

Supporting Information

Synthesis of Decahydropyrrolo[1,2-*a*]tetrazolo[1, 5-*d*]pyrazines via Strecker Reaction and Intramolecular [3+2] Cycloaddition

Shakil N. Afraj,^a Chinpiao Chen,^{*,a,b} Gene-Hsian Lee^c

^a Department of Chemistry, National Dong Hwa University, Hualien 97401, Taiwan

^b Department of Nursing, Tzu Chi University of Science and Technology, Hualien 970, Taiwan

^c National Taiwan University, Instrumentation Center, Taipei 10617, Taiwan

Table of contents

1. General.....S2
2. Crystallographic data of (5*a*S,10*R*)-10-phenyl-5,5*a*,6,7,8,10-hexahydropyrrolo
[1,2-*a*]tetrazolo [1,5-*d*]pyrazine..... S2-S7
3. ¹H and ¹³C NMR Spectra of aminonitriles (**3a–3v**)....S8-S29
4. ¹H and ¹³C NMR Spectra of Major diastereomerS30
5. ¹H and ¹³C NMR Spectra of Minor diastereomer.....S31
6. ¹H and ¹³C NMR Spectra of **4a–4v**.....S32-S53

General

Unless specified otherwise, all starting materials and reagents were obtained from commercial suppliers and used without further purification. All reactions were conducted in oven-dried glassware, in an argon atmosphere with anhydrous solvents, which were dried and distilled before use according to standard procedures. Solvents used for isolating products and chromatography were glass distilled. Reactions were monitored by performing thinlayer chromatography with precoated silica gel 60 glass plates and an F254 indicator. Visualization was accomplished using UV light (254 nm) combined with iodine, potassium permanganate, or anisaldehyde staining solutions. The products were purified using neutral column chromatography on 230–400 mesh silica gels. Yields refer to a chromatographically and spectrographically pure material, unless otherwise noted. ^1H NMR and ^{13}C NMR spectra were obtained using 400 and 100.6 MHz NMR spectrometers, respectively. Chemical shifts (δ) are reported in parts per million (ppm) relative to CDCl_3 (7.26 and 77.00 ppm); coupling constants are reported in Hertz (Hz); and multiplicities are indicated as br = broad, s = singlet, d = doublet, dd = doublet of doublet, t = triplet, and m = multiplet. Infrared spectra were recorded using an FT/IR spectrometer. High resolution mass spectra (HRMS-EI) were determined using a Thermo Quest MAT 95XL mass spectrometer.

Crystal structure of

(5a*S*,10*R*)-10-phenyl-5,5a,6,7,8,10-hexahydropyrrolo[1,2-*a*]tetrazolo[1,5-*d*]pyrazine and its absolute configuration (Major diastereomer,). CCDC: 1041454

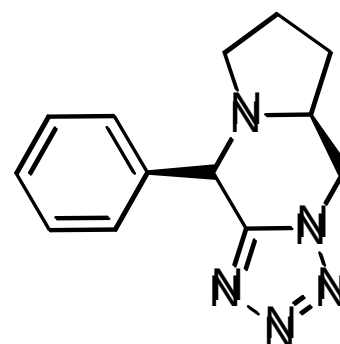
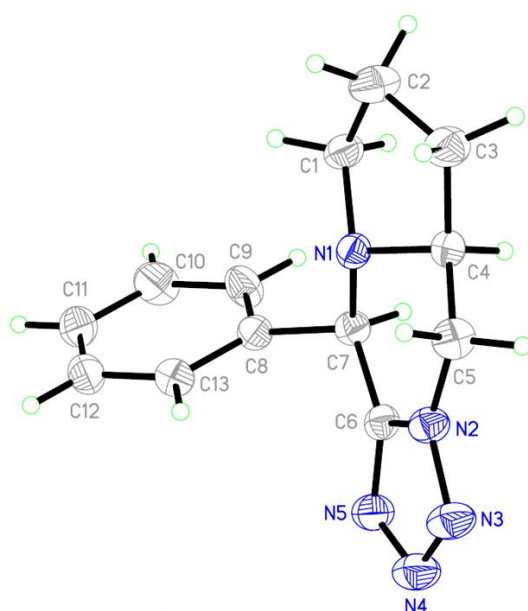


Fig. : The molecular structure of IC16489, thermal ellipsoids drawn at the 50% probability level.

Table 1. Crystal data and structure refinement for ic16489.

