

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

Xianfu Li, Andrew T. Reeder, Federica Torri, Harry Adams and Simon Jones*

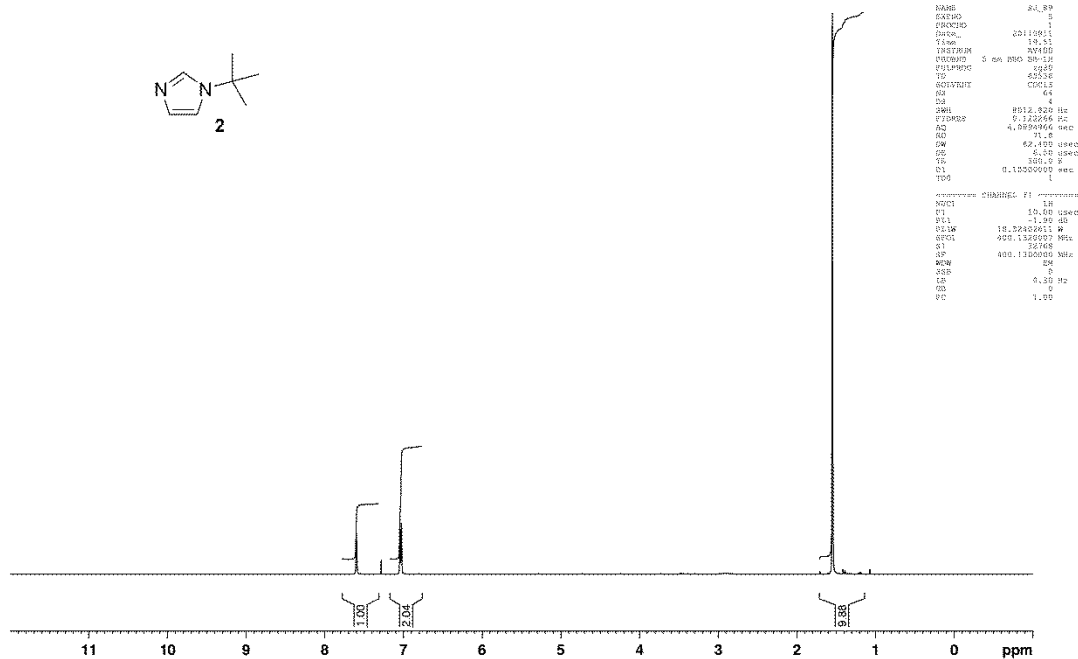
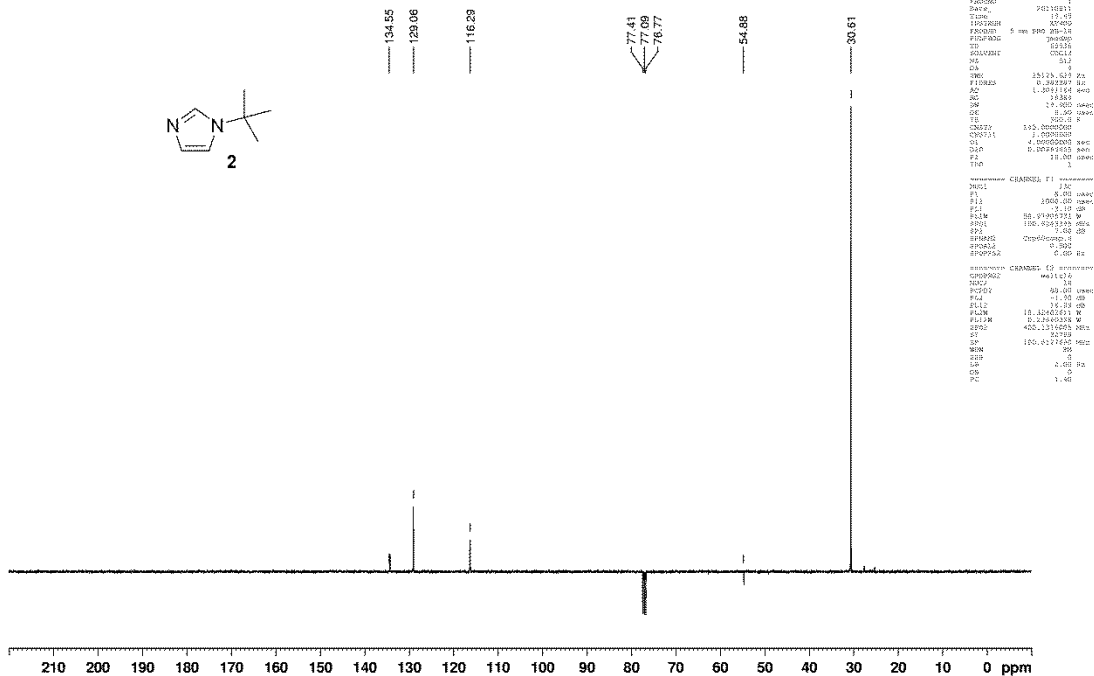
Department of Chemistry, University of Sheffield, Dainton Building, Brook Hill, Sheffield, UK. S3
7HF

Email: simon.jones@sheffield.ac.uk

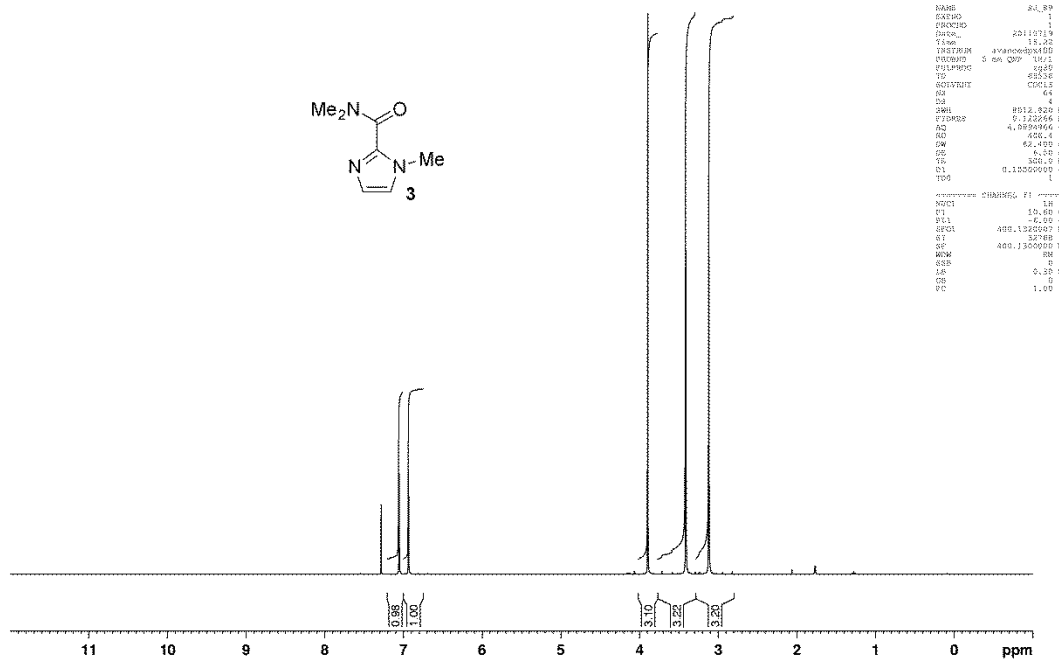
Copies of ^1H and ^{13}C NMR data	2
Copies of HPLC data	22
Thermal ellipsoid plot of catalyst 17 (CCDC 1517809)	34

CC1(C)N2C=CC=CC2=C1

2

CC(C)(C)n1ccncc1

XL5-78
PRO CDC13 {C:07|y2011} ch3sj 29

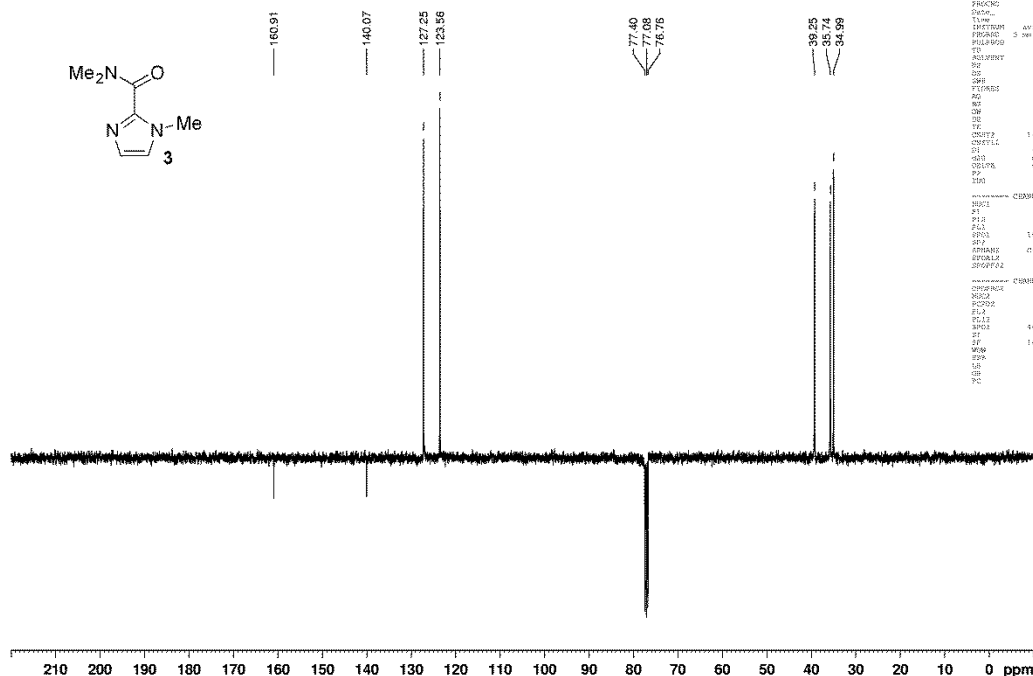


The University of Sheffield

NAME: XL5-78
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PROCNO: 1
DATE_: 20110719
TIME: 15.02
INSTRUM: avance400
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 4
DS: 4
SWH: 8512.820 Hz
F2: 101.625 MHz
AQ: 4.0594966 sec
RG: 655.4
SQ: 62.470 sec
DE: 6.500 sec
TE: 300.2 K
D1: 0.10000000 sec
TD0: 1

===== CHANNEL f1 =====
NUC1: 1H
P1: 12.00 usec
PL1: -6.00 dB
SFO1: 400.1300000 MHz
NUC2: 13C
P2: 100.000000 usec
PL2: 0.00 dB
SFO2: 101.6250000 MHz

XL5-78
A4JMOD250PPM CDC13 {C:07|y2011} ch3sj 30



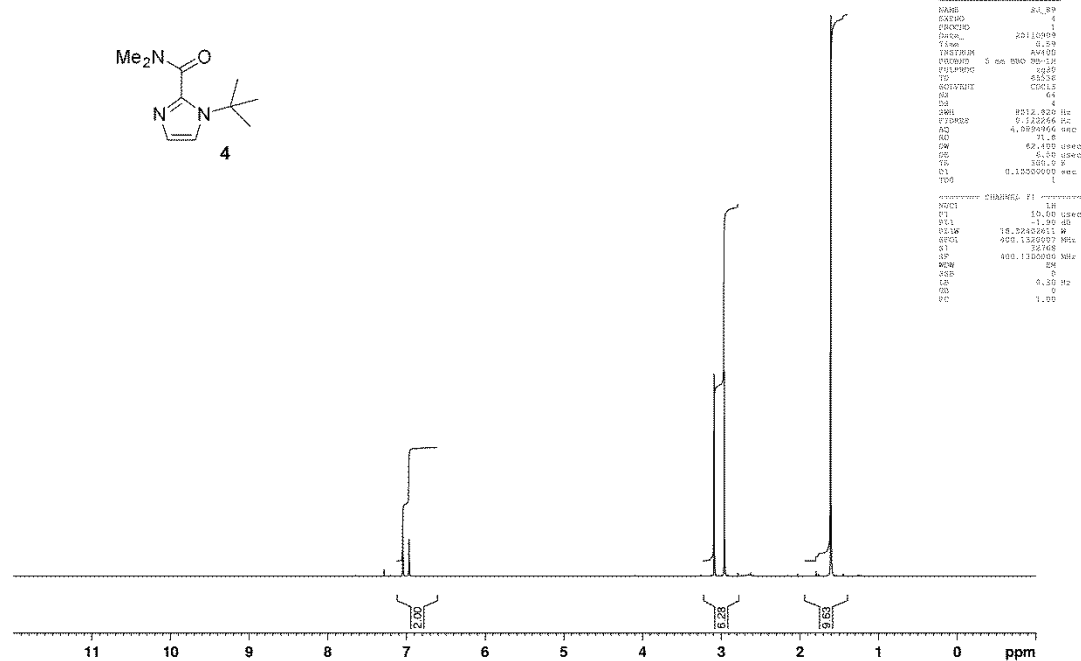
The University of Sheffield

NAME: XL5-78
EXPNO: 2
PROCNO: 1
DATE_: 20110719
TIME: 15.02
INSTRUM: avance400
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 4
DS: 4
SWH: 25125.145 Hz
F2: 101.625 MHz
AQ: 1.0181144 sec
RG: 12360.4
SQ: 19.100 sec
DE: 6.500 sec
TE: 300.2 K
D1: 145.0000000 sec
D11: 0.00000000 sec
D12: 0.00000000 sec
DELTA: 0.00001713 sec
PP: 20.00 usec
TD0: 1

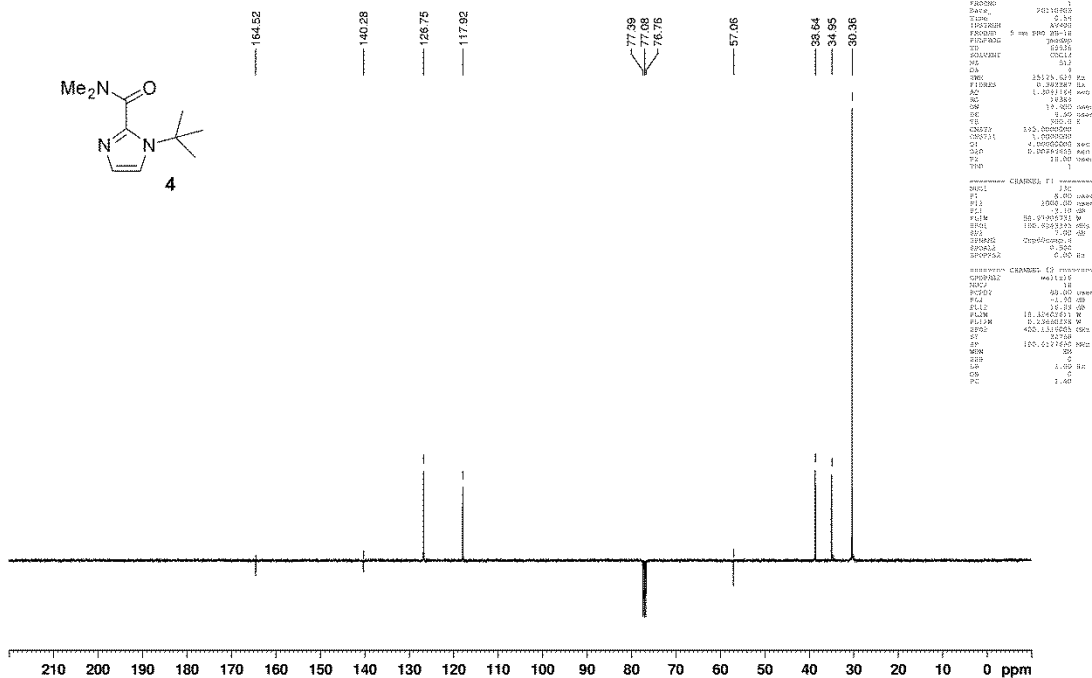
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NUC1: 13C
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 101.6250000 MHz
NUC2: 1H
P2: 12.00 usec
PL2: 0.00 dB
SFO2: 400.1300000 MHz

===== CHANNEL f2 =====
NUC3: 13C
P3: 10.00 usec
PL3: 0.00 dB
SFO3: 101.6250000 MHz

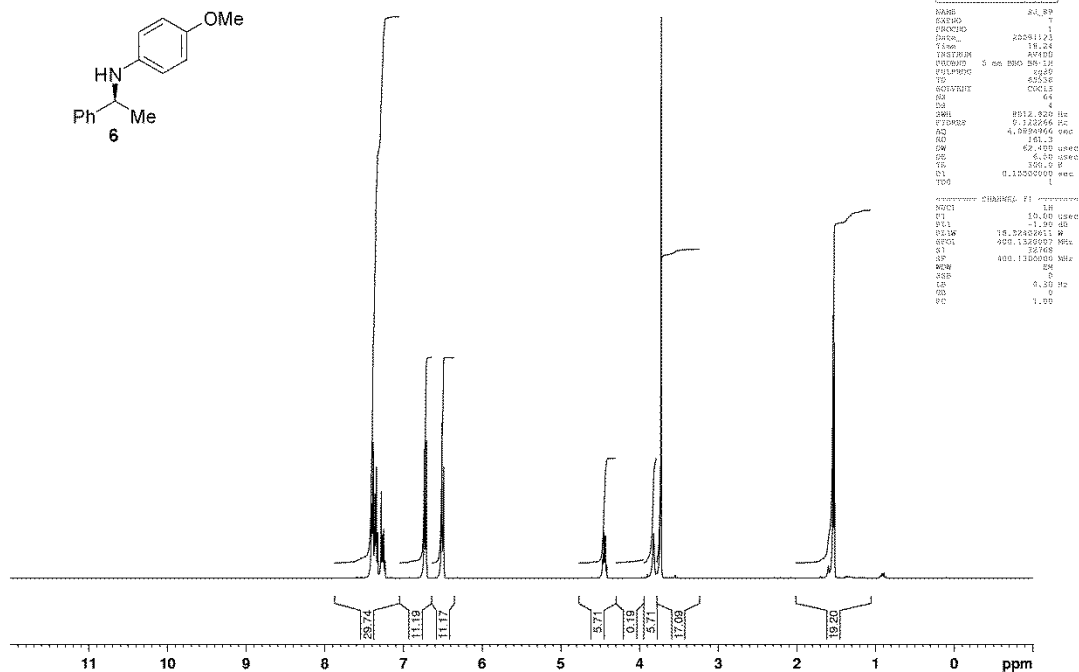
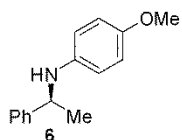
XL6-07
PRO CDCl3 {C:\09se2011\} ch3sj 4



XL6-07
JMOD250PPM CDCl3 {C:\09se2011\} ch3sj 4



x1018 after column
PRO CDCl₃ {C:\11no2008} ch3sj 31

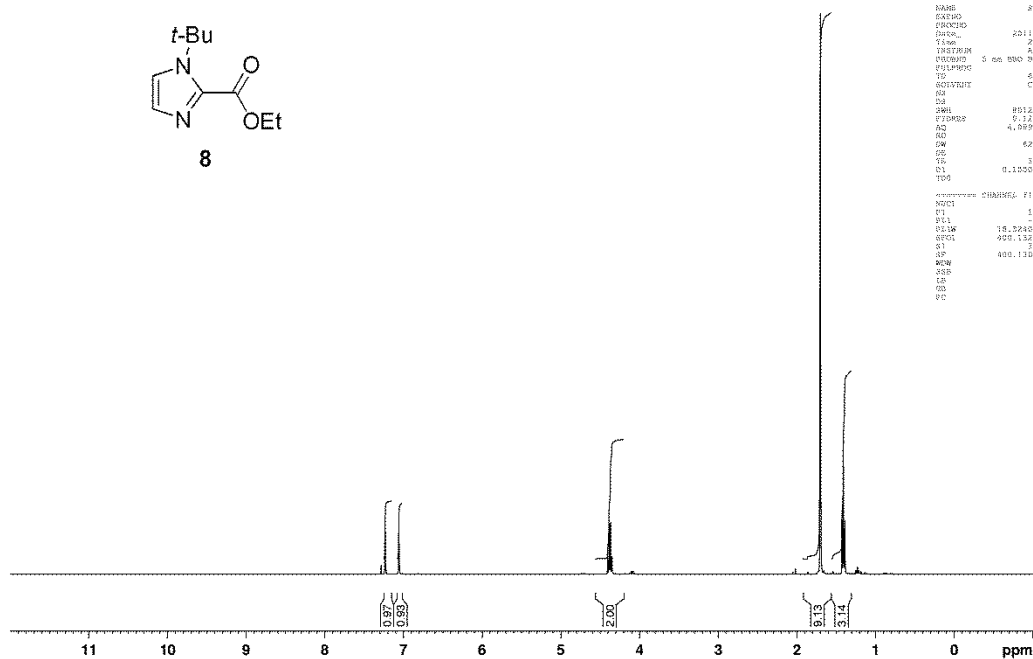
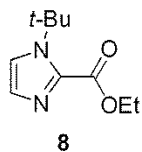


The University of Sheffield

NAME: A1_89
EXPER: 1
PROCNO: 20081113
Date_: 18.12
Time: 15.24
INSTRUM: spect
PULPROG: zgpg30
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 64
DS: 4
SWH: 8512.820 Hz
FIDRES: 0.116058 Hz
AQ: 4.059966 sec
RG: 655.3
SN: 62.480 spec
DS: 6.00 spec
SS: 320.0 Hz
SI: 0.1000000 sec
RG: 1

