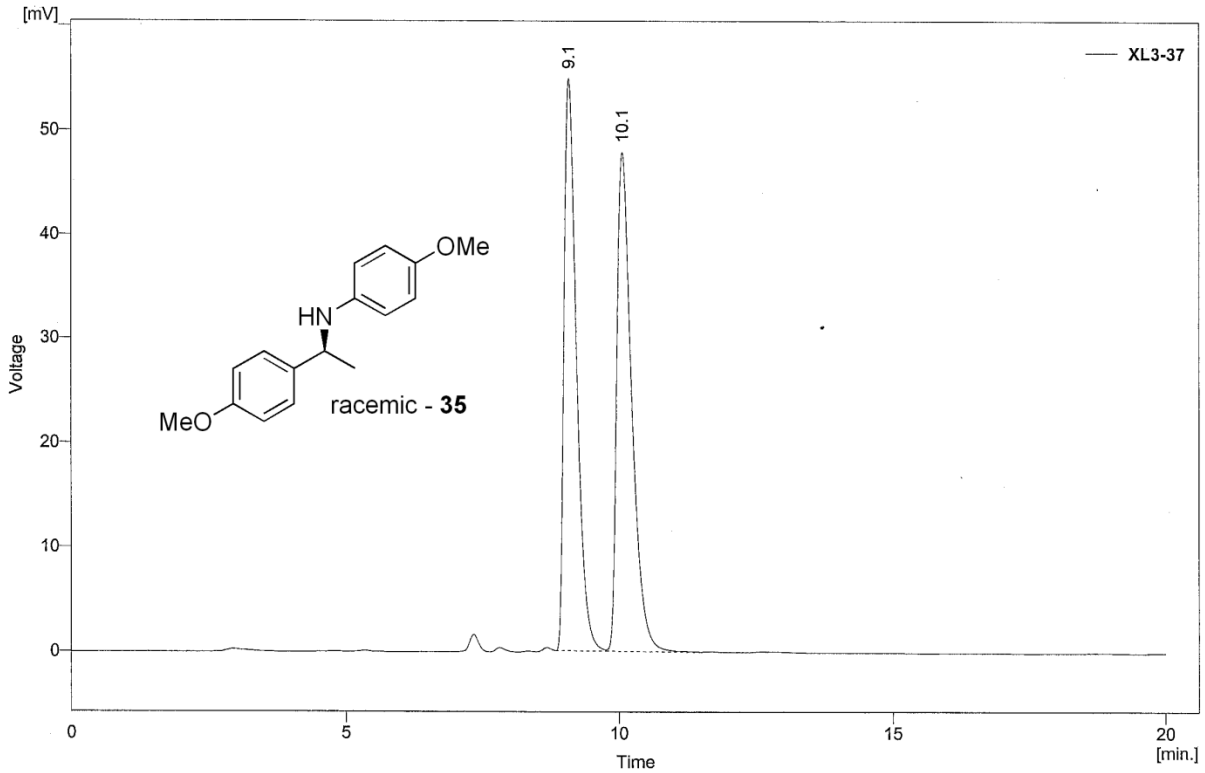
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.547	468.409	31.917	6.6	7.9	0.22
2	7.427	6612.641	369.652	93.4	92.1	0.27
	Total	7081.050	401.569	100.0	100.0	

86.8% ee

Created	: 18/01/2010 12:49:13	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-37	Sample	: XL3-37
Calibration	: XL3-37	Chromatogram	: DATA\XL3-37

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 18/01/2010 15:26
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 10% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 20.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