Identification code	ic16489
---------------------	---------

Empirical formula	C13 H15 N5	
Formula weight	241.30	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.2273(6) Å	$\alpha = 90^\circ$.
	b = 10.6788(7) Å	$\beta = 90^\circ$.
	c = 11.1734(7) Å	$\gamma = 90^\circ$.
Volume	1220.31(13) Å ³	
Z	4	
Density (calculated)	1.313 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	512	
Crystal size	0.40 x 0.25 x 0.25 mm ³	
Theta range for data collection	2.64 to 27.50°.	
Index ranges	-13<=h<=13, -13<=k<=13, -14<=l<=14	
Reflections collected	11035	
Independent reflections	2798 [R(int) = 0.0428]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9793 and 0.9671	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2798 / 0 / 163	
Goodness-of-fit on F ²	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0931	
R indices (all data)	R1 = 0.0463, wR2 = 0.0959	
Absolute structure parameter	0(2)	
Largest diff. peak and hole	0.185 and -0.207 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ic16489. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
N(1)	2488(1)	9307(1)	2454(1)	25(1)
N(2)	1569(1)	7691(1)	4084(1)	28(1)
N(3)	1230(2)	6717(1)	4783(1)	36(1)

N(4)	2258(2)	6008(1)	4840(1)	37(1)
N(5)	3263(1)	6496(1)	4192(1)	32(1)
C(1)	3000(2)	10439(2)	1872(2)	30(1)
C(2)	1783(2)	11240(2)	1696(2)	40(1)
C(3)	845(2)	10842(2)	2698(2)	40(1)
C(4)	1556(2)	9785(2)	3350(1)	26(1)
C(5)	694(2)	8722(2)	3760(2)	31(1)
C(6)	2805(2)	7545(2)	3736(1)	25(1)
C(7)	3503(2)	8513(1)	2996(1)	24(1)
C(8)	4383(2)	7963(2)	2041(1)	25(1)
C(9)	5571(2)	8531(2)	1804(2)	33(1)
C(10)	6354(2)	8111(2)	878(2)	40(1)
C(11)	5965(2)	7104(2)	189(2)	35(1)
C(12)	4786(2)	6523(2)	427(2)	32(1)
C(13)	3996(2)	6946(2)	1345(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for ic16489.

N(1)-C(1)	1.4689(19)
N(1)-C(7)	1.4706(19)
N(1)-C(4)	1.4737(19)
N(2)-C(6)	1.332(2)
N(2)-N(3)	1.3469(18)
N(2)-C(5)	1.465(2)
N(3)-N(4)	1.297(2)
N(4)-N(5)	1.361(2)
N(5)-C(6)	1.316(2)
C(1)-C(2)	1.523(2)
C(2)-C(3)	1.534(3)
C(3)-C(4)	1.527(2)
C(4)-C(5)	1.509(2)
C(6)-C(7)	1.504(2)
C(7)-C(8)	1.515(2)
C(8)-C(9)	1.384(2)
C(8)-C(13)	1.393(2)
C(9)-C(10)	1.383(2)
C(10)-C(11)	1.381(3)
C(11)-C(12)	1.382(3)
C(12)-C(13)	1.382(2)

C(1)-N(1)-C(7)	113.88(12)
C(1)-N(1)-C(4)	104.29(12)
C(7)-N(1)-C(4)	112.11(12)
C(6)-N(2)-N(3)	108.87(14)
C(6)-N(2)-C(5)	126.61(13)
N(3)-N(2)-C(5)	124.51(13)
N(4)-N(3)-N(2)	105.65(14)
N(3)-N(4)-N(5)	111.31(13)
C(6)-N(5)-N(4)	105.25(14)
N(1)-C(1)-C(2)	103.16(13)
C(1)-C(2)-C(3)	105.15(14)
C(4)-C(3)-C(2)	104.79(14)
N(1)-C(4)-C(5)	108.92(13)
N(1)-C(4)-C(3)	103.86(13)
C(5)-C(4)-C(3)	115.02(14)
N(2)-C(5)-C(4)	106.47(12)
N(5)-C(6)-N(2)	108.92(14)
N(5)-C(6)-C(7)	128.99(15)
N(2)-C(6)-C(7)	122.01(14)
N(1)-C(7)-C(6)	106.74(12)
N(1)-C(7)-C(8)	110.66(12)
C(6)-C(7)-C(8)	113.71(13)
C(9)-C(8)-C(13)	119.02(15)
C(9)-C(8)-C(7)	119.09(14)
C(13)-C(8)-C(7)	121.78(14)
C(10)-C(9)-C(8)	120.58(16)
C(11)-C(10)-C(9)	120.21(16)
C(10)-C(11)-C(12)	119.60(16)
C(13)-C(12)-C(11)	120.41(16)
C(12)-C(13)-C(8)	120.17(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ic16489. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
----------	----------	----------	----------	----------	----------