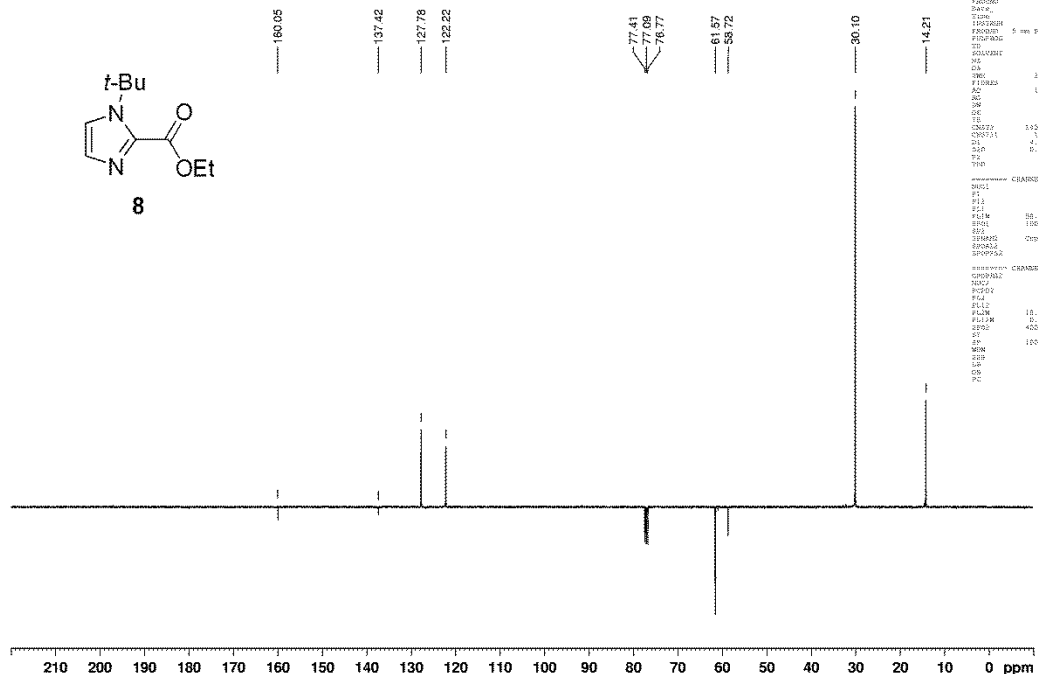
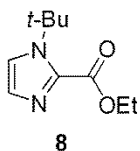
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NUC1: 1H
P1: 12.00 usec
PL1: -1.90 dB
PL12: 19.20dB 1H
RF01: 400.1360007 MHz
SI: 32768
SF: 400.1360000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

XL5-92
PRO CDCl₃ {C:\08au2011\} ch3sj 30



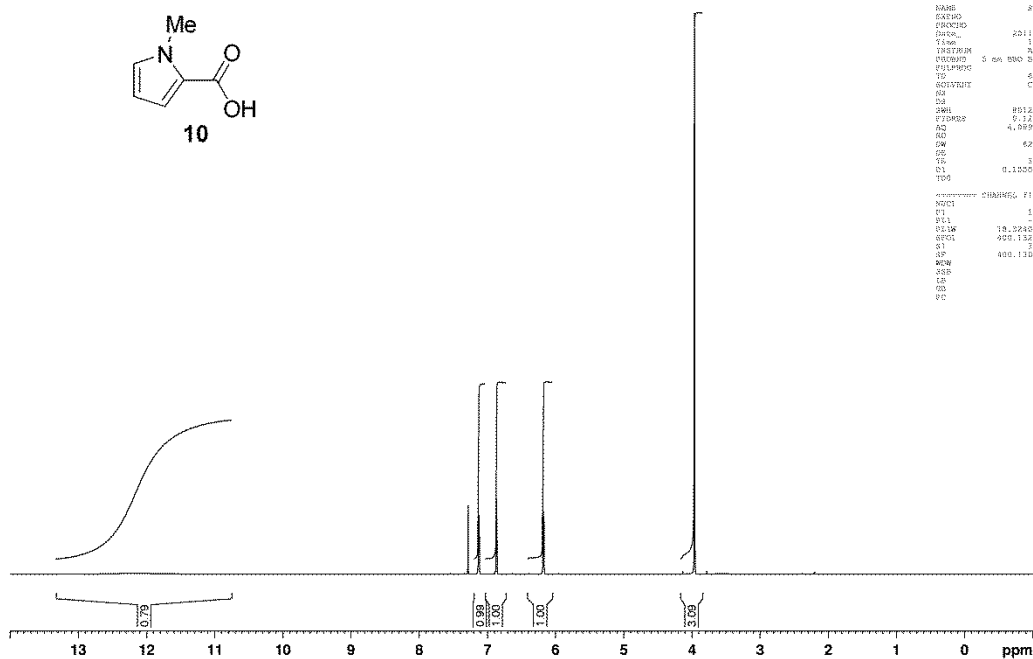
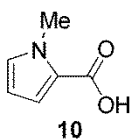
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PROCNO	1
INSTR	2D110914
TIME	20.00
INSTRUM	400MHz
PROBHD	5 mm BBO HD-1H
PULPROG	zgpg30
TD	65536
ROBIN	2
RG	64
SD	4
SWH	1012.820 Hz
F2	514.000 MHz
AQ	4.0000000 sec
RG	64
SW	62.450 sec
DS	6.00 sec
TE	300.2 K
D1	0.1000000 sec
TD1	1
===== CHANNEL F1 =====	
NUC1	1H
PT	10.00 sec
PUL	1.00 sec
PULP	15.0000000 sec
RF1	400.1326000 MHz
SI	32768
RF	400.1326000 MHz
NUC	1H
SD	4
SW	62.450 sec
DS	6.00 sec
TE	300.2 K
D1	0.1000000 sec
TD1	1

XL5-92
JMOD250PPM CDCl₃ {C:\08au2011\} ch3sj 30



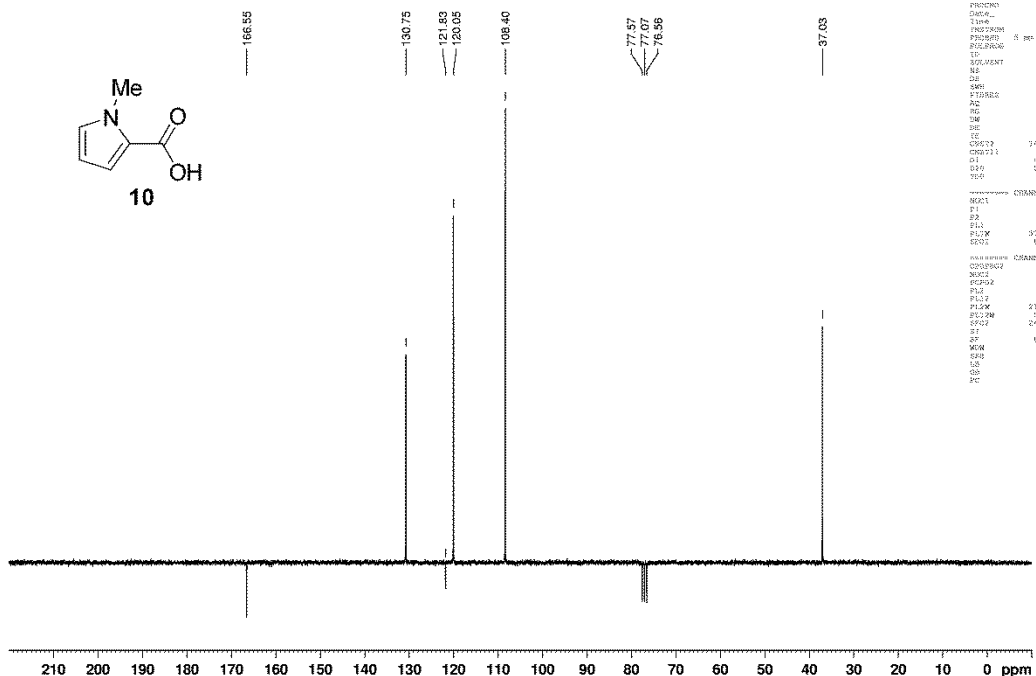
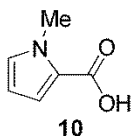
The University of Sheffield	
NAME	XL5-92
EXPNO	1
PROCNO	1
INSTR	2D110914
TIME	20.00
INSTRUM	400MHz
PROBHD	5 mm BBO HD-1H
PULPROG	zgpg30
TD	65536
ROBIN	2
RG	64
SD	4
SWH	1012.820 Hz
F2	514.000 MHz
AQ	4.0000000 sec
RG	64
SW	62.450 sec
DS	6.00 sec
TE	300.2 K
D1	0.1000000 sec
TD1	1
===== CHANNEL F1 =====	
NUC1	13C
PT	8.00 sec
PUL	1.00 sec
PULP	15.0000000 sec
RF1	100.6261200 MHz
SI	32768
RF	100.6261200 MHz
NUC	13C
SD	4
SW	62.450 sec
DS	6.00 sec
TE	300.2 K
D1	0.1000000 sec
TD1	1
===== CHANNEL F2 =====	
NUC2	1H
PT2	8.00 sec
PUL2	1.00 sec
PULP2	15.0000000 sec
RF2	400.1326000 MHz
SI2	32768
RF2	400.1326000 MHz
NUC2	1H
SD2	4
SW2	62.450 sec
DS2	6.00 sec
TE2	300.2 K
D12	0.1000000 sec
TD12	1

XL5-82
PRO CDCl3 {C:\07\y2011\} ch3sj 16



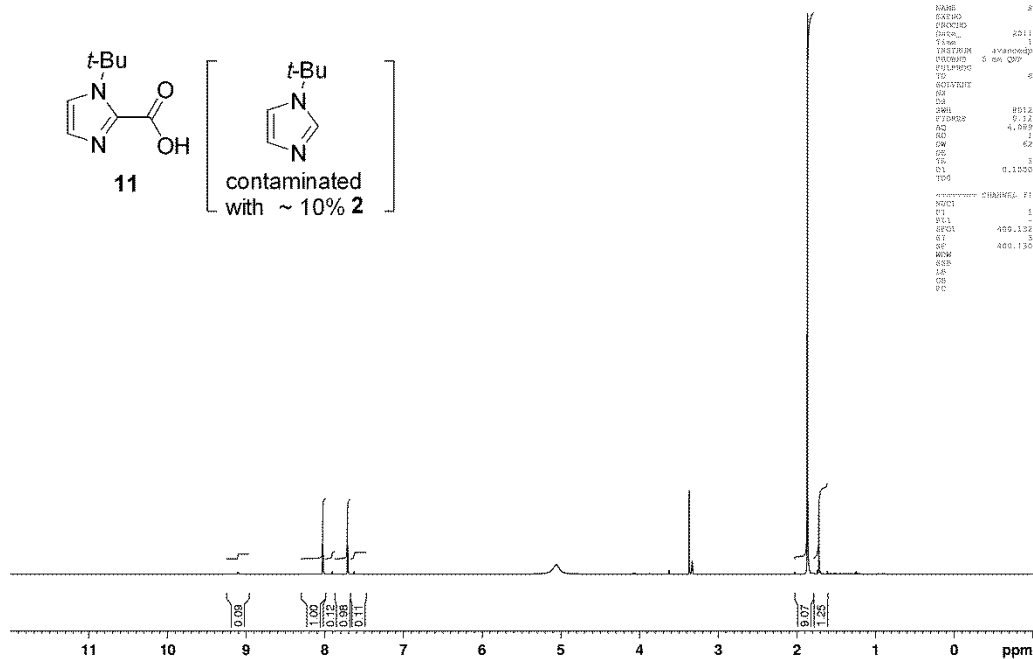
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PROCNO	1
DATE_	20110722
TIME	14.00
INSTRUM	QNP400
PROBHD	5 mm BBO 2D-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	8012.820 Hz
F2HRES	0.140000 Hz
AQ	4.0590466 sec
RG	320
SW	62.400 e/sec
GE	6.000 e/sec
TE	300.2 K
D1	0.10000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	1H
NUC2	13C
NUC3	13C
NUC4	13C
NUC5	13C
NUC6	13C
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XL5-82
JMOD250PPM CDCl3 {C:\08\au2011\} ch3sj 31

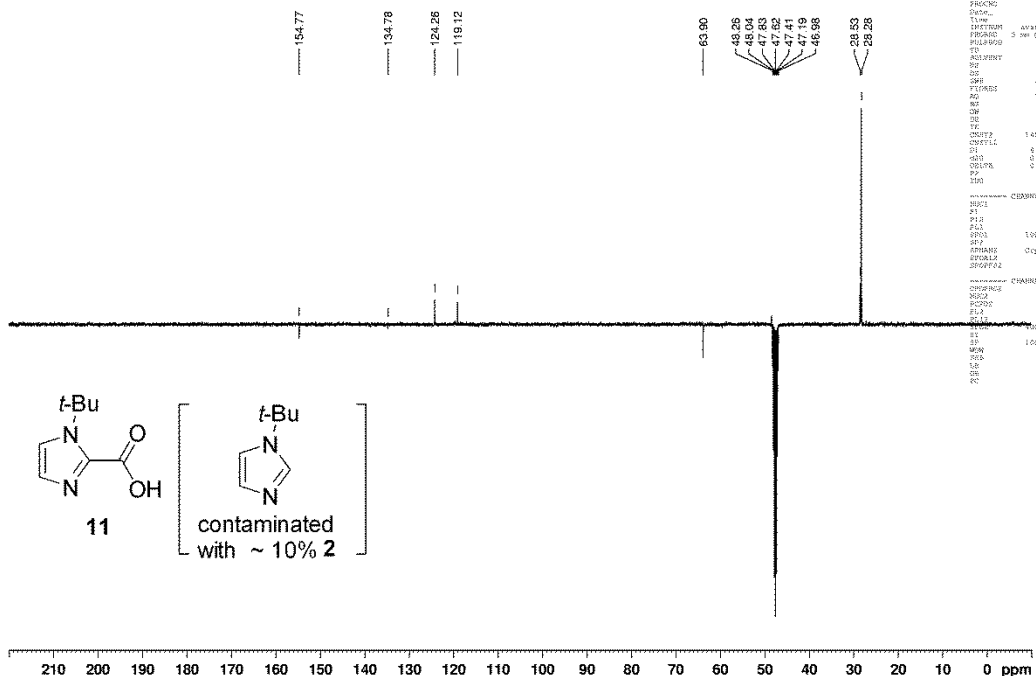


The University of Sheffield	
NAME	XL5-82
EXPNO	2
PROCNO	1
DATE_	20110802
TIME	10.12
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PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	15723.275 Hz
F2HRES	0.4750000 Hz
AQ	1.8440726 sec
RG	320
SW	37.400 e/sec
GE	6.000 e/sec
TE	300.2 K
D1	0.10000000 sec
D11	0.00000000 sec
D12	0.00000000 sec
D13	0.00000000 sec
D14	0.00000000 sec
D15	0.00000000 sec
D16	0.00000000 sec
D17	0.00000000 sec
D18	0.00000000 sec
D19	0.00000000 sec
D20	0.00000000 sec
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D22	0.00000000 sec
D23	0.00000000 sec
D24	0.00000000 sec
D25	0.00000000 sec
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D27	0.00000000 sec
D28	0.00000000 sec
D29	0.00000000 sec
D30	0.00000000 sec
D31	0.00000000 sec
D32	0.00000000 sec
D33	0.00000000 sec
D34	0.00000000 sec
D35	0.00000000 sec
D36	0.00000000 sec
D37	0.00000000 sec
D38	0.00000000 sec
D39	0.00000000 sec
D40	0.00000000 sec
D41	0.00000000 sec
D42	0.00000000 sec
D43	0.00000000 sec
D44	0.00000000 sec
D45	0.00000000 sec
D46	0.00000000 sec
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D50	0.00000000 sec
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D53	0.00000000 sec
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D99	0.00000000 sec
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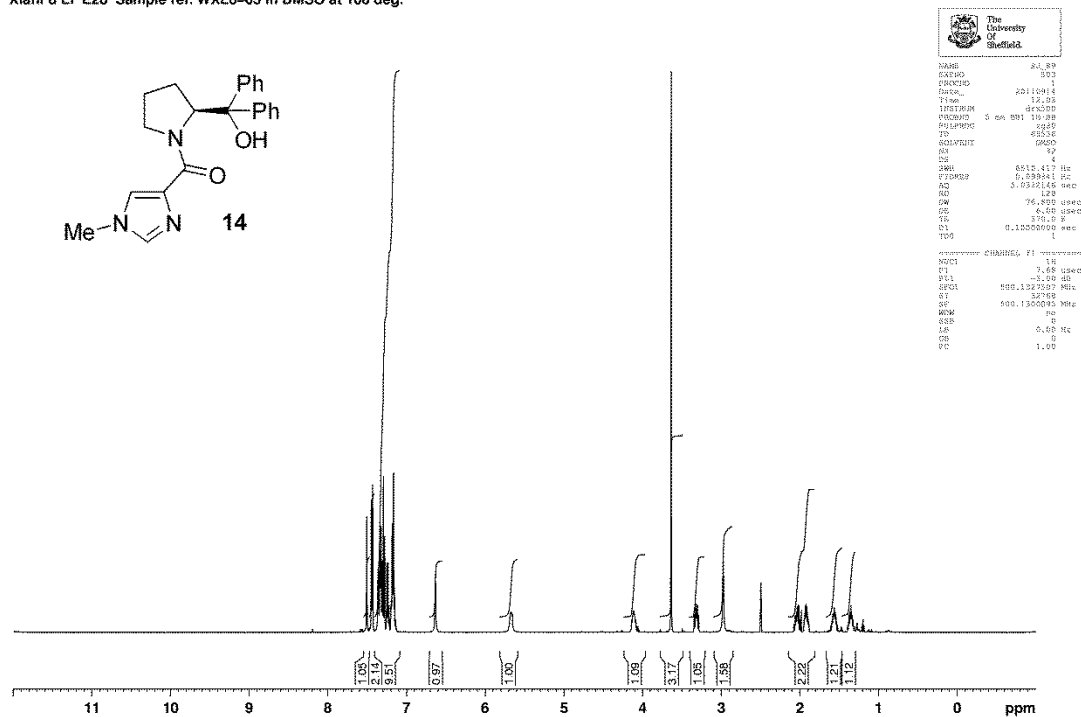
XL5-94
PRO MeOD (C:\08au2011) ch3s] 25



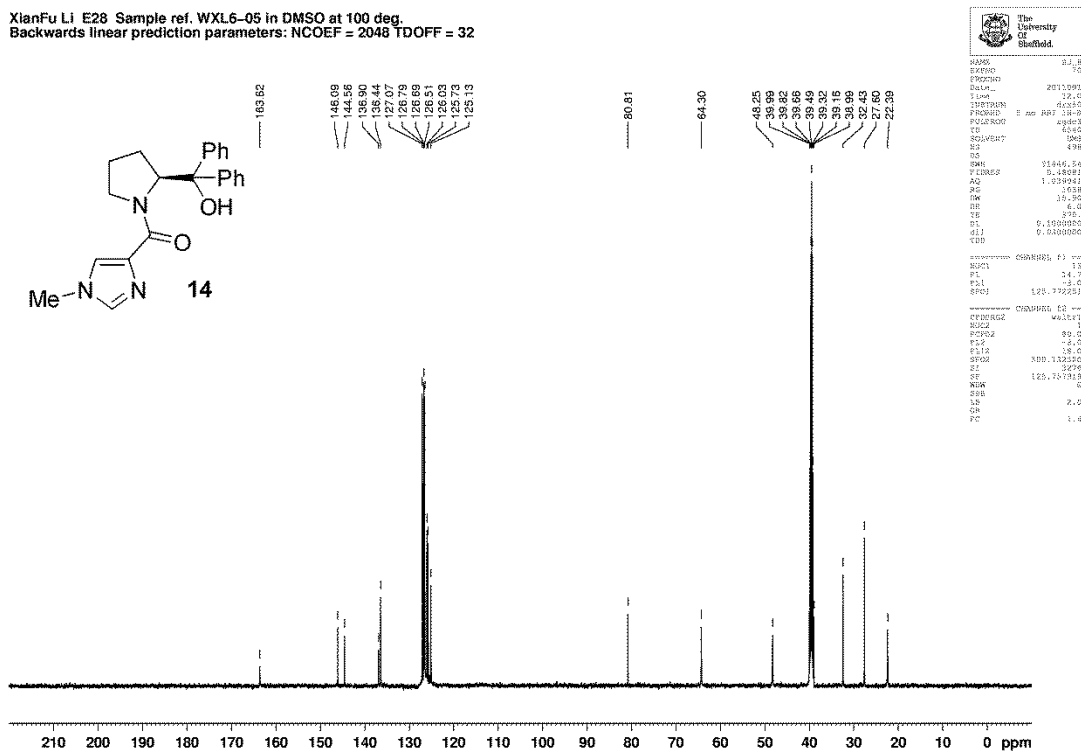
XL5-94
A4JMOD250PPM MeOD (C:\08au2011) ch3s] 30



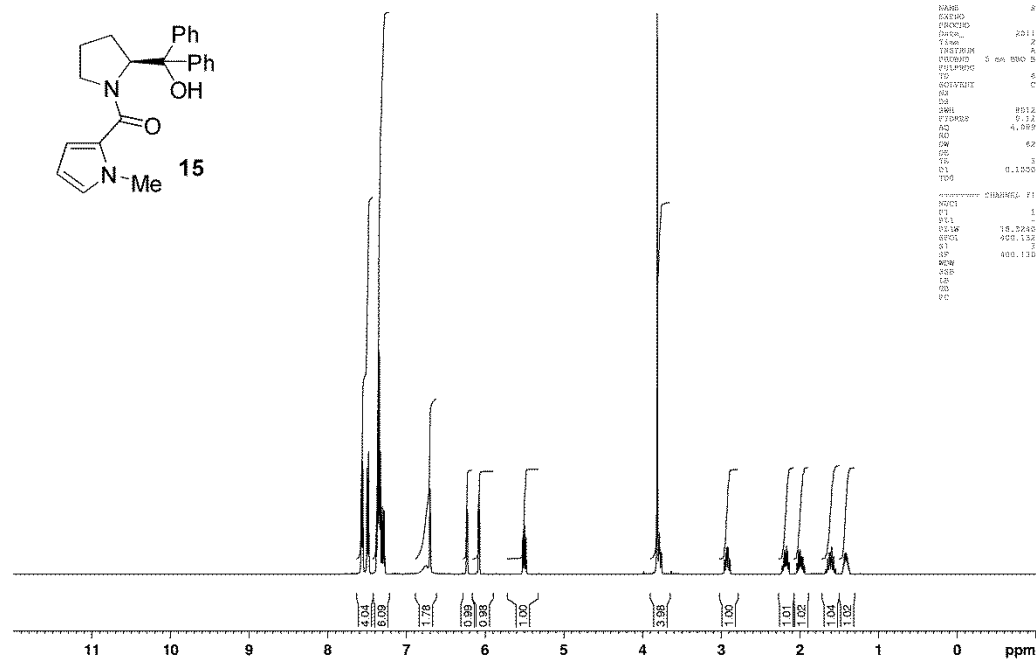
XianFu Li E28 Sample ref. WXL6-05 in DMSO at 100 deg.