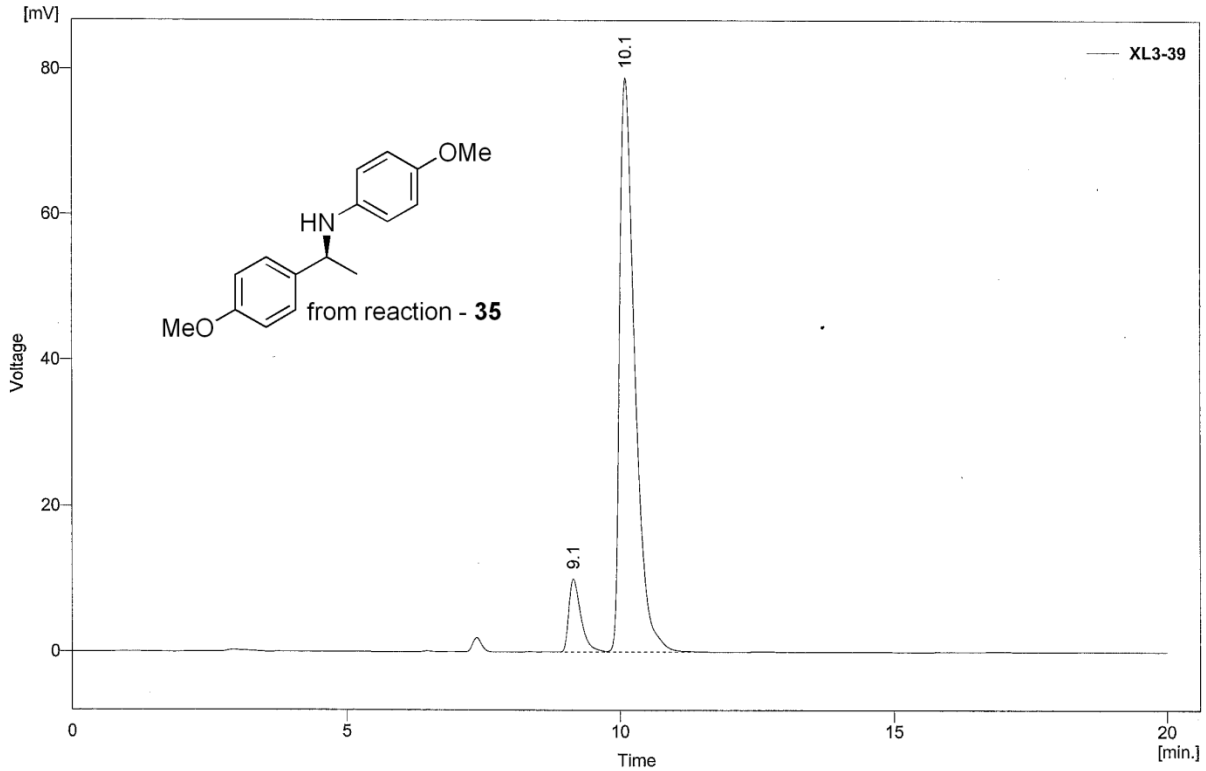
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.077	8811.267	548.372	49.1	53.4	0.25
2	10.063	9137.374	478.874	50.9	46.6	0.29
	Total	17948.641	1027.246	100.0	100.0	

Created	: 18/01/2010 15:50:54	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-39	Sample	: XL3-39
Calibration	: XL3-39	Chromatogram	: DATA\XL3-39

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 18/01/2010 15:50
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 10% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 20.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