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

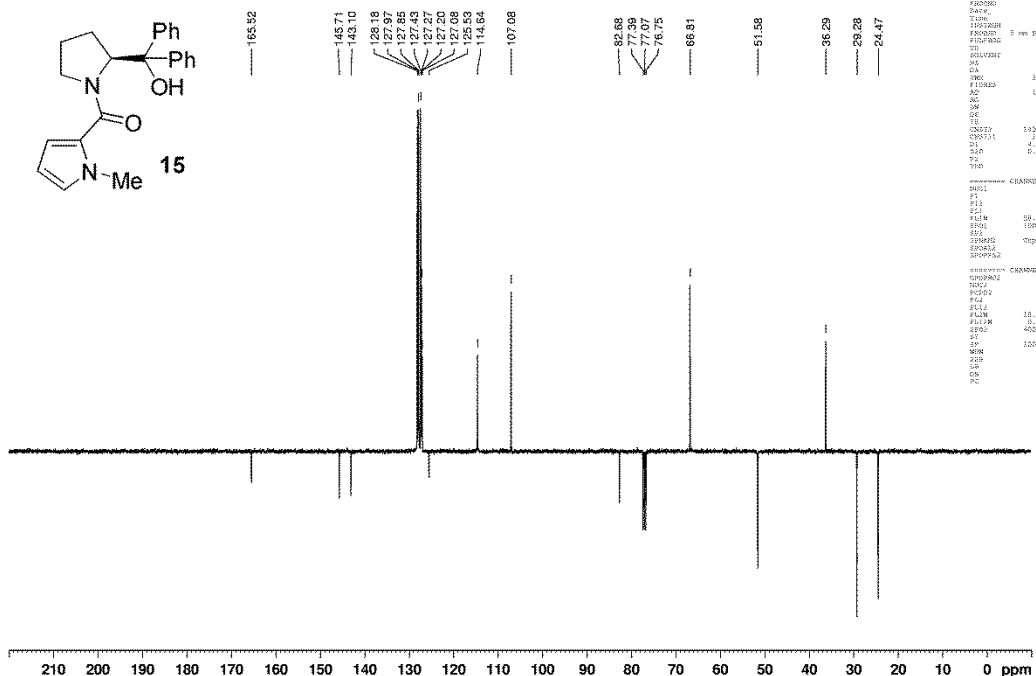


The University of Sheffield

NAME: AL 89
EXPNO: 2
PROCNO: 20110803
Date_: 22.10
Time: 09:00
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCL3
NS: 64
DS: 4
SWH: 8512.820 Hz
FIDRES: 0.146000 Hz
AQ: 4.0590966 sec
RG: 60.0
RW: 62.4700 sec
GB: 6.00 sec
PC: 100.0
DT: 0.1000000 sec
TE: 1

===== CHANNEL f1 =====
NUC1: 1H
P1: 12.00 usec
PL1: -1.90 dB
NUC2: 13C
P2: 10.00 usec
PL2: -1.90 dB
NUC3: 13C
P3: 10.00 usec
PL3: -1.90 dB
NUC4: 13C
P4: 10.00 usec
PL4: -1.90 dB
NUC5: 13C
P5: 10.00 usec
PL5: -1.90 dB
NUC6: 13C
P6: 10.00 usec
PL6: -1.90 dB
NUC7: 13C
P7: 10.00 usec
PL7: -1.90 dB
NUC8: 13C
P8: 10.00 usec
PL8: -1.90 dB
NUC9: 13C
P9: 10.00 usec
PL9: -1.90 dB
NUC10: 13C
P10: 10.00 usec
PL10: -1.90 dB
NUC11: 13C
P11: 10.00 usec
PL11: -1.90 dB
NUC12: 13C
P12: 10.00 usec
PL12: -1.90 dB
NUC13: 13C
P13: 10.00 usec
PL13: -1.90 dB
NUC14: 13C
P14: 10.00 usec
PL14: -1.90 dB
NUC15: 13C
P15: 10.00 usec
PL15: -1.90 dB
NUC16: 13C
P16: 10.00 usec
PL16: -1.90 dB
NUC17: 13C
P17: 10.00 usec
PL17: -1.90 dB
NUC18: 13C
P18: 10.00 usec
PL18: -1.90 dB
NUC19: 13C
P19: 10.00 usec
PL19: -1.90 dB
NUC20: 13C
P20: 10.00 usec
PL20: -1.90 dB
NUC21: 13C
P21: 10.00 usec
PL21: -1.90 dB
NUC22: 13C
P22: 10.00 usec
PL22: -1.90 dB
NUC23: 13C
P23: 10.00 usec
PL23: -1.90 dB
NUC24: 13C
P24: 10.00 usec
PL24: -1.90 dB
NUC25: 13C
P25: 10.00 usec
PL25: -1.90 dB
NUC26: 13C
P26: 10.00 usec
PL26: -1.90 dB
NUC27: 13C
P27: 10.00 usec
PL27: -1.90 dB
NUC28: 13C
P28: 10.00 usec
PL28: -1.90 dB
NUC29: 13C
P29: 10.00 usec
PL29: -1.90 dB
NUC30: 13C
P30: 10.00 usec
PL30: -1.90 dB
NUC31: 13C
P31: 10.00 usec
PL31: -1.90 dB
NUC32: 13C
P32: 10.00 usec
PL32: -1.90 dB
NUC33: 13C
P33: 10.00 usec
PL33: -1.90 dB
NUC34: 13C
P34: 10.00 usec
PL34: -1.90 dB
NUC35: 13C
P35: 10.00 usec
PL35: -1.90 dB
NUC36: 13C
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PL36: -1.90 dB
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PL37: -1.90 dB
NUC38: 13C
P38: 10.00 usec
PL38: -1.90 dB
NUC39: 13C
P39: 10.00 usec
PL39: -1.90 dB
NUC40: 13C
P40: 10.00 usec
PL40: -1.90 dB
NUC41: 13C
P41: 10.00 usec
PL41: -1.90 dB
NUC42: 13C
P42: 10.00 usec
PL42: -1.90 dB
NUC43: 13C
P43: 10.00 usec
PL43: -1.90 dB
NUC44: 13C
P44: 10.00 usec
PL44: -1.90 dB
NUC45: 13C
P45: 10.00 usec
PL45: -1.90 dB
NUC46: 13C
P46: 10.00 usec
PL46: -1.90 dB
NUC47: 13C
P47: 10.00 usec
PL47: -1.90 dB
NUC48: 13C
P48: 10.00 usec
PL48: -1.90 dB
NUC49: 13C
P49: 10.00 usec
PL49: -1.90 dB
NUC50: 13C
P50: 10.00 usec
PL50: -1.90 dB
NUC51: 13C
P51: 10.00 usec
PL51: -1.90 dB
NUC52: 13C
P52: 10.00 usec
PL52: -1.90 dB
NUC53: 13C
P53: 10.00 usec
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NUC56: 13C
P56: 10.00 usec
PL56: -1.90 dB
NUC57: 13C
P57: 10.00 usec
PL57: -1.90 dB
NUC58: 13C
P58: 10.00 usec
PL58: -1.90 dB
NUC59: 13C
P59: 10.00 usec
PL59: -1.90 dB
NUC60: 13C
P60: 10.00 usec
PL60: -1.90 dB
NUC61: 13C
P61: 10.00 usec
PL61: -1.90 dB
NUC62: 13C
P62: 10.00 usec
PL62: -1.90 dB
NUC63: 13C
P63: 10.00 usec
PL63: -1.90 dB
NUC64: 13C
P64: 10.00 usec
PL64: -1.90 dB
NUC65: 13C
P65: 10.00 usec
PL65: -1.90 dB
NUC66: 13C
P66: 10.00 usec
PL66: -1.90 dB
NUC67: 13C
P67: 10.00 usec
PL67: -1.90 dB
NUC68: 13C
P68: 10.00 usec
PL68: -1.90 dB
NUC69: 13C
P69: 10.00 usec
PL69: -1.90 dB
NUC70: 13C
P70: 10.00 usec
PL70: -1.90 dB
NUC71: 13C
P71: 10.00 usec
PL71: -1.90 dB
NUC72: 13C
P72: 10.00 usec
PL72: -1.90 dB
NUC73: 13C
P73: 10.00 usec
PL73: -1.90 dB
NUC74: 13C
P74: 10.00 usec
PL74: -1.90 dB
NUC75: 13C
P75: 10.00 usec
PL75: -1.90 dB
NUC76: 13C
P76: 10.00 usec
PL76: -1.90 dB
NUC77: 13C
P77: 10.00 usec
PL77: -1.90 dB
NUC78: 13C
P78: 10.00 usec
PL78: -1.90 dB
NUC79: 13C
P79: 10.00 usec
PL79: -1.90 dB
NUC80: 13C
P80: 10.00 usec
PL80: -1.90 dB
NUC81: 13C
P81: 10.00 usec
PL81: -1.90 dB
NUC82: 13C
P82: 10.00 usec
PL82: -1.90 dB
NUC83: 13C
P83: 10.00 usec
PL83: -1.90 dB
NUC84: 13C
P84: 10.00 usec
PL84: -1.90 dB
NUC85: 13C
P85: 10.00 usec
PL85: -1.90 dB
NUC86: 13C
P86: 10.00 usec
PL86: -1.90 dB
NUC87: 13C
P87: 10.00 usec
PL87: -1.90 dB
NUC88: 13C
P88: 10.00 usec
PL88: -1.90 dB
NUC89: 13C
P89: 10.00 usec
PL89: -1.90 dB
NUC90: 13C
P90: 10.00 usec
PL90: -1.90 dB
NUC91: 13C
P91: 10.00 usec
PL91: -1.90 dB
NUC92: 13C
P92: 10.00 usec
PL92: -1.90 dB
NUC93: 13C
P93: 10.00 usec
PL93: -1.90 dB
NUC94: 13C
P94: 10.00 usec
PL94: -1.90 dB
NUC95: 13C
P95: 10.00 usec
PL95: -1.90 dB
NUC96: 13C
P96: 10.00 usec
PL96: -1.90 dB
NUC97: 13C
P97: 10.00 usec
PL97: -1.90 dB
NUC98: 13C
P98: 10.00 usec
PL98: -1.90 dB
NUC99: 13C
P99: 10.00 usec
PL99: -1.90 dB
NUC100: 13C
P100: 10.00 usec
PL100: -1.90 dB

XL5-89
JMOD250PPM CDCl3 {C:\08au2011\} ch3sj 52

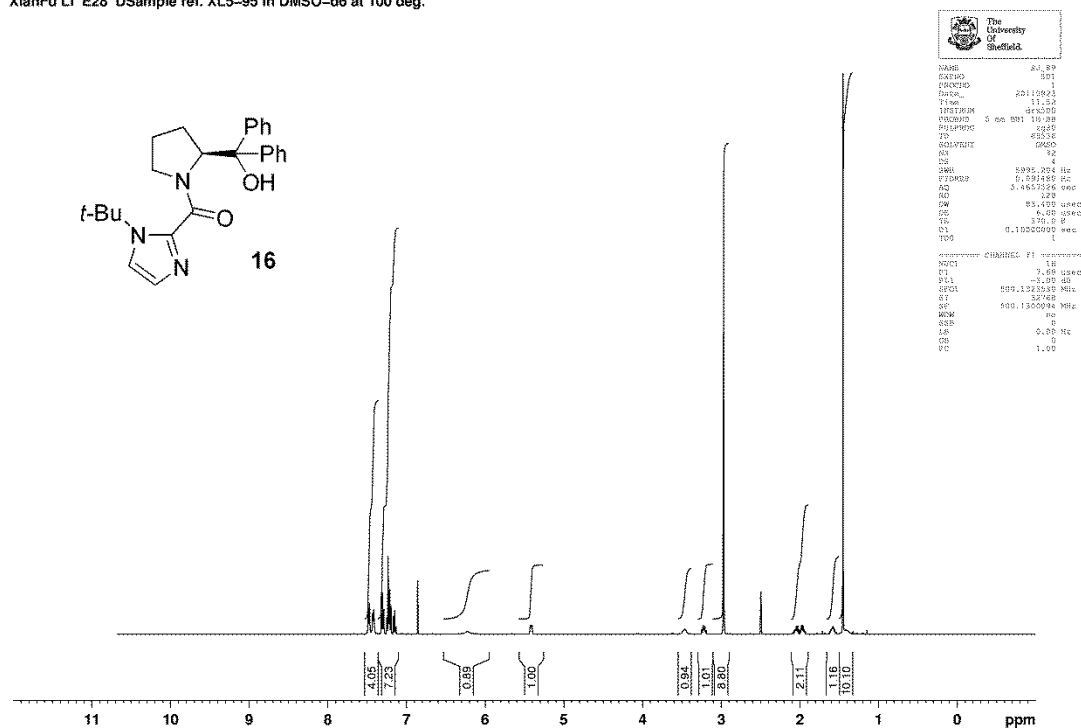


The University of Sheffield

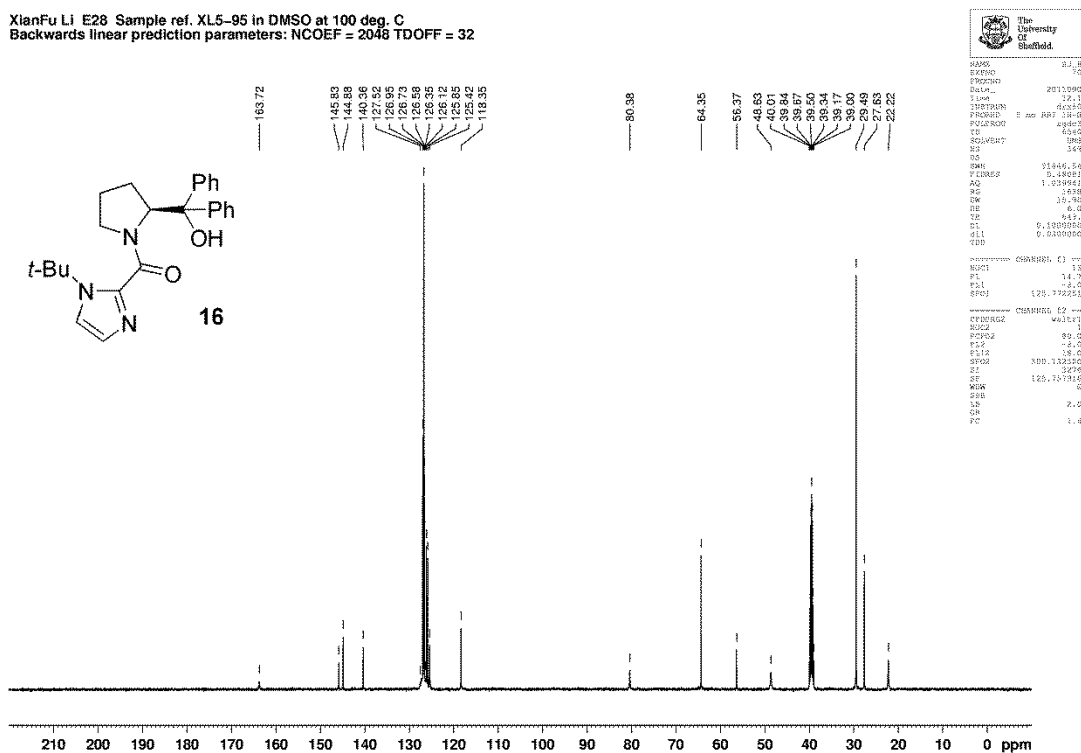
NAME: AL 89
EXPNO: 1
PROCNO: 20110803
Date_: 22.10
Time: 09:00
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCL3
NS: 64
DS: 4
SWH: 15133.639 Hz
FIDRES: 0.146000 Hz
AQ: 4.0590966 sec
RG: 60.0
RW: 62.4700 sec
GB: 6.00 sec
PC: 100.0
DT: 0.1000000 sec
TE: 1

===== CHANNEL f1 =====
NUC1: 13C
P1: 12.00 usec
PL1: -1.90 dB
NUC2: 13C
P2: 10.00 usec
PL2: -1.90 dB
NUC3: 13C
P3: 10.00 usec
PL3: -1.90 dB
NUC4: 13C
P4: 10.00 usec
PL4: -1.90 dB
NUC5: 13C
P5: 10.00 usec
PL5: -1.90 dB
NUC6: 13C
P6: 10.00 usec
PL6: -1.90 dB
NUC7: 13C
P7: 10.00 usec
PL7: -1.90 dB
NUC8: 13C
P8: 10.00 usec
PL8: -1.90 dB
NUC9: 13C
P9: 10.00 usec
PL9: -1.90 dB
NUC10: 13C
P10: 10.00 usec
PL10: -1.90 dB
NUC11: 13C
P11: 10.00 usec
PL11: -1.90 dB
NUC12: 13C
P12: 10.00 usec
PL12: -1.90 dB
NUC13: 13C
P13: 10.00 usec
PL13: -1.90 dB
NUC14: 13C
P14: 10.00 usec
PL14: -1.90 dB
NUC15: 13C
P15: 10.00 usec
PL15: -1.90 dB
NUC16: 13C
P16: 10.00 usec
PL16: -1.90 dB
NUC17: 13C
P17: 10.00 usec
PL17: -1.90 dB
NUC18: 13C
P18: 10.00 usec
PL18: -1.90 dB
NUC19: 13C
P19: 10.00 usec
PL19: -1.90 dB
NUC20: 13C
P20: 10.00 usec
PL20: -1.90 dB
NUC21: 13C
P21: 10.00 usec
PL21: -1.90 dB
NUC22: 13C
P22: 10.00 usec
PL22: -1.90 dB
NUC23: 13C
P23: 10.00 usec
PL23: -1.90 dB
NUC24: 13C
P24: 10.00 usec
PL24: -1.90 dB
NUC25: 13C
P25: 10.00 usec
PL25: -1.90 dB
NUC26: 13C
P26: 10.00 usec
PL26: -1.90 dB
NUC27: 13C
P27: 10.00 usec
PL27: -1.90 dB
NUC28: 13C
P28: 10.00 usec
PL28: -1.90 dB
NUC29: 13C
P29: 10.00 usec
PL29: -1.90 dB
NUC30: 13C
P30: 10.00 usec
PL30: -1.90 dB
NUC31: 13C
P31: 10.00 usec
PL31: -1.90 dB
NUC32: 13C
P32: 10.00 usec
PL32: -1.90 dB
NUC33: 13C
P33: 10.00 usec
PL33: -1.90 dB
NUC34: 13C
P34: 10.00 usec
PL34: -1.90 dB
NUC35: 13C
P35: 10.00 usec
PL35: -1.90 dB
NUC36: 13C
P36: 10.00 usec
PL36: -1.90 dB
NUC37: 13C
P37: 10.00 usec
PL37: -1.90 dB
NUC38: 13C
P38: 10.00 usec
PL38: -1.90 dB
NUC39: 13C
P39: 10.00 usec
PL39: -1.90 dB
NUC40: 13C
P40: 10.00 usec
PL40: -1.90 dB
NUC41: 13C
P41: 10.00 usec
PL41: -1.90 dB
NUC42: 13C
P42: 10.00 usec
PL42: -1.90 dB
NUC43: 13C
P43: 10.00 usec
PL43: -1.90 dB
NUC44: 13C
P44: 10.00 usec
PL44: -1.90 dB
NUC45: 13C
P45: 10.00 usec
PL45: -1.90 dB
NUC46: 13C
P46: 10.00 usec
PL46: -1.90 dB
NUC47: 13C
P47: 10.00 usec
PL47: -1.90 dB
NUC48: 13C
P48: 10.00 usec
PL48: -1.90 dB
NUC49: 13C
P49: 10.00 usec
PL49: -1.90 dB
NUC50: 13C
P50: 10.00 usec
PL50: -1.90 dB
NUC51: 13C
P51: 10.00 usec
PL51: -1.90 dB
NUC52: 13C
P52: 10.00 usec
PL52: -1.90 dB
NUC53: 13C
P53: 10.00 usec
PL53: -1.90 dB
NUC54: 13C
P54: 10.00 usec
PL54: -1.90 dB
NUC55: 13C
P55: 10.00 usec
PL55: -1.90 dB
NUC56: 13C
P56: 10.00 usec
PL56: -1.90 dB
NUC57: 13C
P57: 10.00 usec
PL57: -1.90 dB
NUC58: 13C
P58: 10.00 usec
PL58: -1.90 dB
NUC59: 13C
P59: 10.00 usec
PL59: -1.90 dB
NUC60: 13C
P60: 10.00 usec
PL60: -1.90 dB
NUC61: 13C
P61: 10.00 usec
PL61: -1.90 dB
NUC62: 13C
P62: 10.00 usec
PL62: -1.90 dB
NUC63: 13C
P63: 10.00 usec
PL63: -1.90 dB
NUC64: 13C
P64: 10.00 usec
PL64: -1.90 dB
NUC65: 13C
P65: 10.00 usec
PL65: -1.90 dB
NUC66: 13C
P66: 10.00 usec
PL66: -1.90 dB
NUC67: 13C
P67: 10.00 usec
PL67: -1.90 dB
NUC68: 13C
P68: 10.00 usec
PL68: -1.90 dB
NUC69: 13C
P69: 10.00 usec
PL69: -1.90 dB
NUC70: 13C
P70: 10.00 usec
PL70: -1.90 dB
NUC71: 13C
P71: 10.00 usec
PL71: -1.90 dB
NUC72: 13C
P72: 10.00 usec
PL72: -1.90 dB
NUC73: 13C
P73: 10.00 usec
PL73: -1.90 dB
NUC74: 13C
P74: 10.00 usec
PL74: -1.90 dB
NUC75: 13C
P75: 10.00 usec
PL75: -1.90 dB
NUC76: 13C
P76: 10.00 usec
PL76: -1.90 dB
NUC77: 13C
P77: 10.00 usec
PL77: -1.90 dB
NUC78: 13C
P78: 10.00 usec
PL78: -1.90 dB
NUC79: 13C
P79: 10.00 usec
PL79: -1.90 dB
NUC80: 13C
P80: 10.00 usec
PL80: -1.90 dB
NUC81: 13C
P81: 10.00 usec
PL81: -1.90 dB
NUC82: 13C
P82: 10.00 usec
PL82: -1.90 dB
NUC83: 13C
P83: 10.00 usec
PL83: -1.90 dB
NUC84: 13C
P84: 10.00 usec
PL84: -1.90 dB
NUC85: 13C
P85: 10.00 usec
PL85: -1.90 dB
NUC86: 13C
P86: 10.00 usec
PL86: -1.90 dB
NUC87: 13C
P87: 10.00 usec
PL87: -1.90 dB
NUC88: 13C
P88: 10.00 usec
PL88: -1.90 dB
NUC89: 13C
P89: 10.00 usec
PL89: -1.90 dB
NUC90: 13C
P90: 10.00 usec
PL90: -1.90 dB
NUC91: 13C
P91: 10.00 usec
PL91: -1.90 dB
NUC92: 13C
P92: 10.00 usec
PL92: -1.90 dB
NUC93: 13C
P93: 10.00 usec
PL93: -1.90 dB
NUC94: 13C
P94: 10.00 usec
PL94: -1.90 dB
NUC95: 13C
P95: 10.00 usec
PL95: -1.90 dB
NUC96: 13C
P96: 10.00 usec
PL96: -1.90 dB
NUC97: 13C
P97: 10.00 usec
PL97: -1.90 dB
NUC98: 13C
P98: 10.00 usec
PL98: -1.90 dB
NUC99: 13C
P99: 10.00 usec
PL99: -1.90 dB
NUC100: 13C
P100: 10.00 usec
PL100: -1.90 dB

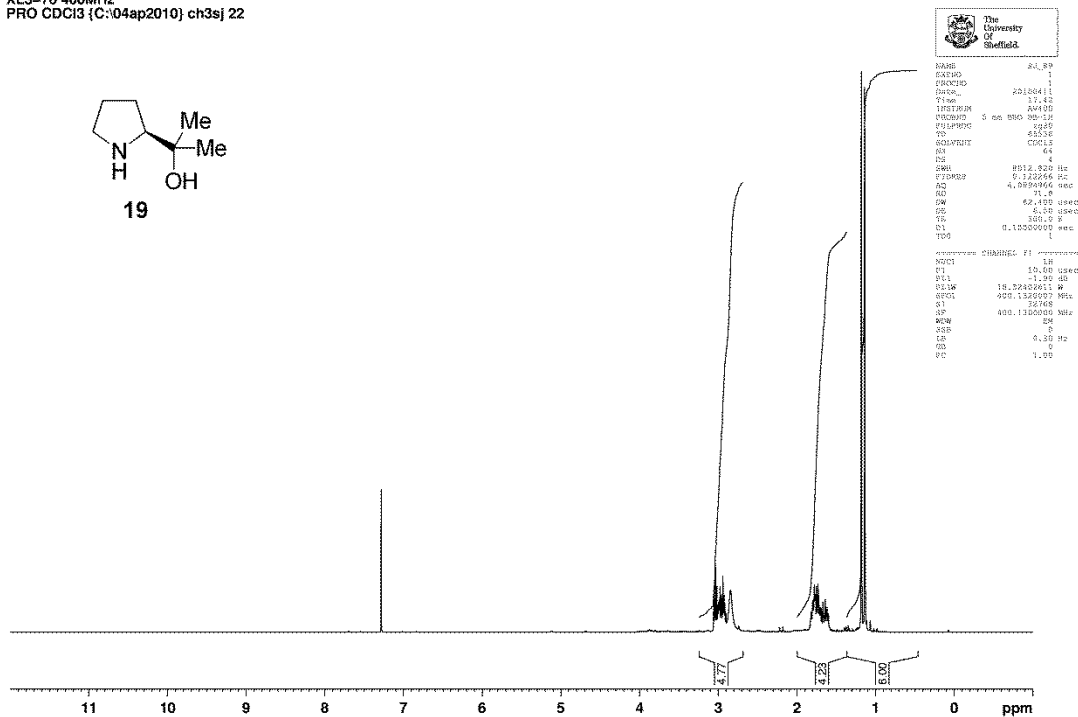
XianFu Li E28 DSAMPLE ref. XL5-95 in DMSO-d6 at 100 deg.



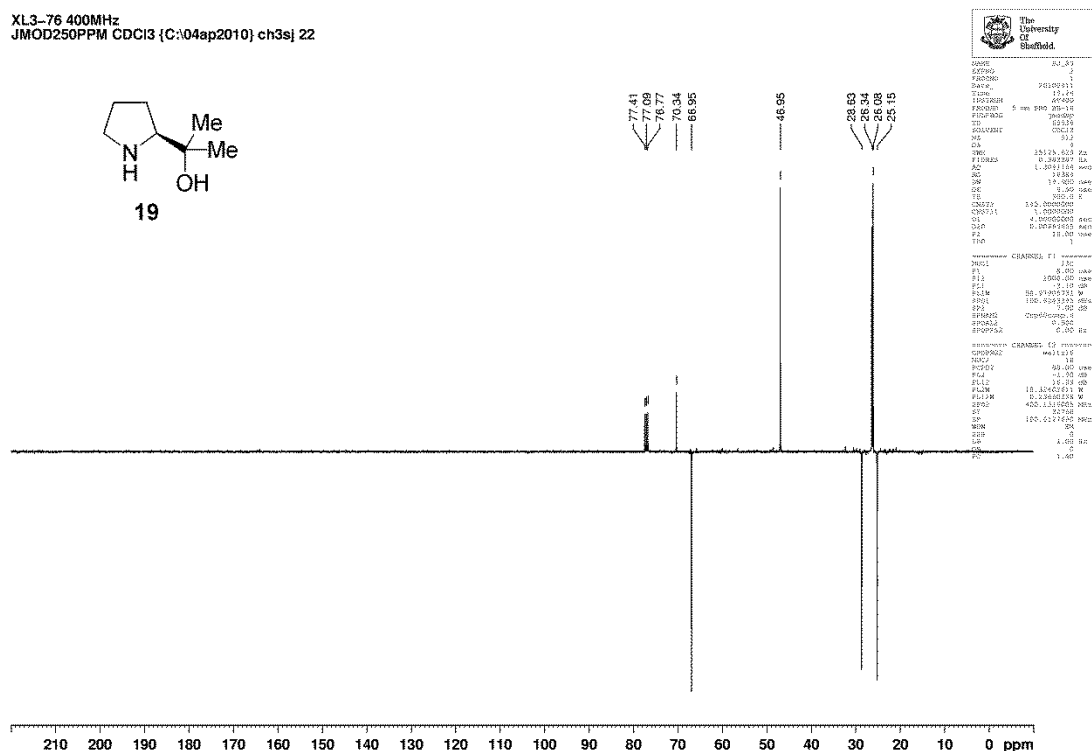
XianFu Li E28 Sample ref. XL5-95 in DMSO at 100 deg. C
Backwards linear prediction parameters: NCOEF = 2048 TDOFF = 32



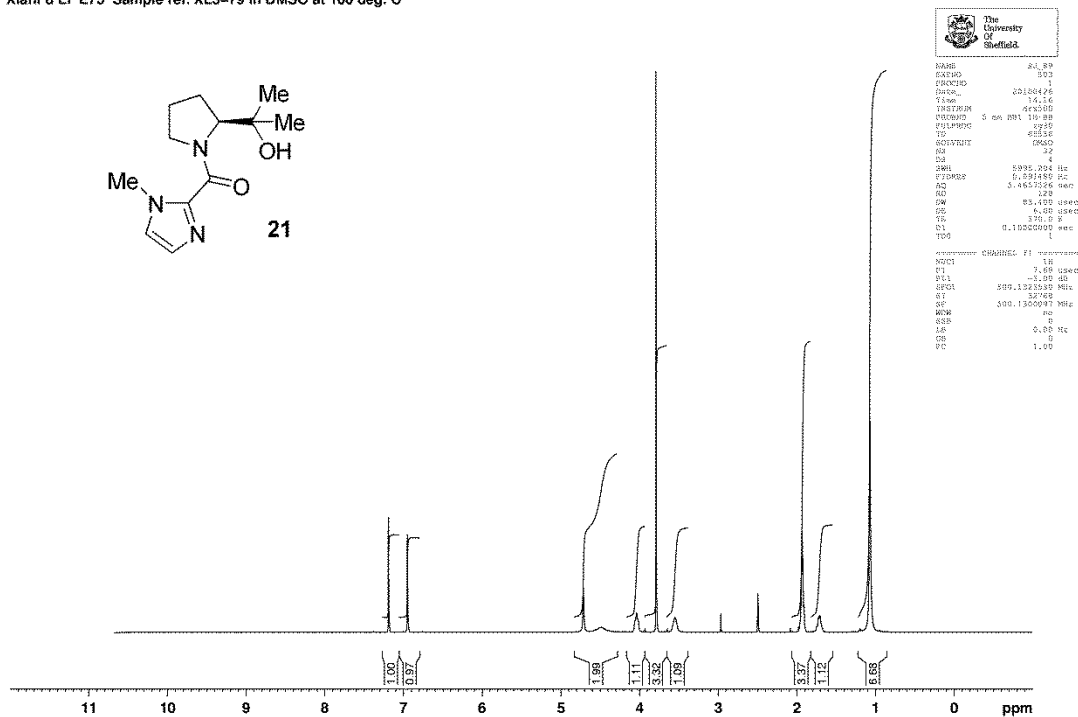
XL3-76 400MHz
PRO CDCl₃ {C:04ap2010} ch3sj 22



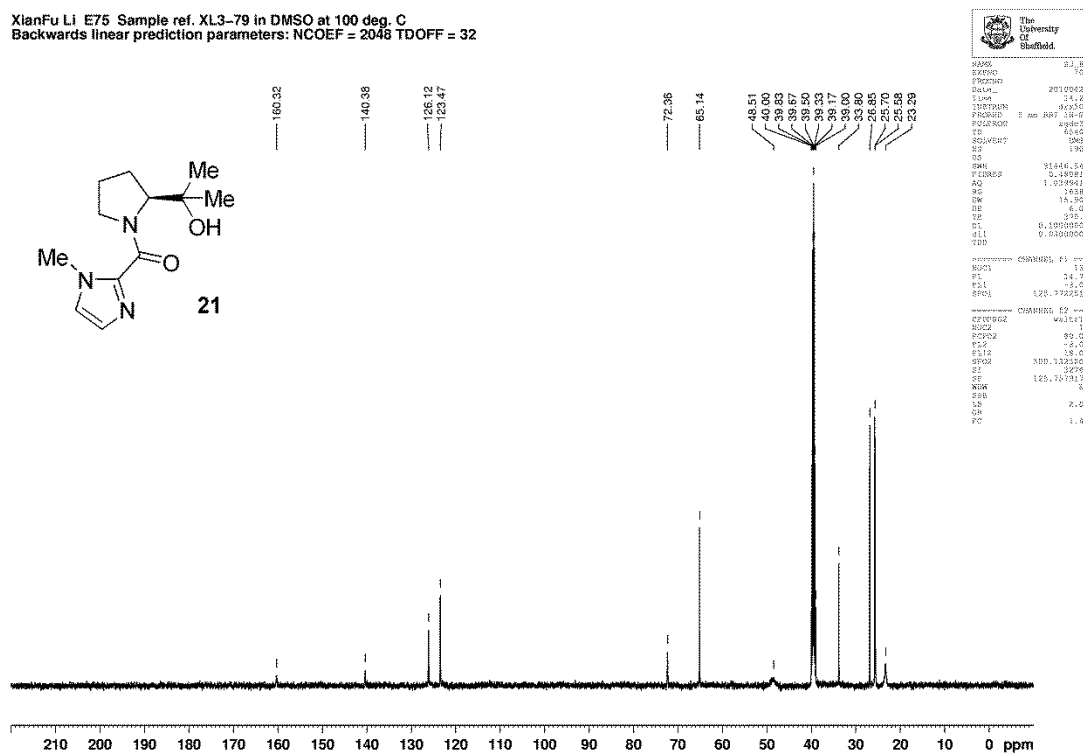
XL3-76 400MHz
JMOD250PPM CDCl₃ {C:04ap2010} ch3sj 22



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



XianFu Li E75 Sample ref. XL3-79 in DMSO at 100 deg. C
Backwards linear prediction parameters: NCOEF = 2048 TDOFF = 32

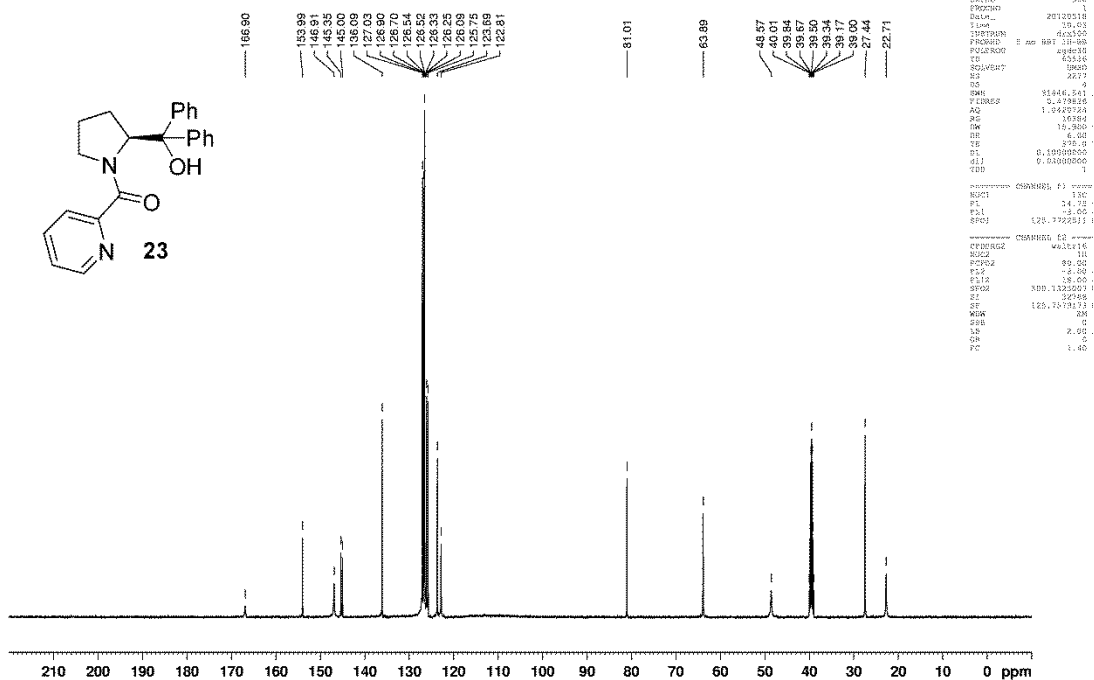




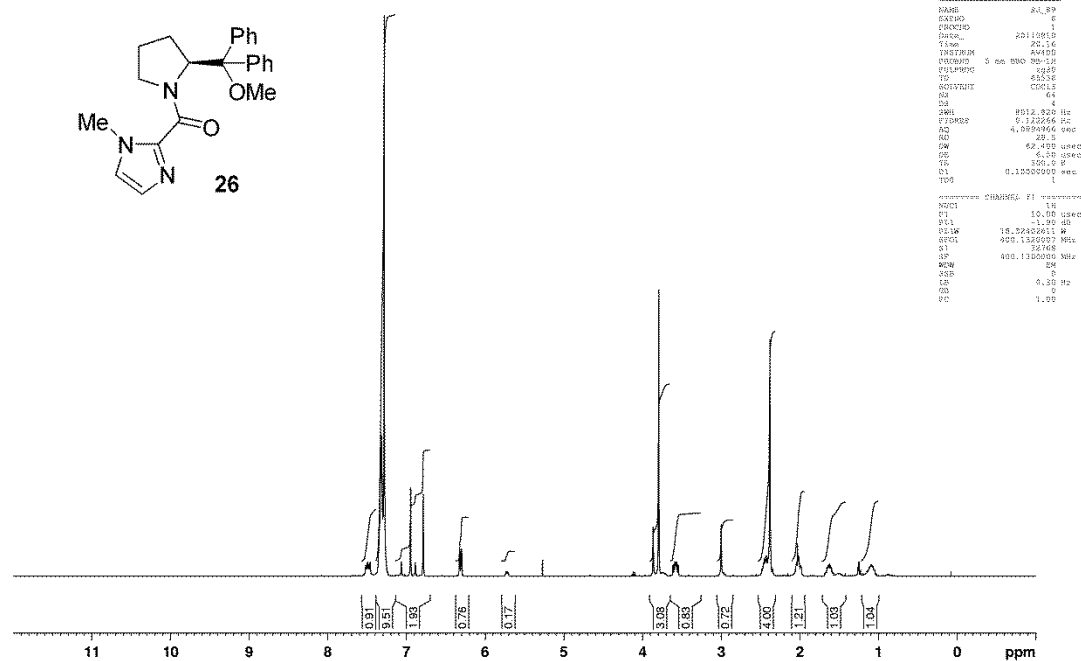
The University
Of
Sheffield.



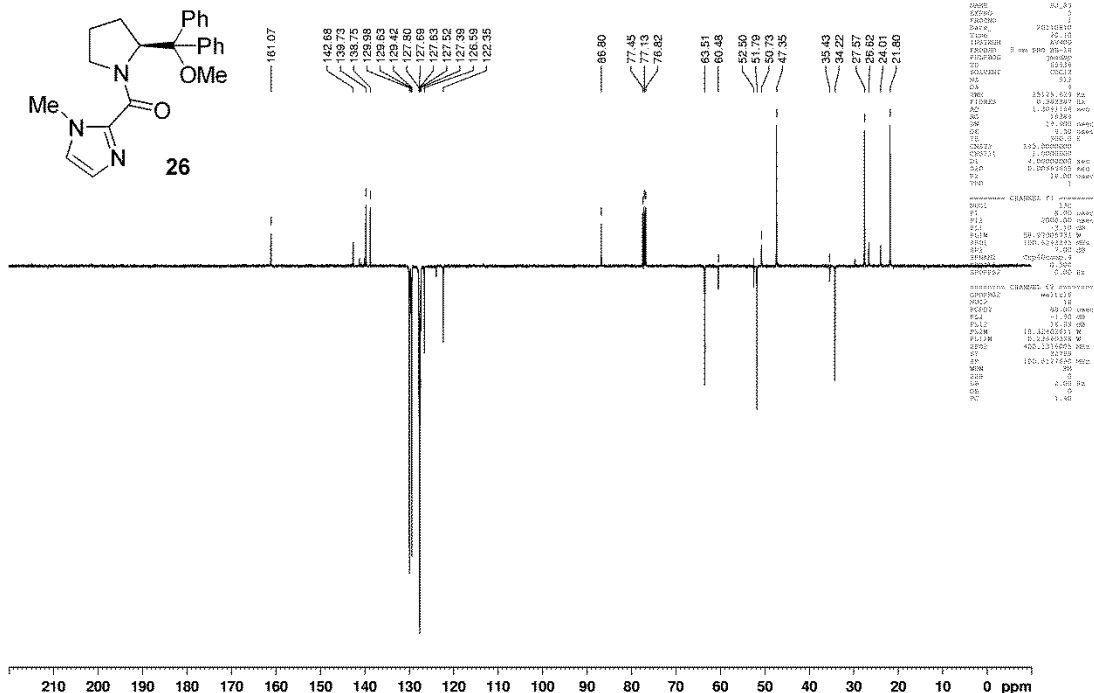
The
University
of
Sheffield.