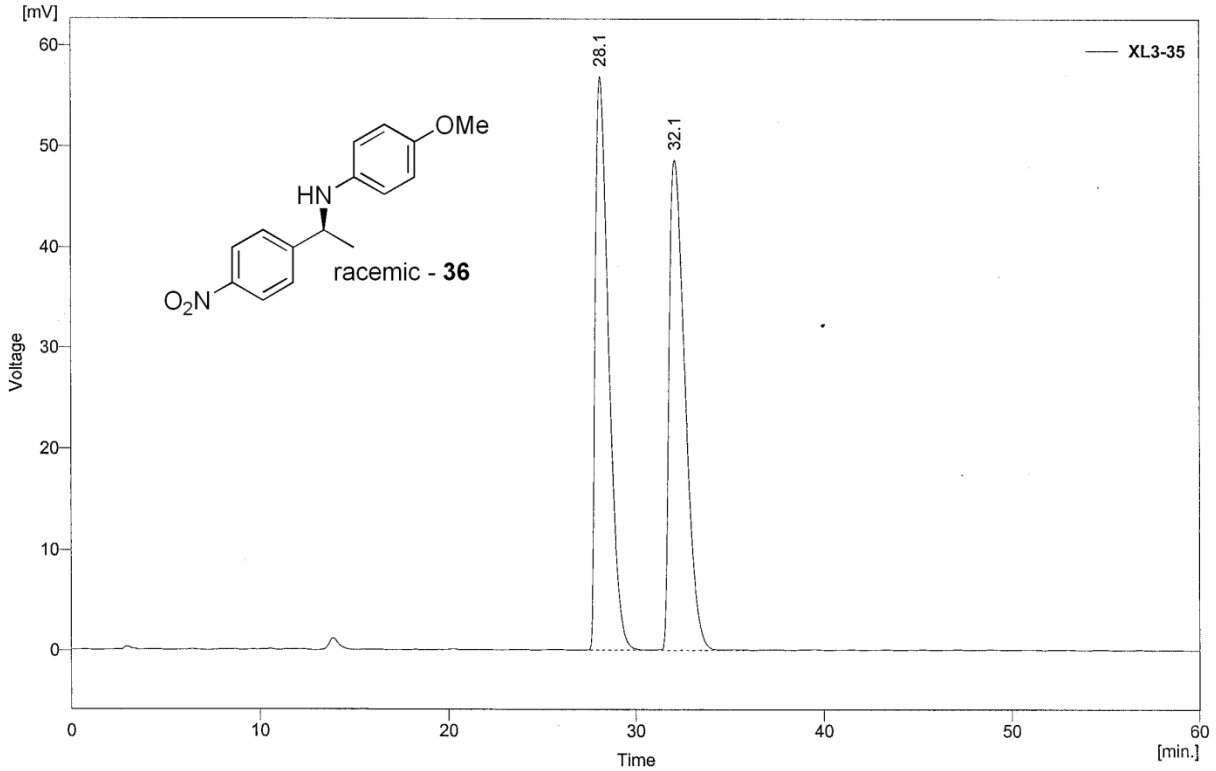
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.140	1559.629	100.719	9.3	11.3	0.23
2	10.103	15275.953	788.398	90.7	88.7	0.29
	Total	16835.583	889.117	100.0	100.0	

Created	: 15/01/2010 11:10:21	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-35	Sample	: XL3-35
Calibration	: XL3-35	Chromatogram	: DATA\XL3-35

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 15/01/2010 11:10
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 10% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 80.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



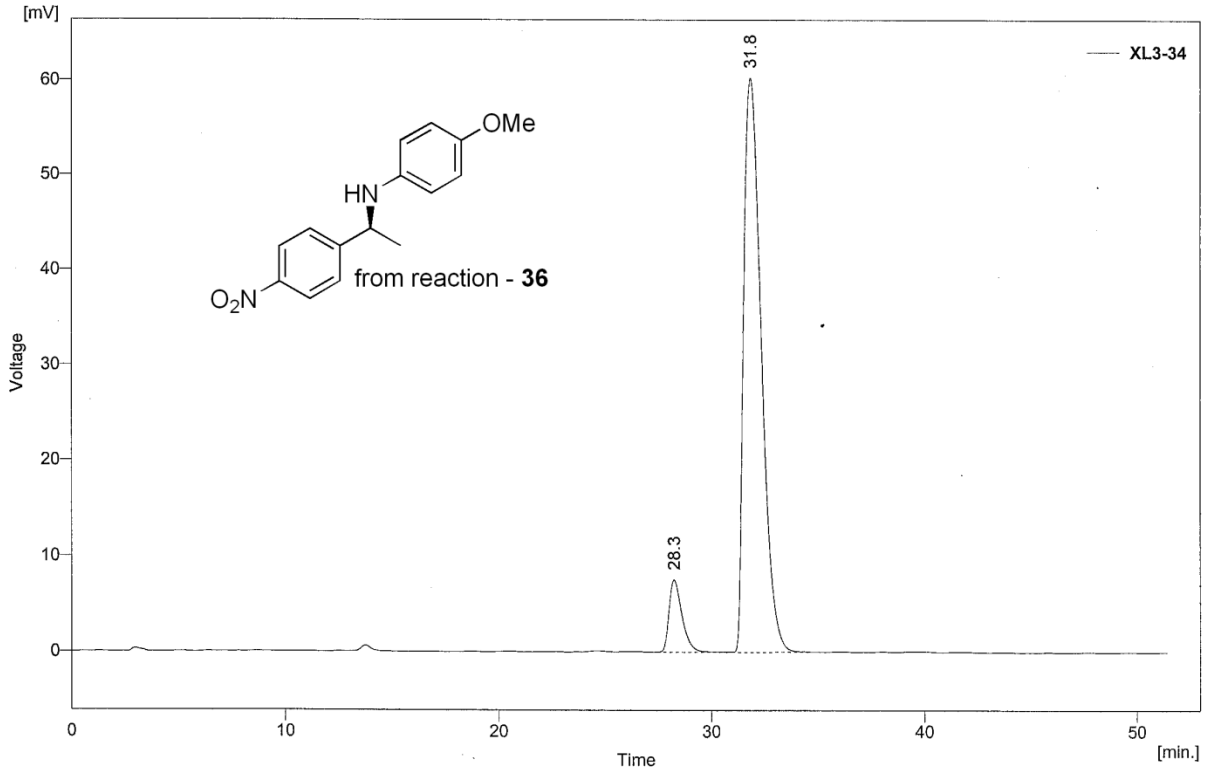
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	28.110	28290.391	568.854	50.0	53.9	0.78
2	32.103	28339.401	486.131	50.0	46.1	0.92
	Total	56629.793	1054.985	100.0	100.0	