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



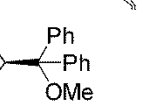
XL5-75
JMOD250PPM CDCl3 {C:\08au2011\} ch3sj 47



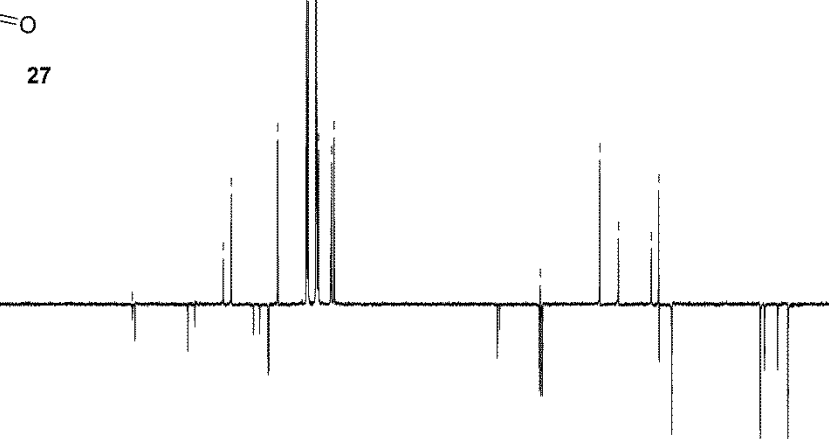
COC(=O)N1CCCC1[C@H](C1=CC=CC=C1)C1=CC=CC=C1

1H NMR spectrum (400 MHz, CDCl₃) of compound 27. The chemical structure of 27 is shown above the spectrum. The spectrum displays peaks in the aromatic region (7.0-7.5 ppm), a methoxy singlet (3.8 ppm), and aliphatic signals (1.5-2.5 ppm). Integration values are provided below the baseline.

Chemical Shift (ppm)	Integration
7.40	0.53
7.35	0.98
7.25	2.07
7.20	1.11
7.15	1.26
7.10	20.82
5.80	0.99
5.60	0.52
3.80	1.00
3.20	0.56
3.00	1.63
2.80	0.54
2.20	7.40
1.80	2.27
1.50	1.66

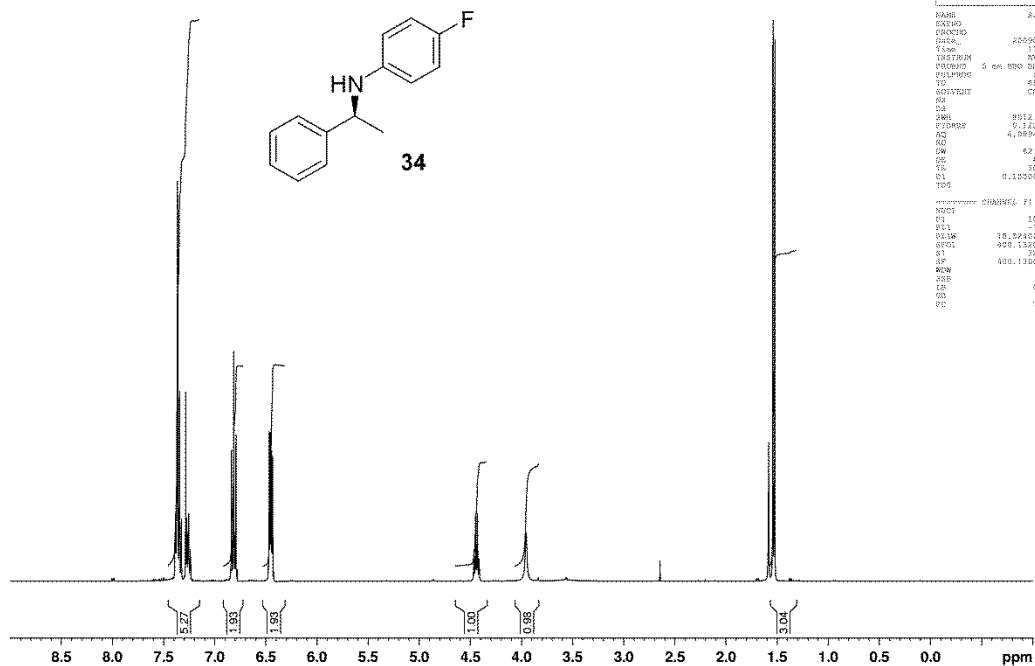


27



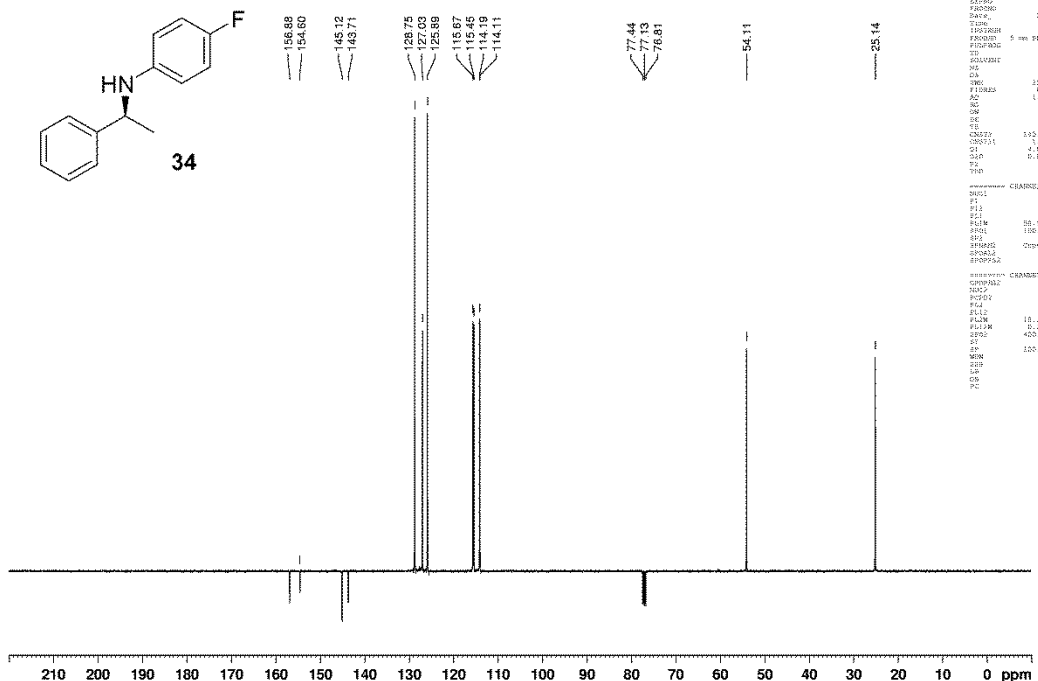
Chemical Shift (ppm)
165.18
163.54
156.62
155.00
148.68
148.87
148.87
140.48
139.57
138.40
138.49
138.57
138.89
138.89
129.75
129.56
127.86
127.86
127.70
127.65
127.55
127.33
127.26
127.26
124.28
123.73
87.00
86.48
77.49
77.37
77.17
76.85
63.95
59.76
52.34
50.69
50.59
47.74
27.84
26.89
23.96
21.61

XLp-F using XI006 as catalyst
PRO CDCl₃ [C:\04ap2009] ch3sj 8



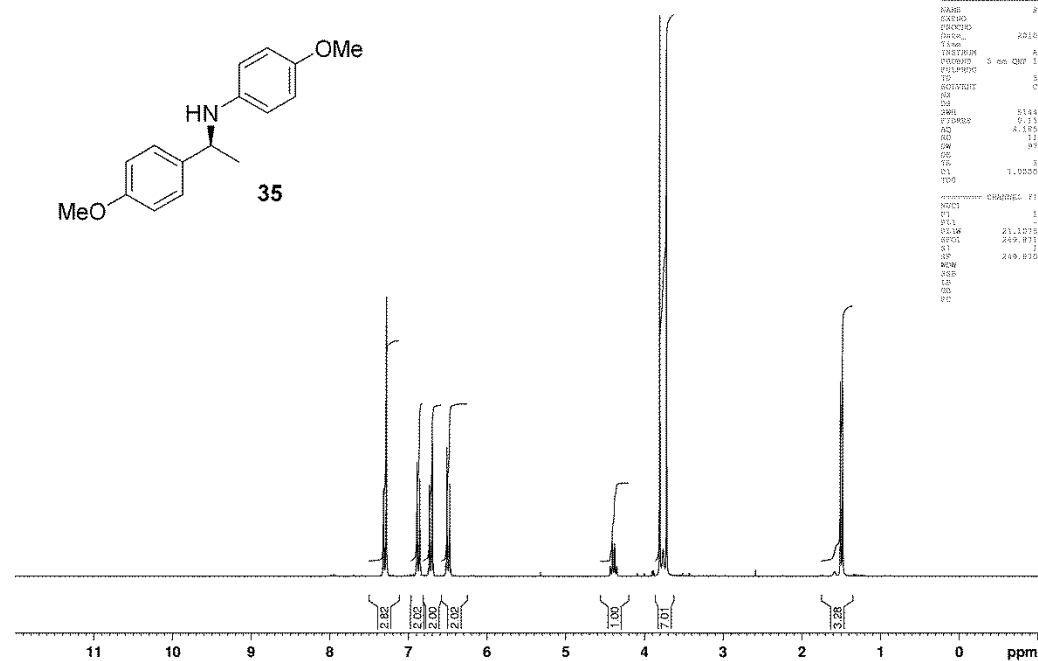
The University of Sheffield	
NAME	34_89
EXPNO	2
PROCNO	1
INSTR	200004032
TIME	11.17
INSTRUM	QNP400
PROBHD	5 mm BBO BB-1H
NUC1	13C
TD	43236
SOLVENT	CDCl3
DS	4
SWH	1012.820 Hz
F2	50.140000 MHz
RG	4.000000 sec
AD	256
SW	62.150000 sec
DE	6.000000 sec
TE	300.2 K
Q1	0.1000000 sec
Q2	1
===== CHANNEL F1 =====	
NUC1	1H
TD	10.000000
PUL	1.000000
PL1	18.000000 dB
PL2	18.000000 dB
PL3	18.000000 dB
PL4	18.000000 dB
PL5	18.000000 dB
PL6	18.000000 dB
PL7	18.000000 dB
PL8	18.000000 dB
PL9	18.000000 dB
PL10	18.000000 dB
PL11	18.000000 dB
PL12	18.000000 dB
PL13	18.000000 dB
PL14	18.000000 dB
PL15	18.000000 dB
PL16	18.000000 dB
PL17	18.000000 dB
PL18	18.000000 dB
PL19	18.000000 dB
PL20	18.000000 dB
PL21	18.000000 dB
PL22	18.000000 dB
PL23	18.000000 dB
PL24	18.000000 dB
PL25	18.000000 dB
PL26	18.000000 dB
PL27	18.000000 dB
PL28	18.000000 dB
PL29	18.000000 dB
PL30	18.000000 dB
PL31	18.000000 dB
PL32	18.000000 dB
PL33	18.000000 dB
PL34	18.000000 dB
PL35	18.000000 dB
PL36	18.000000 dB
PL37	18.000000 dB
PL38	18.000000 dB
PL39	18.000000 dB
PL40	18.000000 dB
PL41	18.000000 dB
PL42	18.000000 dB
PL43	18.000000 dB
PL44	18.000000 dB
PL45	18.000000 dB
PL46	18.000000 dB
PL47	18.000000 dB
PL48	18.000000 dB
PL49	18.000000 dB
PL50	18.000000 dB
PL51	18.000000 dB
PL52	18.000000 dB
PL53	18.000000 dB
PL54	18.000000 dB
PL55	18.000000 dB
PL56	18.000000 dB
PL57	18.000000 dB
PL58	18.000000 dB
PL59	18.000000 dB
PL60	18.000000 dB
PL61	18.000000 dB
PL62	18.000000 dB
PL63	18.000000 dB
PL64	18.000000 dB
PL65	18.000000 dB
PL66	18.000000 dB
PL67	18.000000 dB
PL68	18.000000 dB
PL69	18.000000 dB
PL70	18.000000 dB
PL71	18.000000 dB
PL72	18.000000 dB
PL73	18.000000 dB
PL74	18.000000 dB
PL75	18.000000 dB
PL76	18.000000 dB
PL77	18.000000 dB
PL78	18.000000 dB
PL79	18.000000 dB
PL80	18.000000 dB
PL81	18.000000 dB
PL82	18.000000 dB
PL83	18.000000 dB
PL84	18.000000 dB
PL85	18.000000 dB
PL86	18.000000 dB
PL87	18.000000 dB
PL88	18.000000 dB
PL89	18.000000 dB
PL90	18.000000 dB
PL91	18.000000 dB
PL92	18.000000 dB
PL93	18.000000 dB
PL94	18.000000 dB
PL95	18.000000 dB
PL96	18.000000 dB
PL97	18.000000 dB
PL98	18.000000 dB
PL99	18.000000 dB
PL100	18.000000 dB

XL078 400MHz
JMOD250PPM CDCl₃ [C:\04ap2009] ch3sj 53



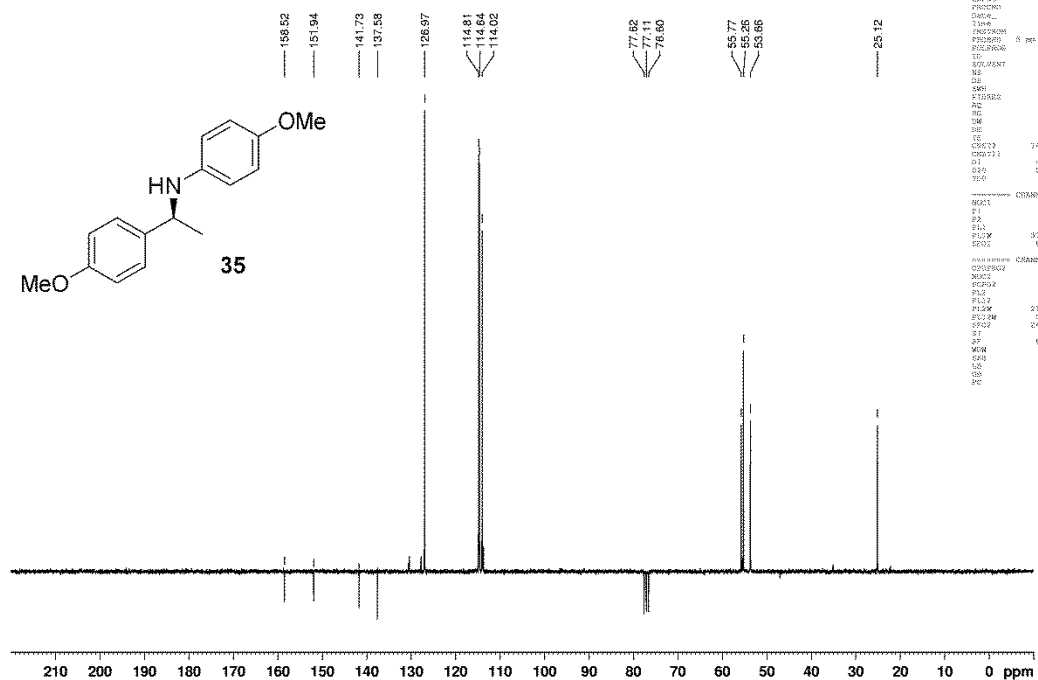
The University of Sheffield	
NAME	34_53
EXPNO	2
PROCNO	1
INSTR	200004032
TIME	11.17
INSTRUM	QNP400
PROBHD	5 mm BBO BB-1H
NUC1	13C
TD	43236
SOLVENT	CDCl3
DS	4
SWH	1012.820 Hz
F2	50.140000 MHz
RG	4.000000 sec
AD	256
SW	62.150000 sec
DE	6.000000 sec
TE	300.2 K
Q1	0.1000000 sec
Q2	1
===== CHANNEL F1 =====	
NUC1	13C
TD	10.000000
PUL	1.000000
PL1	18.000000 dB
PL2	18.000000 dB
PL3	18.000000 dB
PL4	18.000000 dB
PL5	18.000000 dB
PL6	18.000000 dB
PL7	18.000000 dB
PL8	18.000000 dB
PL9	18.000000 dB
PL10	18.000000 dB
PL11	18.000000 dB
PL12	18.000000 dB
PL13	18.000000 dB
PL14	18.000000 dB
PL15	18.000000 dB
PL16	18.000000 dB
PL17	18.000000 dB
PL18	18.000000 dB
PL19	18.000000 dB
PL20	18.000000 dB
PL21	18.000000 dB
PL22	18.000000 dB
PL23	18.000000 dB
PL24	18.000000 dB
PL25	18.000000 dB
PL26	18.000000 dB
PL27	18.000000 dB
PL28	18.000000 dB
PL29	18.000000 dB
PL30	18.000000 dB
PL31	18.000000 dB
PL32	18.000000 dB
PL33	18.000000 dB
PL34	18.000000 dB
PL35	18.000000 dB
PL36	18.000000 dB
PL37	18.000000 dB
PL38	18.000000 dB
PL39	18.000000 dB
PL40	18.000000 dB
PL41	18.000000 dB
PL42	18.000000 dB
PL43	18.000000 dB
PL44	18.000000 dB
PL45	18.000000 dB
PL46	18.000000 dB
PL47	18.000000 dB
PL48	18.000000 dB
PL49	18.000000 dB
PL50	18.000000 dB
PL51	18.000000 dB
PL52	18.000000 dB
PL53	18.000000 dB
PL54	18.000000 dB
PL55	18.000000 dB
PL56	18.000000 dB
PL57	18.000000 dB
PL58	18.000000 dB
PL59	18.000000 dB
PL60	18.000000 dB
PL61	18.000000 dB
PL62	18.000000 dB
PL63	18.000000 dB
PL64	18.000000 dB
PL65	18.000000 dB
PL66	18.000000 dB
PL67	18.000000 dB
PL68	18.000000 dB
PL69	18.000000 dB
PL70	18.000000 dB
PL71	18.000000 dB
PL72	18.000000 dB
PL73	18.000000 dB
PL74	18.000000 dB
PL75	18.000000 dB
PL76	18.000000 dB
PL77	18.000000 dB
PL78	18.000000 dB
PL79	18.000000 dB
PL80	18.000000 dB
PL81	18.000000 dB
PL82	18.000000 dB
PL83	18.000000 dB
PL84	18.000000 dB
PL85	18.000000 dB
PL86	18.000000 dB
PL87	18.000000 dB
PL88	18.000000 dB
PL89	18.000000 dB
PL90	18.000000 dB
PL91	18.000000 dB
PL92	18.000000 dB
PL93	18.000000 dB
PL94	18.000000 dB
PL95	18.000000 dB
PL96	18.000000 dB
PL97	18.000000 dB
PL98	18.000000 dB
PL99	18.000000 dB
PL100	18.000000 dB

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



NAME	XL3-37
EXPNO	1
PROCNO	1
DATE_	20100120
TIME	9.23
INSTRUM	AVANCE
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
DELTA	0.001
RG	64
DS	4
SWH	514.033 Hz
F2	125.761 MHz
NUC1	13C
NUC2	1H
PC	1.00
PD	1.00
PE	1.00
PF	1.00
PG	1.00
PH	1.00
PI	1.00
PJ	1.00
PK	1.00
PL	1.00
PM	1.00
PN	1.00
PO	1.00
PP	1.00
PQ	1.00
PR	1.00
PS	1.00
PT	1.00
PV	1.00
PW	1.00
PX	1.00
PY	1.00
PZ	1.00