Created	: 15/01/2010 14:09:53	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-34	Sample	: XL3-34
Calibration	: XL3-34	Chromatogram	: DATA\XL3-34

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 15/01/2010 14:11
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 10% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 60.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



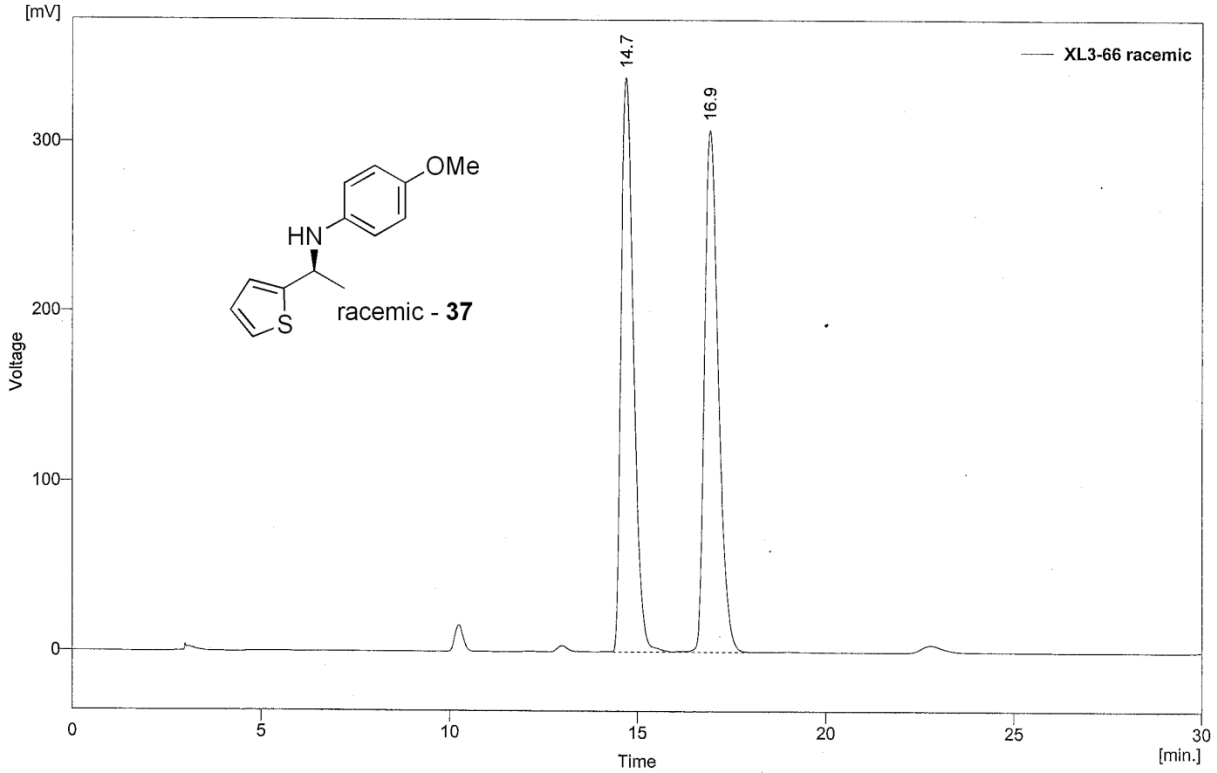
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	28.250	3245.013	75.631	8.6	11.1	0.65
2	31.830	34463.271	602.775	91.4	88.9	0.91
	Total	37708.284	678.406	100.0	100.0	

Created	: 04/03/2010 10:06:40	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-66	Sample	: XL3-66
Calibration	: XL3-66 racemic	Chromatogram	: DATA\XL3-66 racemic

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 04/03/2010 10:08
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 2% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 60.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



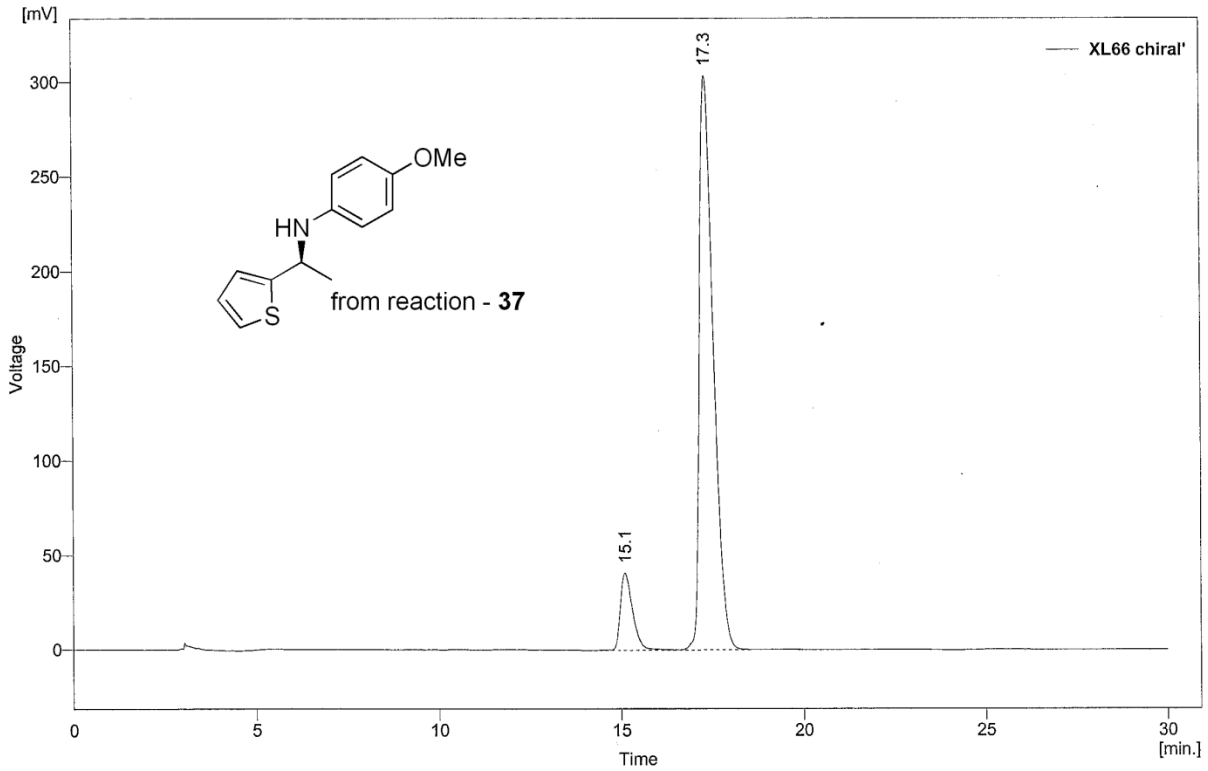
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	14.690	7854.266	338.065	49.8	52.4	0.37
2	16.920	7902.793	307.130	50.2	47.6	0.40
	Total	15757.059	645.195	100.0	100.0	