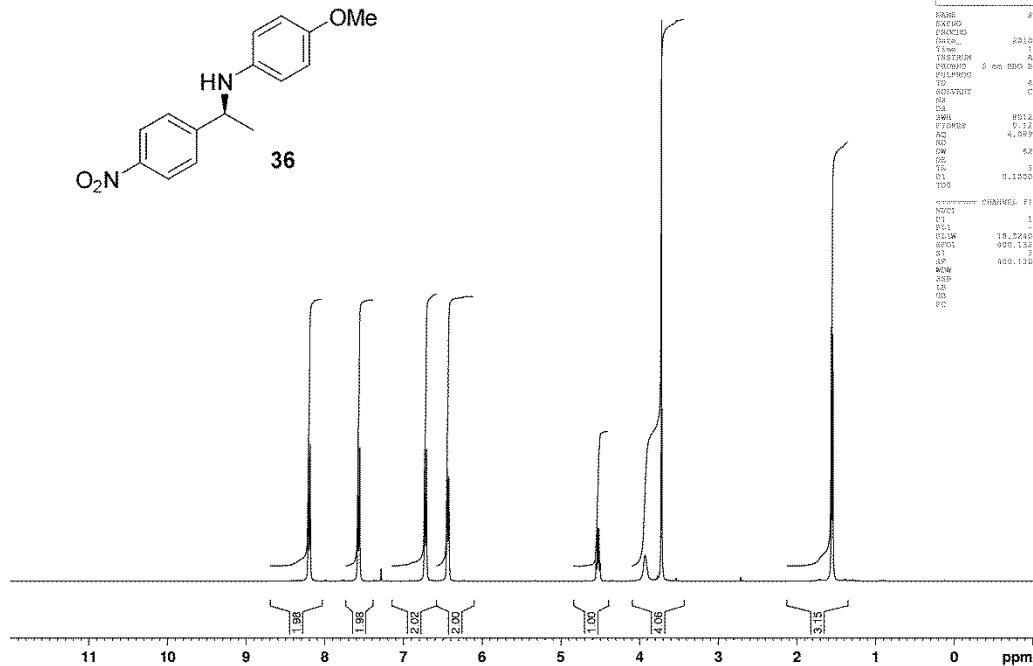
XL3-39 250MHz
JMOD250PPM CDCl₃ {C:01ja2010} ch3sj 48



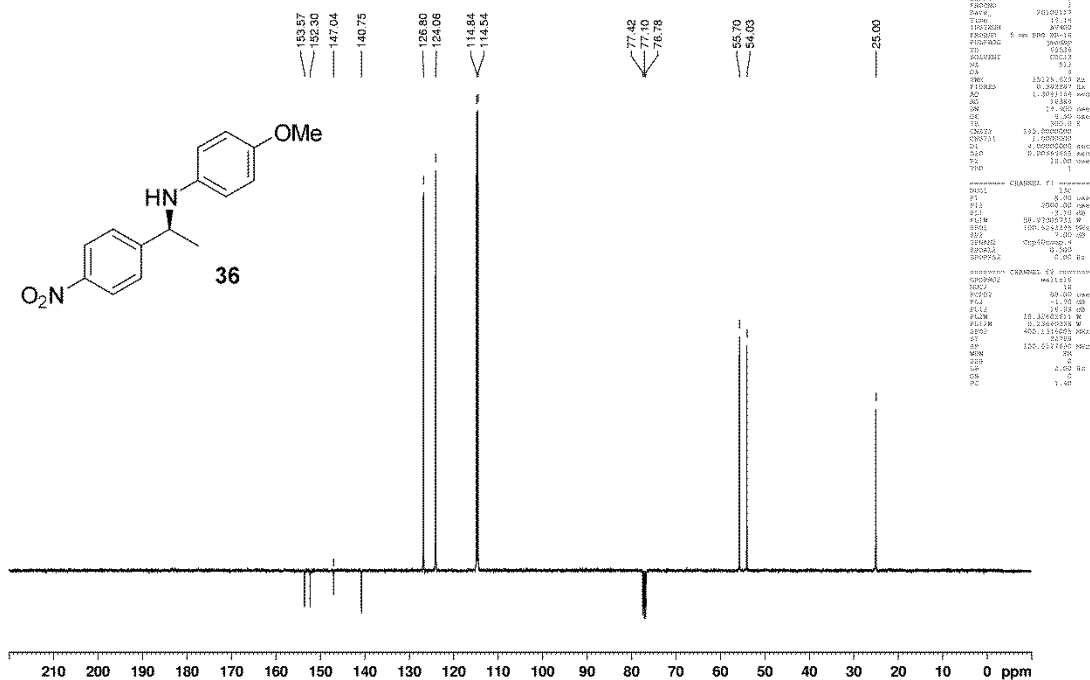
NAME	XL3-39
EXPNO	1
PROCNO	1
DATE_	20100120
TIME	9.23
INSTRUM	AVANCE
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
DELTA	0.001
RG	64
DS	4
SWH	15723.271 Hz
F2	125.761 MHz
NUC1	13C
NUC2	1H
PC	1.00
PD	1.00
PE	1.00
PF	1.00
PG	1.00
PH	1.00
PI	1.00
PJ	1.00
PK	1.00
PL	1.00
PM	1.00
PN	1.00
PO	1.00
PP	1.00
PQ	1.00
PR	1.00
PS	1.00
PT	1.00
PV	1.00
PW	1.00
PX	1.00
PY	1.00
PZ	1.00

COc1ccc(N[C@H](C)c2ccc([N+](=O)[O-])cc2)cc1

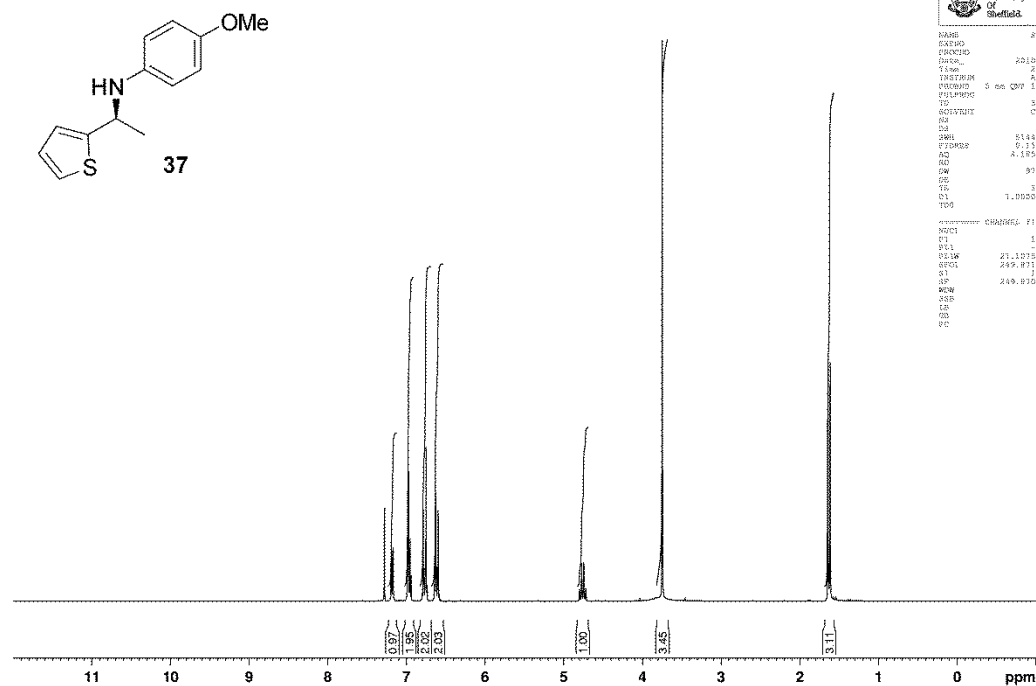
36



36

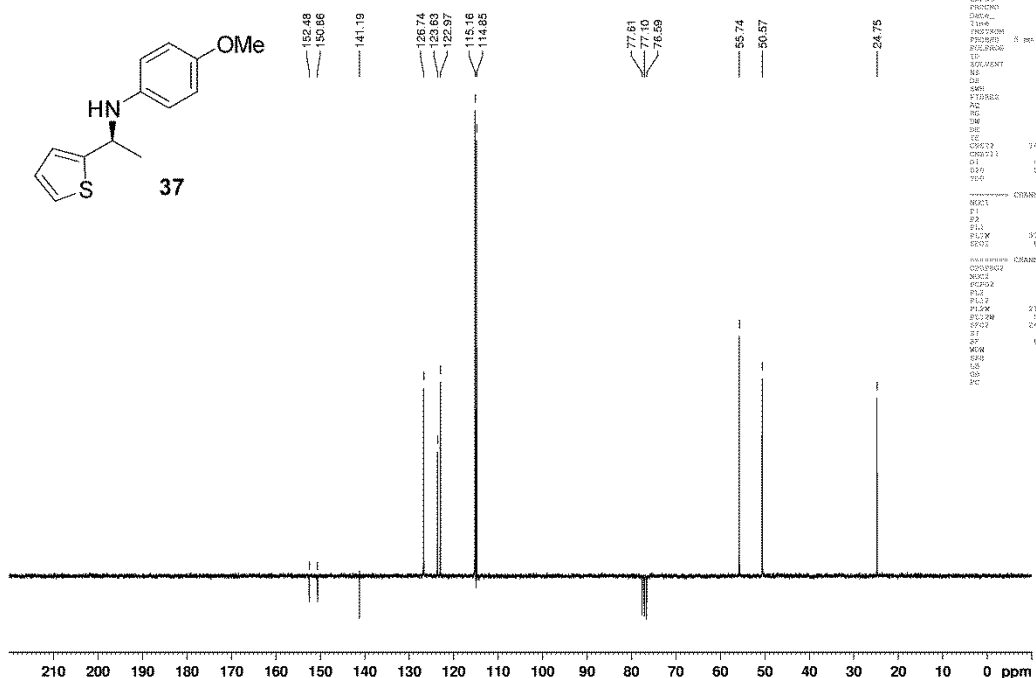
C[C@H](Nc1ccc(OC)cc1)c2ccc([N+](=O)[O-])cc2

XL3-66 250MHz
PRO CDCl3 {C:03mr2010} ch3s] 58



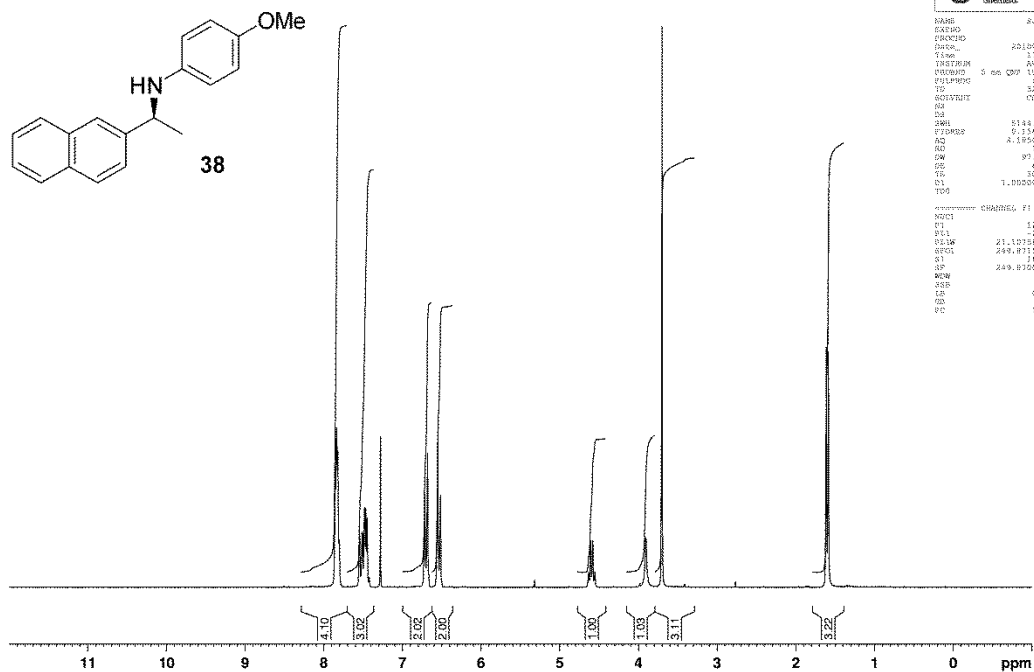
The University of Sheffield	
NAME	37
EXPNO	1
PROCNO	1
DATE_	20100304
TIME	20.29
INSTRUM	QNP1H
PROBHD	5 mm QNP 1H/13
NUC1	13C
NUC2	1H
Q1	1.00000000
Q2	1.00000000
Q3	1.00000000
Q4	1.00000000
Q5	1.00000000
Q6	1.00000000
Q7	1.00000000
Q8	1.00000000
Q9	1.00000000
Q10	1.00000000
Q11	1.00000000
Q12	1.00000000
Q13	1.00000000
Q14	1.00000000
Q15	1.00000000
Q16	1.00000000
Q17	1.00000000
Q18	1.00000000
Q19	1.00000000
Q20	1.00000000
Q21	1.00000000
Q22	1.00000000
Q23	1.00000000
Q24	1.00000000
Q25	1.00000000
Q26	1.00000000
Q27	1.00000000
Q28	1.00000000
Q29	1.00000000
Q30	1.00000000
Q31	1.00000000
Q32	1.00000000
Q33	1.00000000
Q34	1.00000000
Q35	1.00000000
Q36	1.00000000
Q37	1.00000000
Q38	1.00000000
Q39	1.00000000
Q40	1.00000000
Q41	1.00000000
Q42	1.00000000
Q43	1.00000000
Q44	1.00000000
Q45	1.00000000
Q46	1.00000000
Q47	1.00000000
Q48	1.00000000
Q49	1.00000000
Q50	1.00000000
Q51	1.00000000
Q52	1.00000000
Q53	1.00000000
Q54	1.00000000
Q55	1.00000000
Q56	1.00000000
Q57	1.00000000
Q58	1.00000000
Q59	1.00000000
Q60	1.00000000
Q61	1.00000000
Q62	1.00000000
Q63	1.00000000
Q64	1.00000000
Q65	1.00000000
Q66	1.00000000
Q67	1.00000000
Q68	1.00000000
Q69	1.00000000
Q70	1.00000000
Q71	1.00000000
Q72	1.00000000
Q73	1.00000000
Q74	1.00000000
Q75	1.00000000
Q76	1.00000000
Q77	1.00000000
Q78	1.00000000
Q79	1.00000000
Q80	1.00000000
Q81	1.00000000
Q82	1.00000000
Q83	1.00000000
Q84	1.00000000
Q85	1.00000000
Q86	1.00000000
Q87	1.00000000
Q88	1.00000000
Q89	1.00000000
Q90	1.00000000
Q91	1.00000000
Q92	1.00000000
Q93	1.00000000
Q94	1.00000000
Q95	1.00000000
Q96	1.00000000
Q97	1.00000000
Q98	1.00000000
Q99	1.00000000
Q100	1.00000000

XL3-66 250MHz
JMOD250PPM CDCl3 {C:03mr2010} ch3s] 3



The University of Sheffield	
NAME	37
EXPNO	1
PROCNO	1
DATE_	20100304
TIME	20.29
INSTRUM	QNP1H
PROBHD	5 mm QNP 1H/13
NUC1	13C
NUC2	1H
Q1	1.00000000
Q2	1.00000000
Q3	1.00000000
Q4	1.00000000
Q5	1.00000000
Q6	1.00000000
Q7	1.00000000
Q8	1.00000000
Q9	1.00000000
Q10	1.00000000
Q11	1.00000000
Q12	1.00000000
Q13	1.00000000
Q14	1.00000000
Q15	1.00000000
Q16	1.00000000
Q17	1.00000000
Q18	1.00000000
Q19	1.00000000
Q20	1.00000000
Q21	1.00000000
Q22	1.00000000
Q23	1.00000000
Q24	1.00000000
Q25	1.00000000
Q26	1.00000000
Q27	1.00000000
Q28	1.00000000
Q29	1.00000000
Q30	1.00000000
Q31	1.00000000
Q32	1.00000000
Q33	1.00000000
Q34	1.00000000
Q35	1.00000000
Q36	1.00000000
Q37	1.00000000
Q38	1.00000000
Q39	1.00000000
Q40	1.00000000
Q41	1.00000000
Q42	1.00000000
Q43	1.00000000
Q44	1.00000000
Q45	1.00000000
Q46	1.00000000
Q47	1.00000000
Q48	1.00000000
Q49	1.00000000
Q50	1.00000000
Q51	1.00000000
Q52	1.00000000
Q53	1.00000000
Q54	1.00000000
Q55	1.00000000
Q56	1.00000000
Q57	1.00000000
Q58	1.00000000
Q59	1.00000000
Q60	1.00000000
Q61	1.00000000
Q62	1.00000000
Q63	1.00000000
Q64	1.00000000
Q65	1.00000000
Q66	1.00000000
Q67	1.00000000
Q68	1.00000000
Q69	1.00000000
Q70	1.00000000
Q71	1.00000000
Q72	1.00000000
Q73	1.00000000
Q74	1.00000000
Q75	1.00000000
Q76	1.00000000
Q77	1.00000000
Q78	1.00000000
Q79	1.00000000
Q80	1.00000000
Q81	1.00000000
Q82	1.00000000
Q83	1.00000000
Q84	1.00000000
Q85	1.00000000
Q86	1.00000000
Q87	1.00000000
Q88	1.00000000
Q89	1.00000000
Q90	1.00000000
Q91	1.00000000
Q92	1.00000000
Q93	1.00000000
Q94	1.00000000
Q95	1.00000000
Q96	1.00000000
Q97	1.00000000
Q98	1.00000000
Q99	1.00000000
Q100	1.00000000

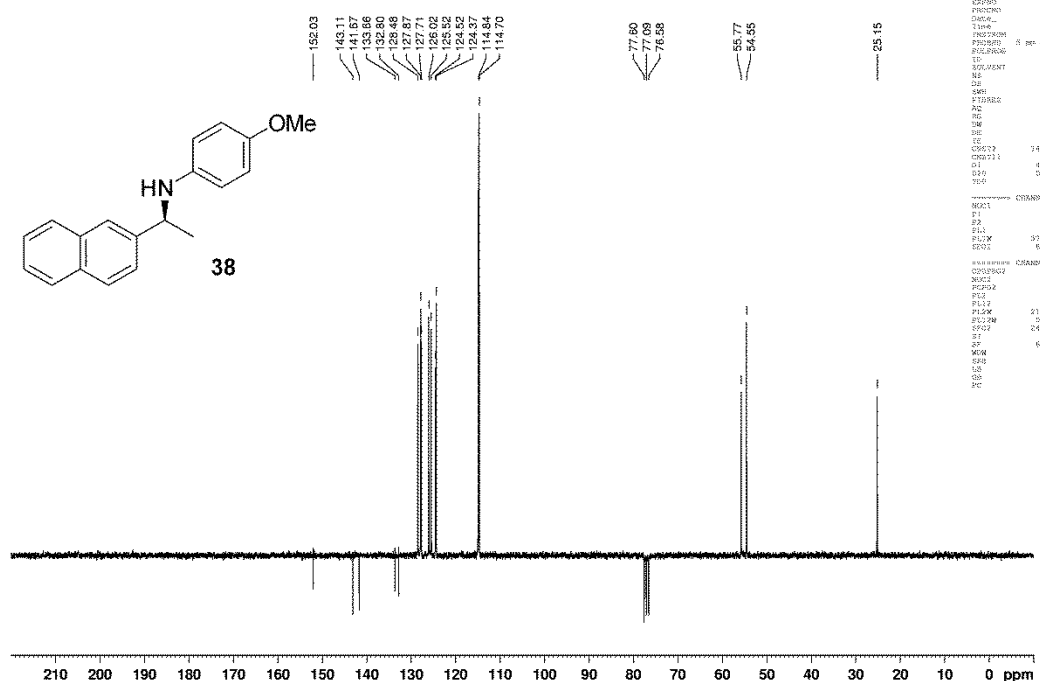
XL3-43 250MHz
PRO CDCl3 {C:01ja2010} ch3sj 21



NAME: AL 89
EXPNO: 2
PROCNO: 1
DATE_: 20100122
TIME: 17.37
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 64
DS: 4
SWH: 5144.033 Hz
F2: 101.625 MHz
AQ: 1.1950396 sec
RG: 1024
RM: 0.17230000 sec
DS: 6.5000000 sec
TE: 300.2 K
D1: 1.00000000 sec
TD0: 1

===== CHANNEL f1 =====
NUC1: 13C
P1: 12.00 usec
PL1: -2.00 dB
PL2: 21.10184931 dB
PL3: 249.8711430 MHz
PL4: 10.00 dB
PL5: 249.8710000 MHz
PL6: 0 dB
PL7: 0.10 MHz
PL8: 0 dB
PL9: 1.00

XL3-43 250MHz
JMOD250PPM CDCl3 {C:01ja2010} ch3sj 24



NAME: AL 89
EXPNO: 2
PROCNO: 1
DATE_: 20100122
TIME: 20.41
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 64
DS: 4
SWH: 15723.271 MHz
F2: 101.625 MHz
AQ: 1.0440768 sec
RG: 1024
RM: 0.17230000 sec
DS: 6.5000000 sec
TE: 300.2 K
D1: 1.00000000 sec
D2: 4.00000000 sec
D3: 0.00649693 sec
TD0: 1

===== CHANNEL f1 =====
NUC1: 13C
P1: 12.00 usec
PL1: -2.00 dB
PL2: 19.99 dB
PL3: 21.10184931 dB
PL4: 10.00 dB
PL5: 249.8710000 MHz
PL6: 0 dB
PL7: 0.10 MHz
PL8: 0 dB
PL9: 1.00

Created : 10/01/2010 16:00:12
Project : Work3
Sample ID : XL3-32
Calibration : XL3-32 racemic

By : Clarity
Report Style : Instrument
Sample : XL3-32
Chromatogram : DATA\XL3-32 racemic

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

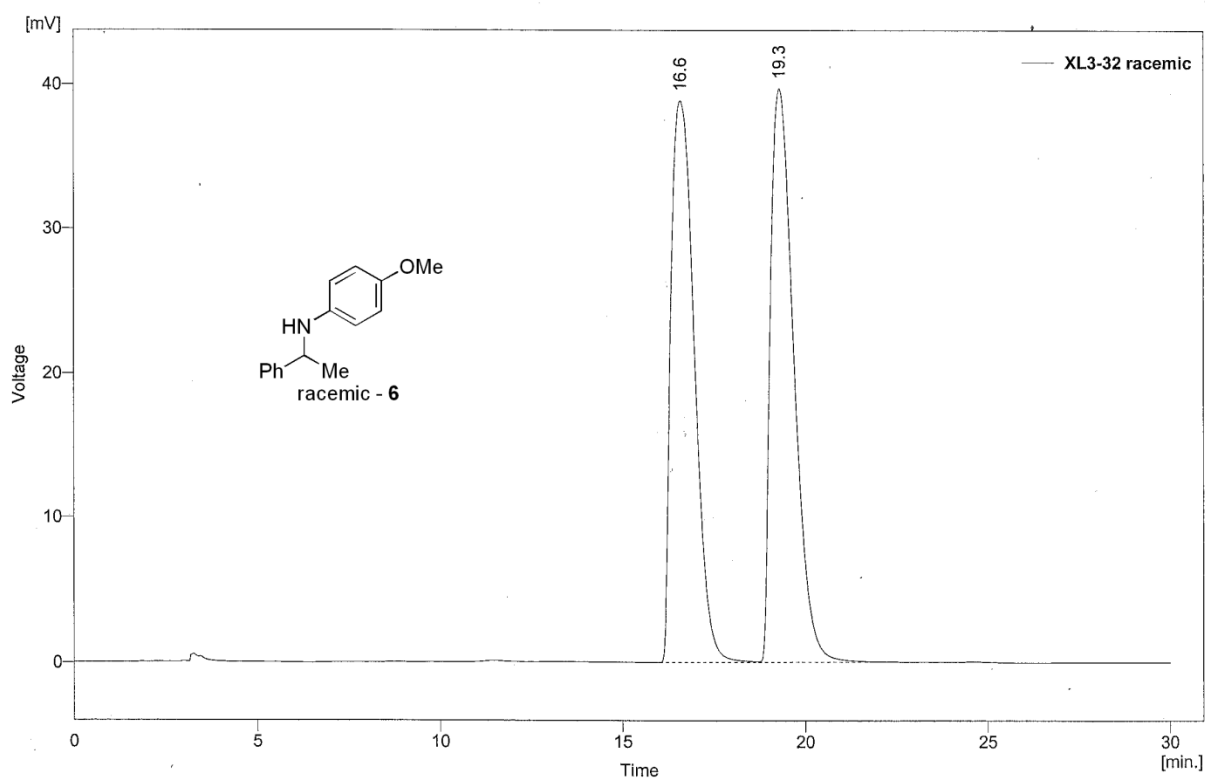
By : Clarity
Modified : 10/01/2010 16:00

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 2% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 30.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-32
Calibration : XL3-32

By : Clarity
Report Style : Instrument
Sample : XL3-32
Chromatogram : DATA\XL3-32

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

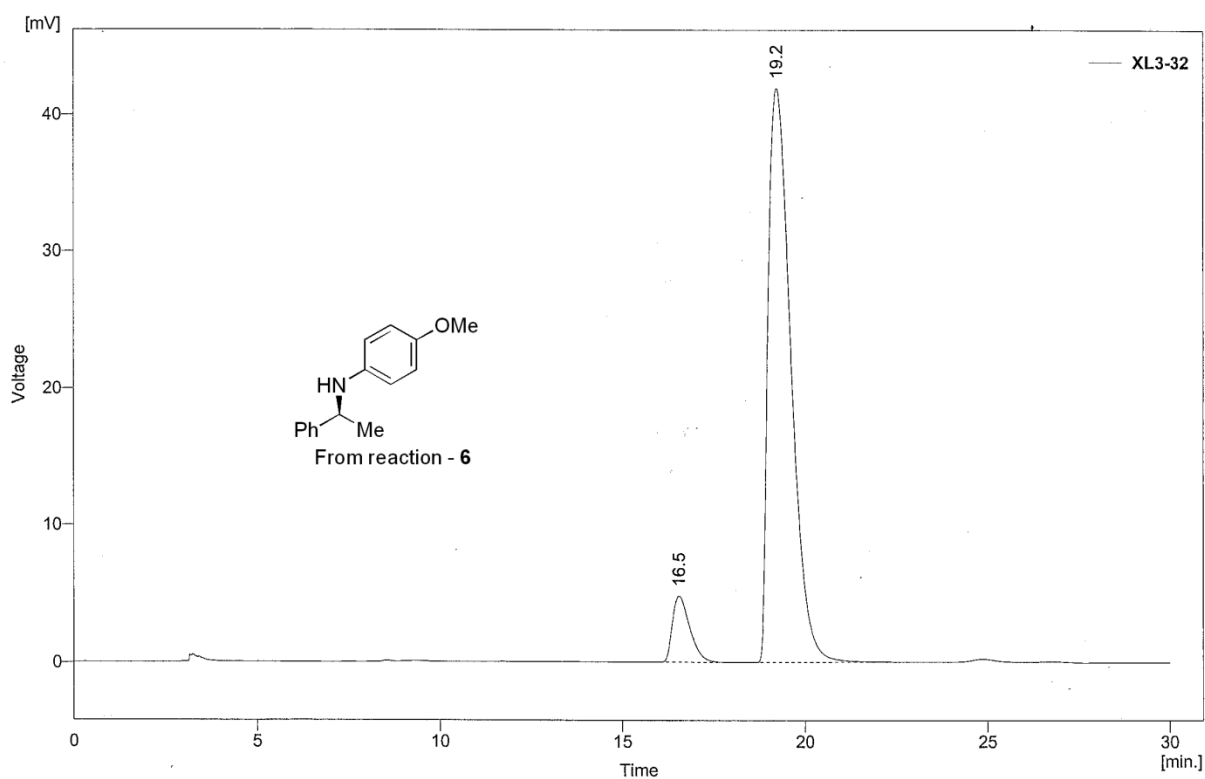
By : Clarity
Modified : 10/01/2010 15:21

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 2% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 30.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL078
Calibration : XL079'

By : Clarity
Report Style : Instrument
Sample : XL078
Chromatogram : DATA\XL079'

Method : Cellucoat
Description : Kromasil OD
Created : 24/08/2004 16:25

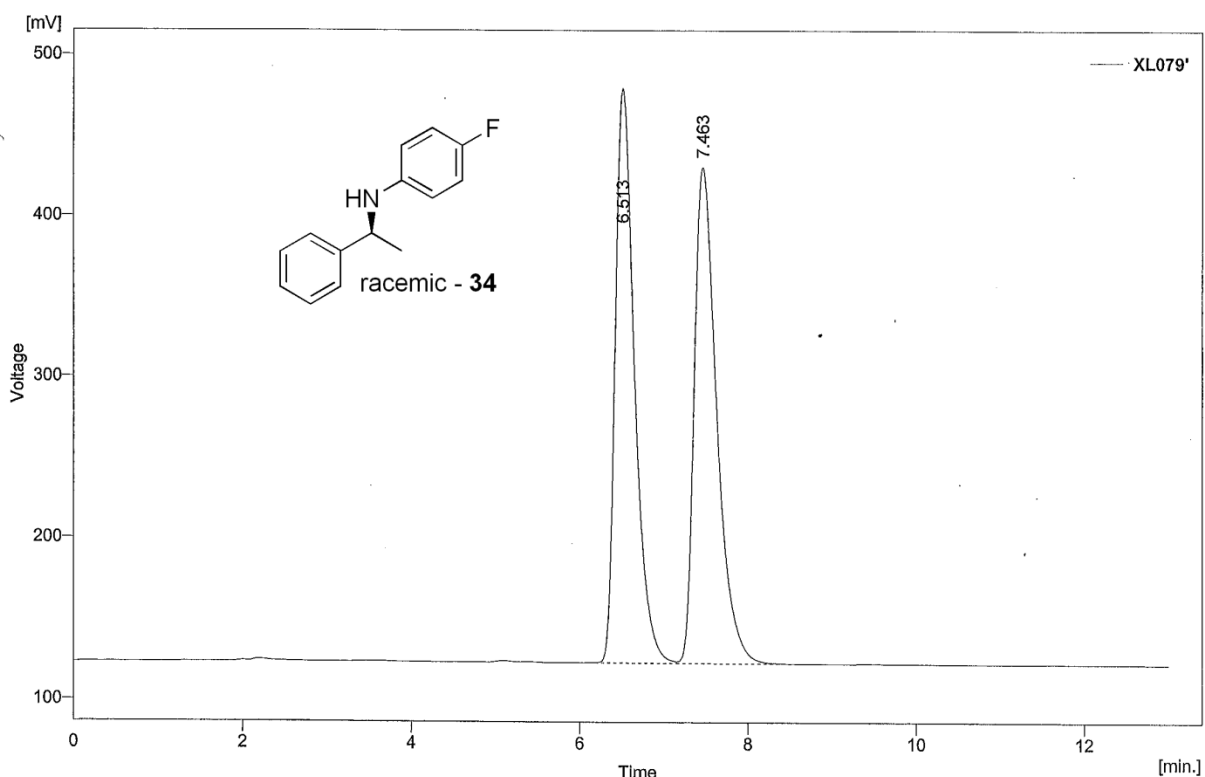
By : Clarity
Modified : 04/04/2009 19:02

Column : Kromasil 3-Cellucoat OD
Mobile Phase : 1% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 13.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL078
Calibration : XL078-2

By : Clarity
Report Style : Instrument
Sample : XL078
Chromatogram : DATA\XL078-2

Method : Cellucoat
Description : Kromasil OD
Created : 24/08/2004 16:25

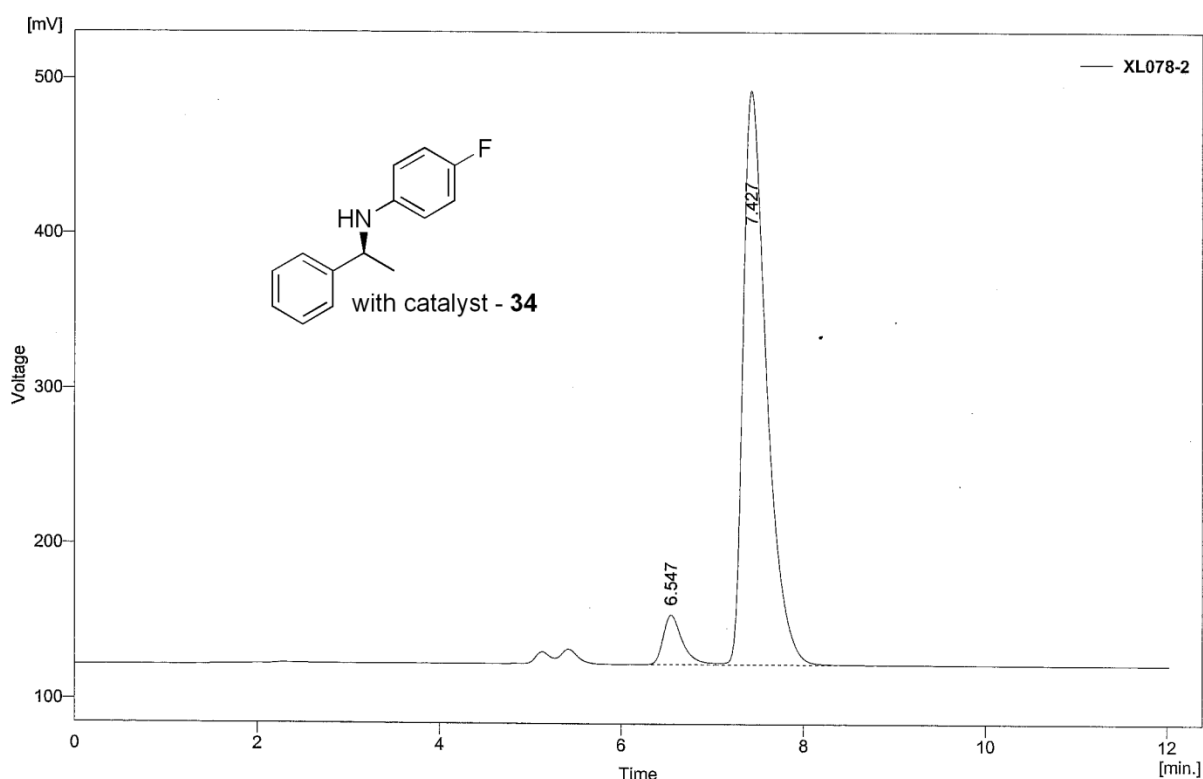
By : Clarity
Modified : 04/04/2009 19:48

Column : Kromasil 3-Cellucoat OD
Mobile Phase : 1% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 13.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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	

86.9%

Created : 18/01/2010 12:49:13
Project : Work3
Sample ID : XL3-37
Calibration : XL3-37

By : Clarity
Report Style : Instrument
Sample : XL3-37
Chromatogram : DATA\XL3-37

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

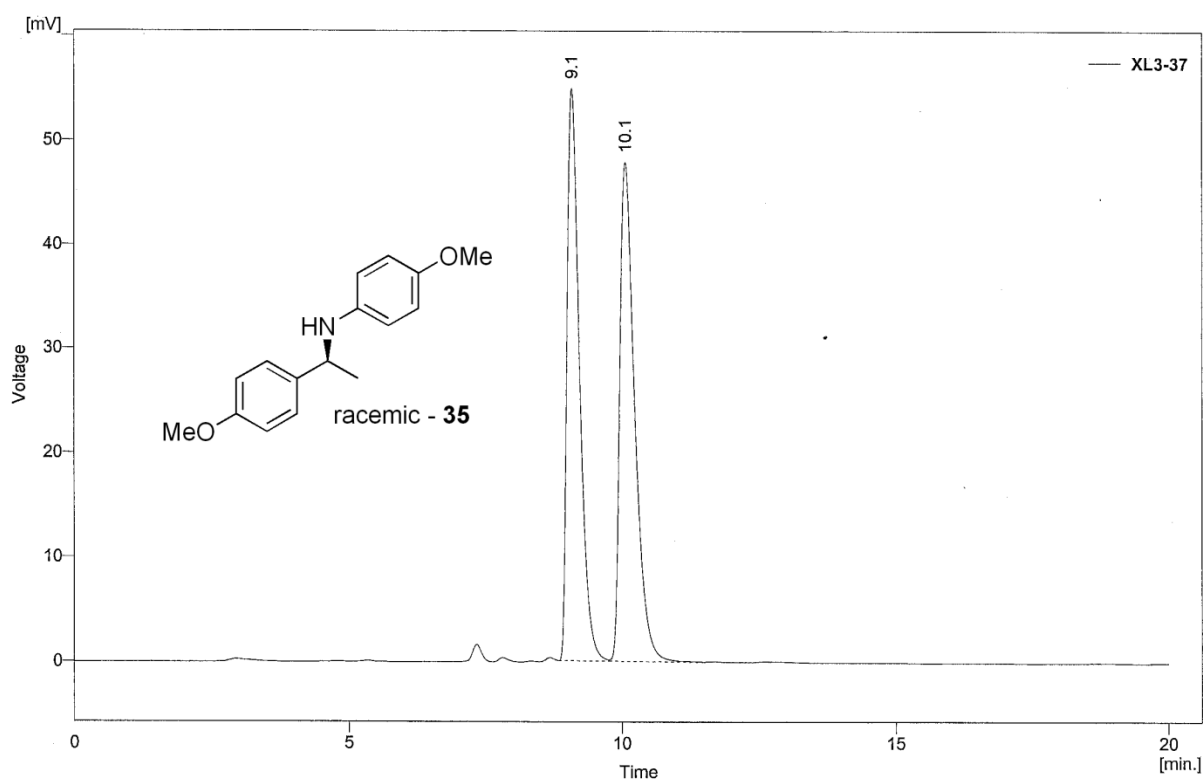
By : Clarity
Modified : 18/01/2010 15:26

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 10% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 20.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-39
Calibration : XL3-39

By : Clarity
Report Style : Instrument
Sample : XL3-39
Chromatogram : DATA\XL3-39

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

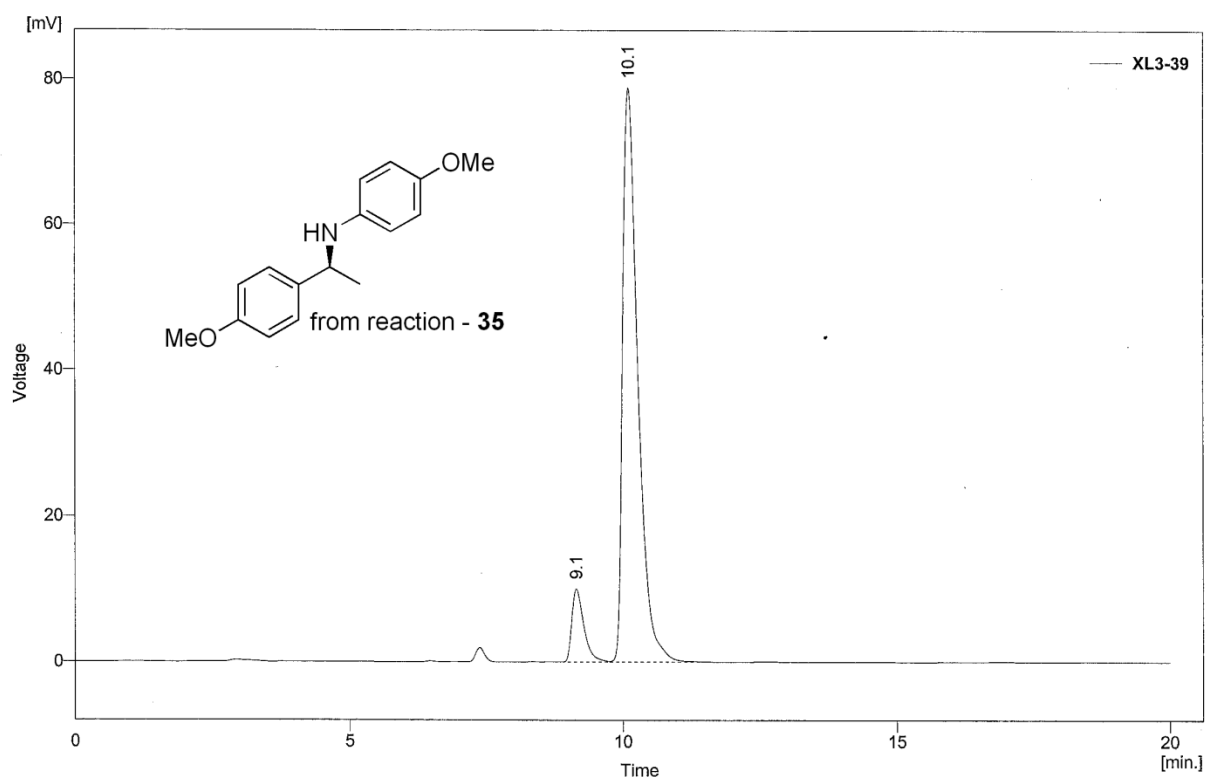
By : Clarity
Modified : 18/01/2010 15:50

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 10% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 20.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-35
Calibration : XL3-35

By : Clarity
Report Style : Instrument
Sample : XL3-35
Chromatogram : DATA\XL3-35

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

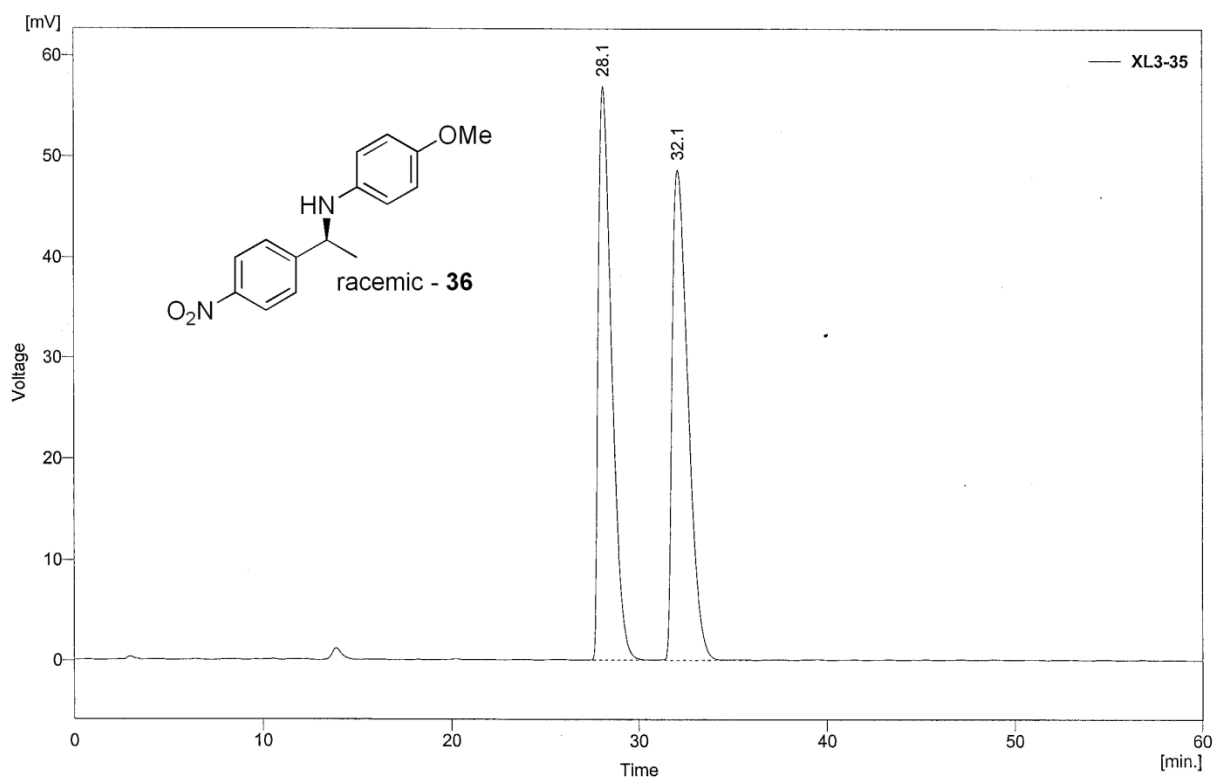
By : Clarity
Modified : 15/01/2010 11:10