Created	: 04/03/2010 19:40:58	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL66 chiral	Sample	: XL66 chiral
Calibration	: XL66 chiral'	Chromatogram	: DATA\XL66 chiral'

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 04/03/2010 19:40
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 2% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 30.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



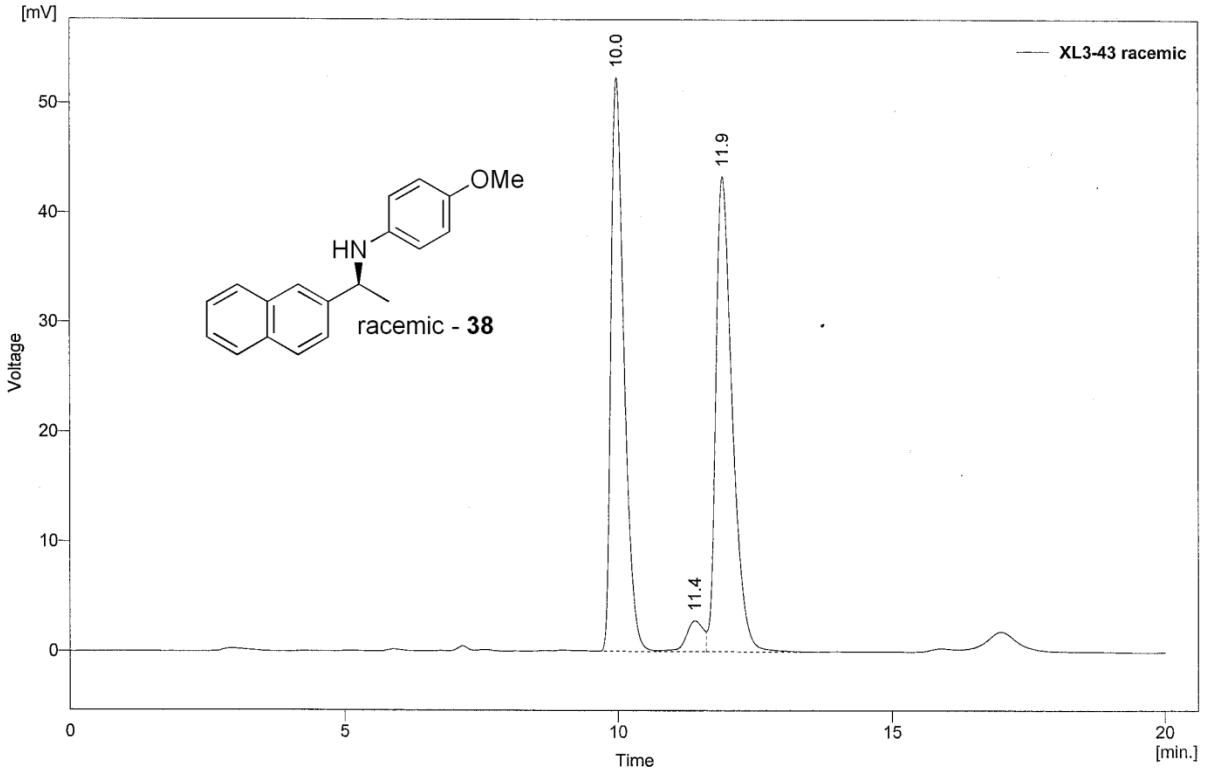
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	15.113	959.038	40.887	10.7	11.9	0.35
2	17.337	8031.051	303.354	89.3	88.1	0.41
	Total	8990.090	344.241	100.0	100.0	

Created	: 22/01/2010 11:26:21	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-43 racemic	Sample	: XL3-43 racemic
Calibration	: XL3-43 racemic	Chromatogram	: DATA\XL3-43 racemic

Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 22/01/2010 11:26
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 10% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 20.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



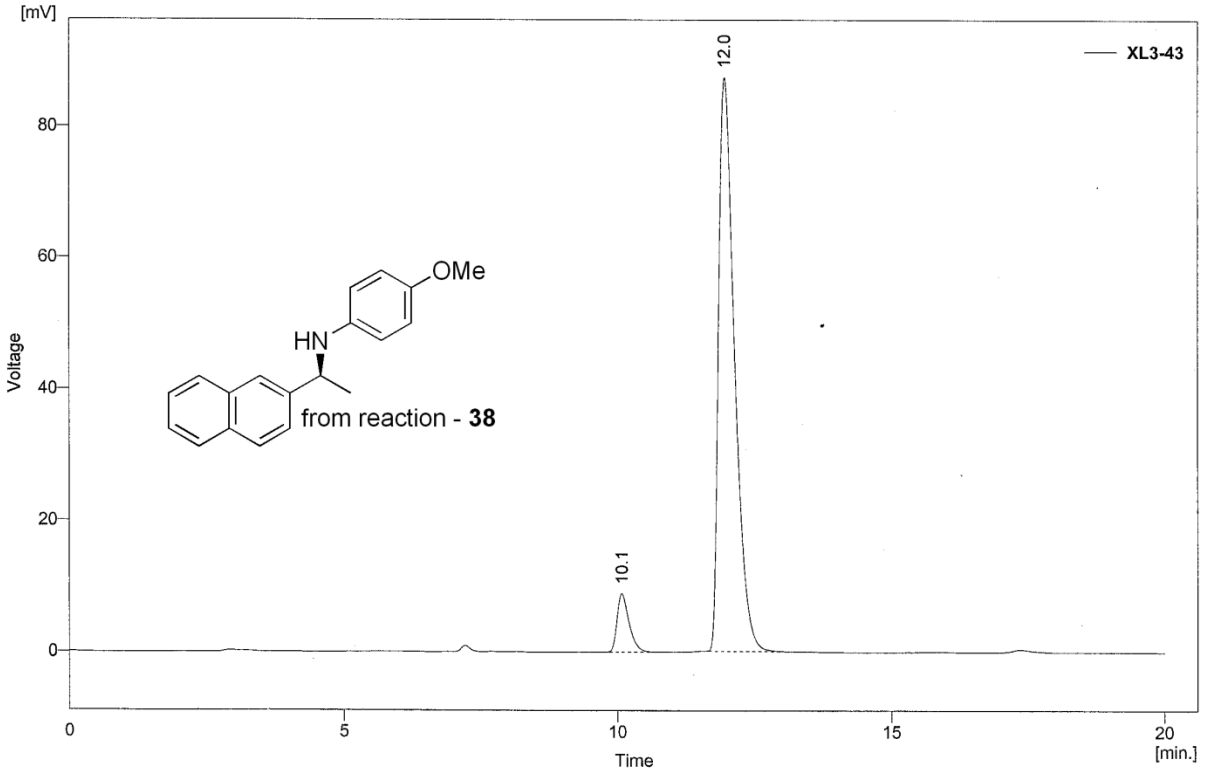
Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.977	8825.033	523.673	47.7	53.1	0.26
2	11.400	607.810	28.245	3.3	2.9	0.37
3	11.913	9052.532	433.507	49.0	44.0	0.32
	Total	18485.375	985.425	100.0	100.0	

Created	: 22/01/2010 12:04:25	By	: Clarity
Project	: Work3	Report Style	: Instrument
Sample ID	: XL3-43	Sample	: XL3-43
Calibration	: XL3-43	Chromatogram	: DATA\XL3-43