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 10% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 80.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-34
Calibration : XL3-34

By : Clarity
Report Style : Instrument
Sample : XL3-34
Chromatogram : DATA\XL3-34

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

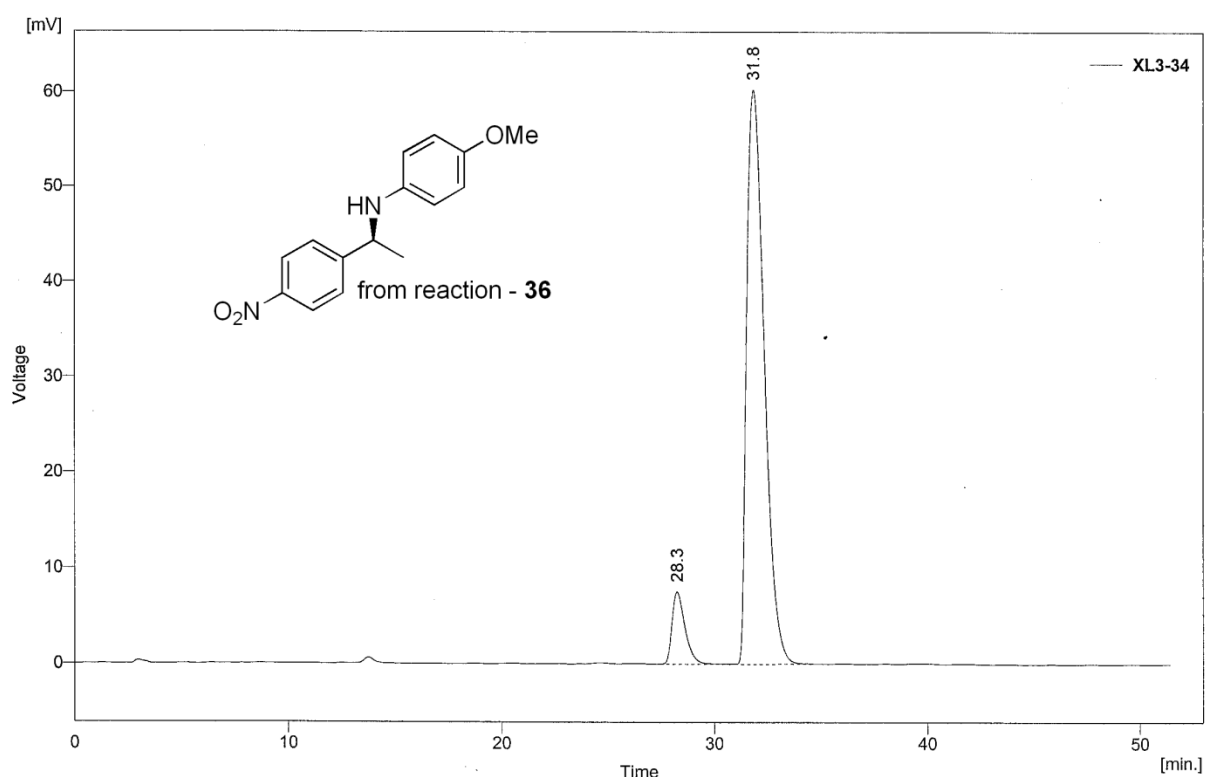
By : Clarity
Modified : 15/01/2010 14:11

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 10% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 60.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-66
Calibration : XL3-66 racemic

By : Clarity
Report Style : Instrument
Sample : XL3-66
Chromatogram : DATA\XL3-66 racemic

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

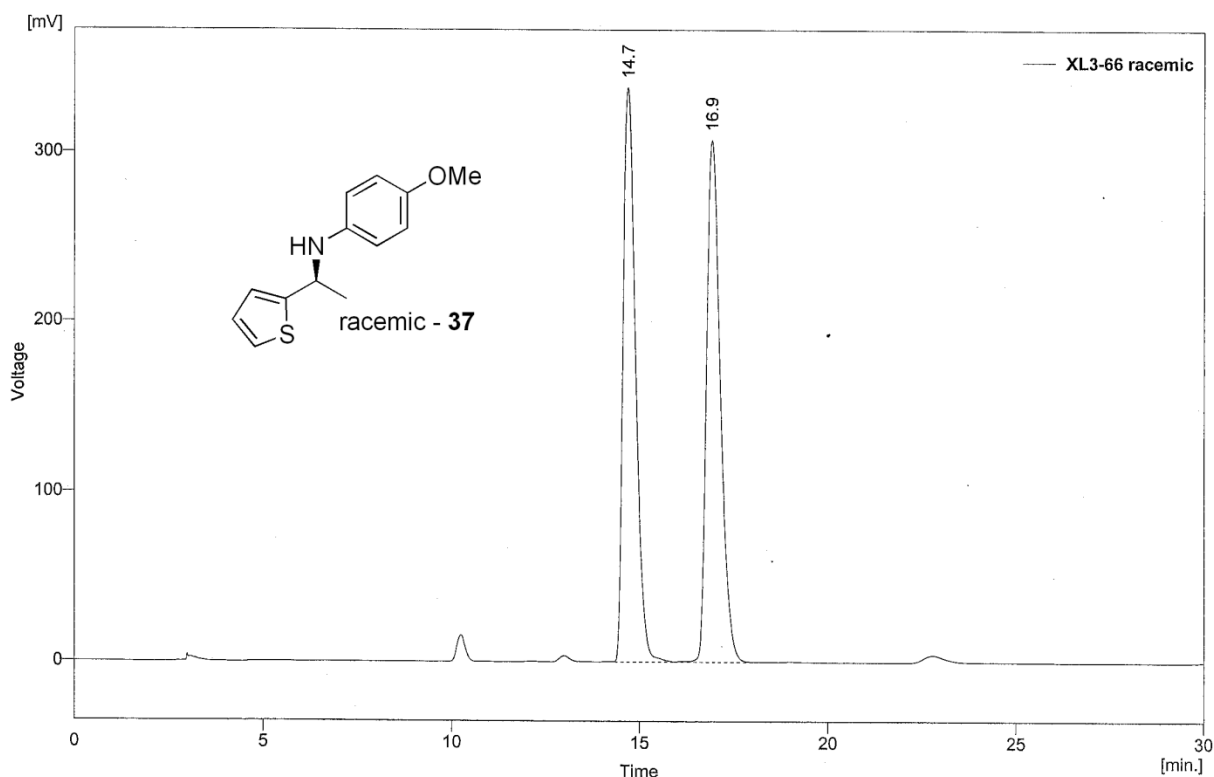
By : Clarity
Modified : 04/03/2010 10:08

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 2% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 60.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL66 chiral
Calibration : XL66 chiral'

By : Clarity
Report Style : Instrument
Sample : XL66 chiral
Chromatogram : DATA\XL66 chiral'

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

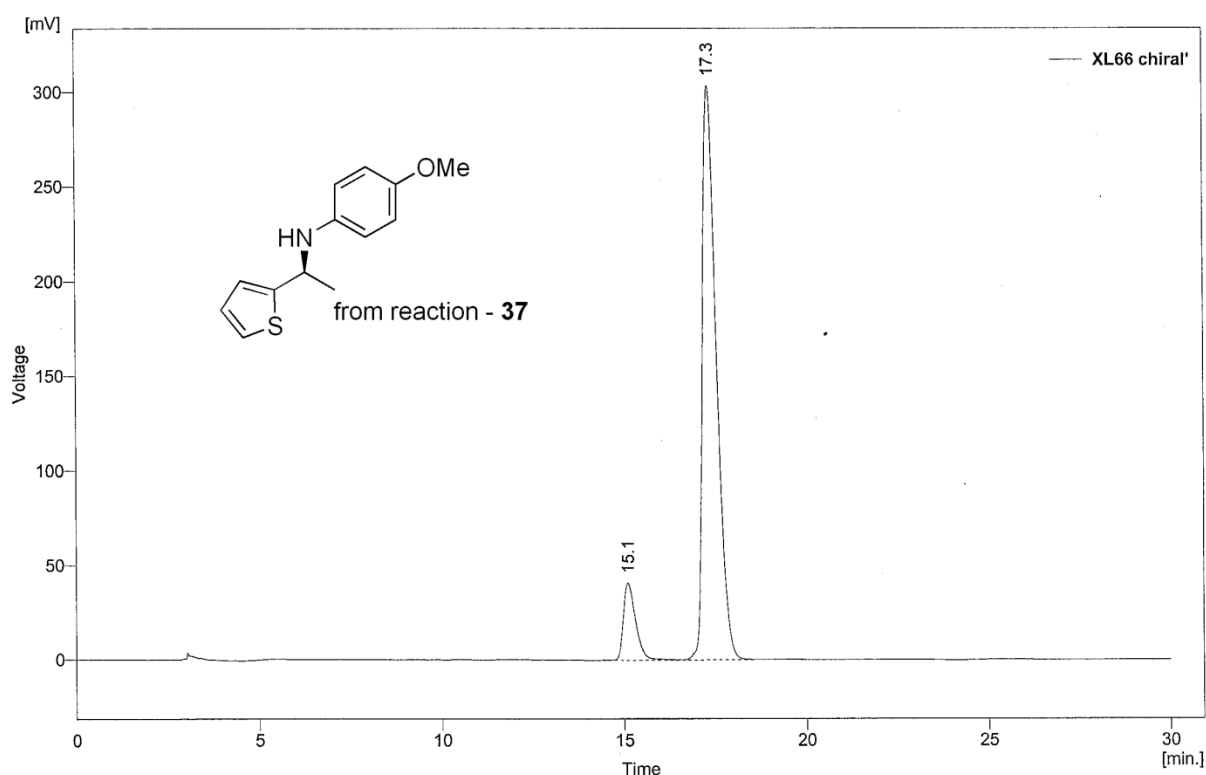
By : Clarity
Modified : 04/03/2010 19:40

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 2% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 30.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-43 racemic
Calibration : XL3-43 racemic

By : Clarity
Report Style : Instrument
Sample : XL3-43 racemic
Chromatogram : DATA\XL3-43 racemic

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

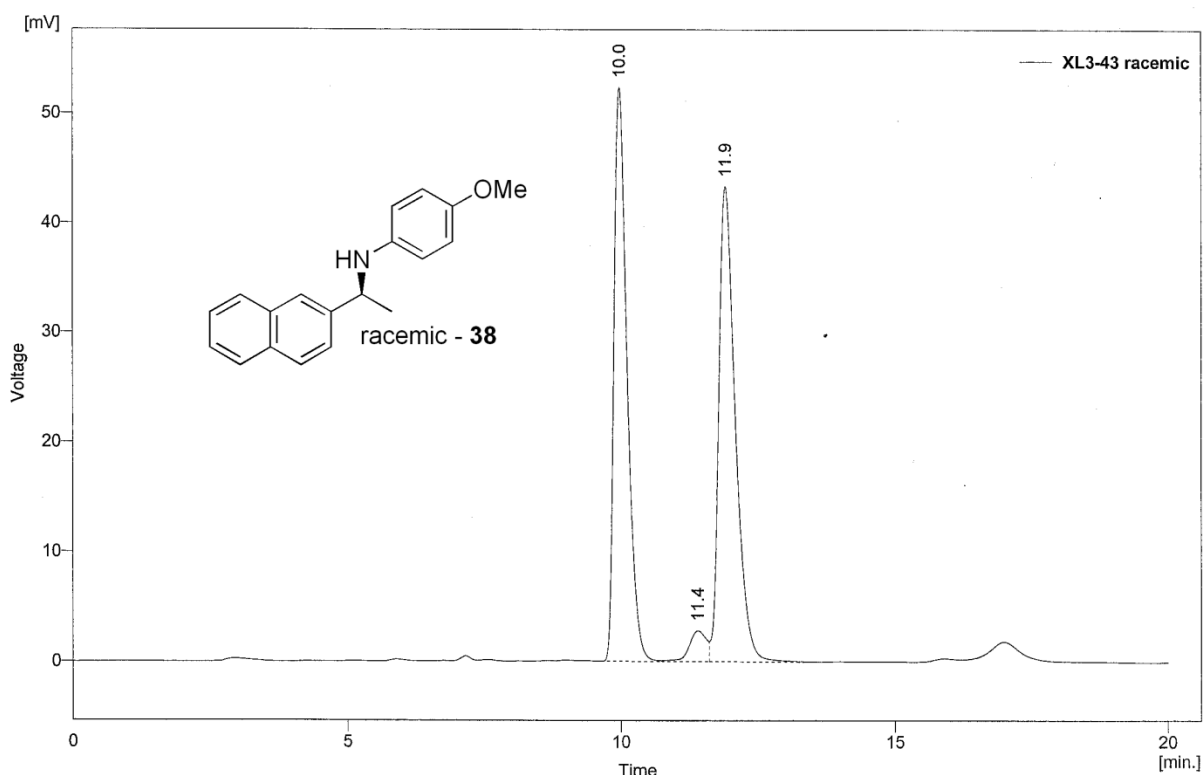
By : Clarity
Modified : 22/01/2010 11:26

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 10% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

Autostop : 20.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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
Project : Work3
Sample ID : XL3-43
Calibration : XL3-43

By : Clarity
Report Style : Instrument
Sample : XL3-43
Chromatogram : DATA\XL3-43

Method : Cellulose-1
Description : Cellulose-1
Created : 24/08/2004 16:25

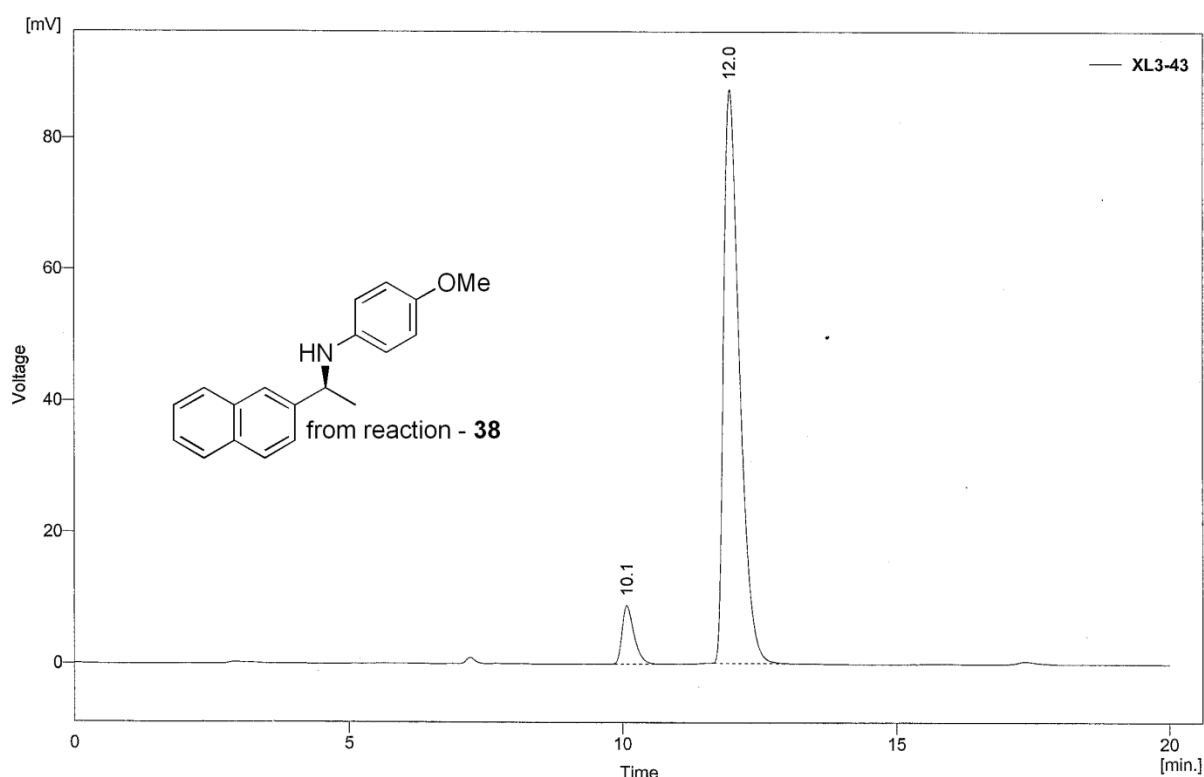
By : Clarity
Modified : 22/01/2010 12:04

Column : Phenomenex Lux 3um Cellulose-1
Mobile Phase : 10% ipa in hexane
Flow Rate : 1mL/min
Note :

Detection : UV@254nm
Temperature : RT
Pressure :

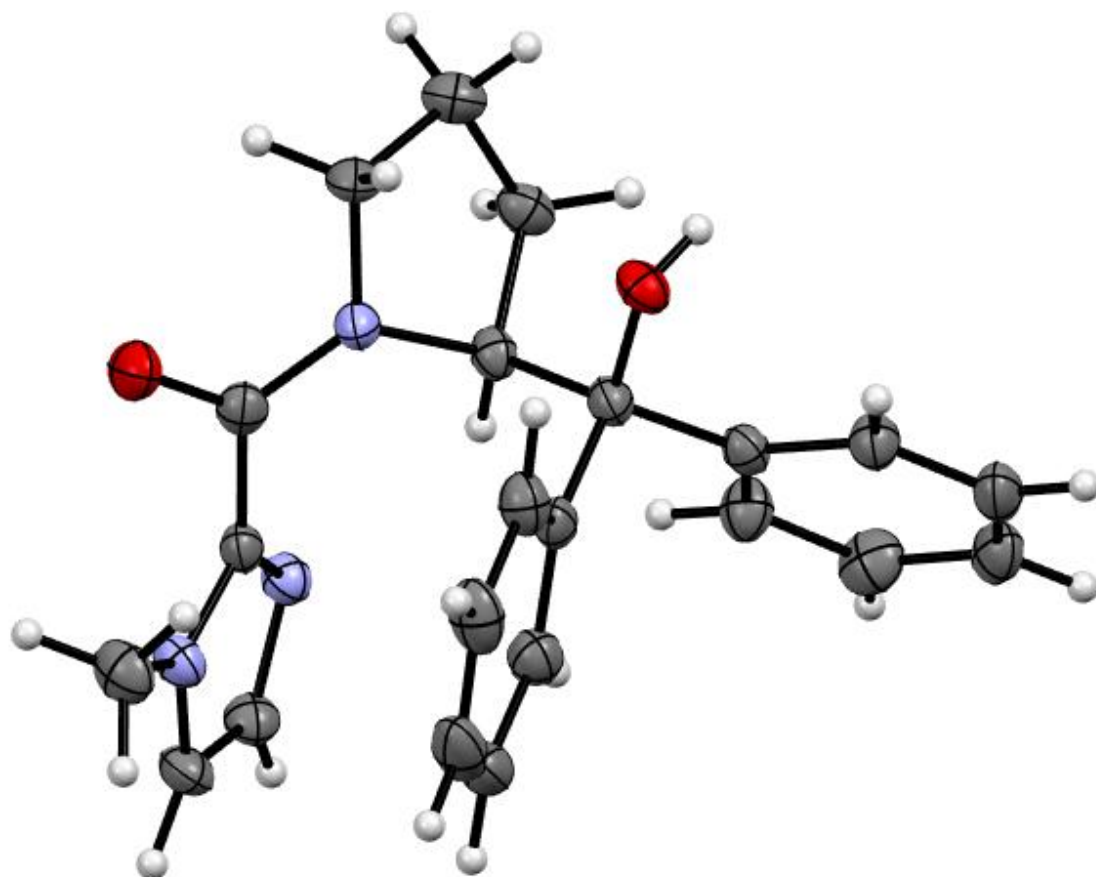
Autostop : 20.00, min
Detector 1 : Signal 1
Subtraction chromatogram : (None)

External Start : Start Only, Down
Range 1 : Bipolar, 10000 mV, 10 Samp. per Sec.
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