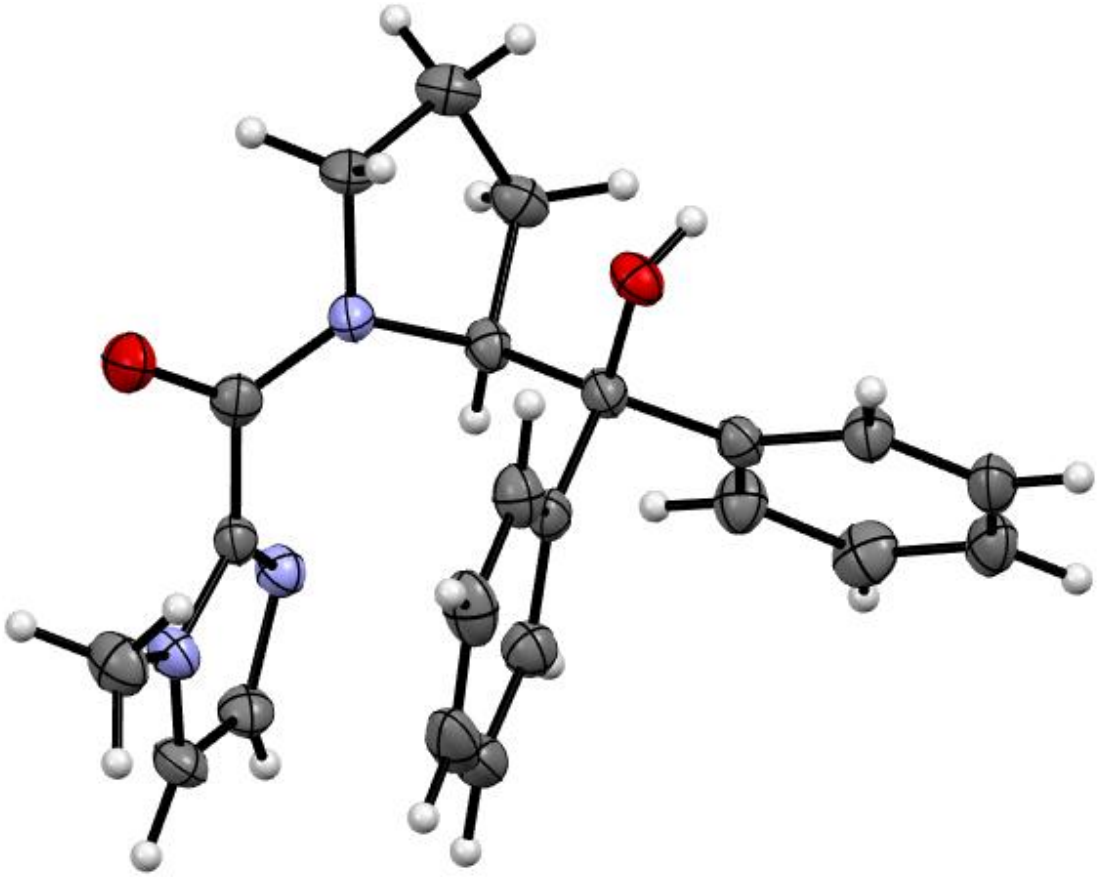
Method	: Cellulose-1	By	: Clarity
Description	: Cellulose-1		
Created	: 24/08/2004 16:25	Modified	: 22/01/2010 12:04
Column	: Phenomenex Lux 3um Cellulose-1	Detection	: UV@254nm
Mobile Phase	: 10% ipa in hexane	Temperature	: RT
Flow Rate	: 1mL/min	Pressure	:
Note	:		

Autostop	: 20.00, min	External Start	: Start Only, Down
Detector 1	: Signal 1	Range 1	: Bipolar, 10000 mV, 10 Samp. per Sec.
Subtraction chromatogram	: (None)	Matching	: No Change



Result Table - Calculation Method Uncal

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	10.080	1370.414	88.888	7.3	9.2	0.24
2	11.963	17476.951	873.441	92.7	90.8	0.31
	Total	18847.365	962.329	100.0	100.0	



X-ray crystallographic representation of catalyst **17**. Thermal ellipsoids are shown at 50% probability. Submitted to the CCDC as 1517809