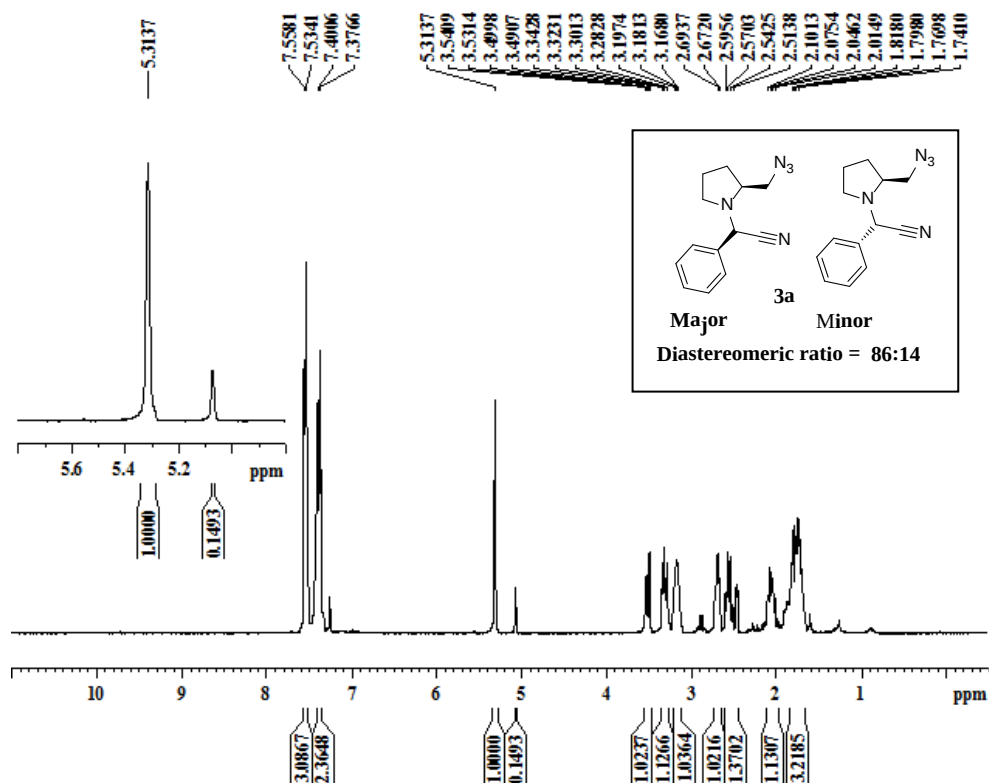
N(1)	25(1)	26(1)	22(1)	0(1)	1(1)	0(1)
N(2)	27(1)	27(1)	29(1)	4(1)	0(1)	-5(1)
N(3)	39(1)	32(1)	38(1)	9(1)	-1(1)	-9(1)
N(4)	43(1)	29(1)	40(1)	8(1)	-1(1)	-6(1)
N(5)	36(1)	28(1)	33(1)	4(1)	-1(1)	0(1)
C(1)	33(1)	29(1)	28(1)	6(1)	3(1)	0(1)
C(2)	39(1)	38(1)	42(1)	14(1)	1(1)	4(1)
C(3)	41(1)	38(1)	40(1)	8(1)	8(1)	14(1)
C(4)	29(1)	26(1)	24(1)	0(1)	3(1)	1(1)
C(5)	23(1)	34(1)	35(1)	3(1)	1(1)	0(1)
C(6)	27(1)	26(1)	22(1)	0(1)	-3(1)	-3(1)
C(7)	24(1)	24(1)	25(1)	1(1)	-2(1)	-2(1)
C(8)	26(1)	25(1)	25(1)	0(1)	1(1)	2(1)
C(9)	32(1)	28(1)	40(1)	-8(1)	6(1)	-5(1)
C(10)	34(1)	36(1)	51(1)	0(1)	16(1)	-5(1)
C(11)	37(1)	34(1)	34(1)	-1(1)	8(1)	8(1)
C(12)	35(1)	30(1)	30(1)	-4(1)	-4(1)	4(1)
C(13)	24(1)	28(1)	32(1)	0(1)	-3(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for ic16489.

	x	y	z	U(eq)
H(1A)	3415	10235	1095	36
H(1B)	3646	10868	2389	36
H(2A)	1389	11084	901	47
H(2B)	1999	12141	1763	47
H(3A)	668	11549	3247	47
H(3B)	6	10542	2361	47
H(4)	2045	10134	4049	32
H(5A)	165	8981	4460	37
H(5B)	95	8463	3110	37
H(7)	4047	9043	3541	29
H(9)	5852	9216	2282	40
H(10)	7162	8516	716	48

H(11)	6505	6813	-444	42
H(12)	4518	5828	-43	38
H(13)	3186	6542	1502	33

¹H, ¹³C, Spectra of aminonitriles

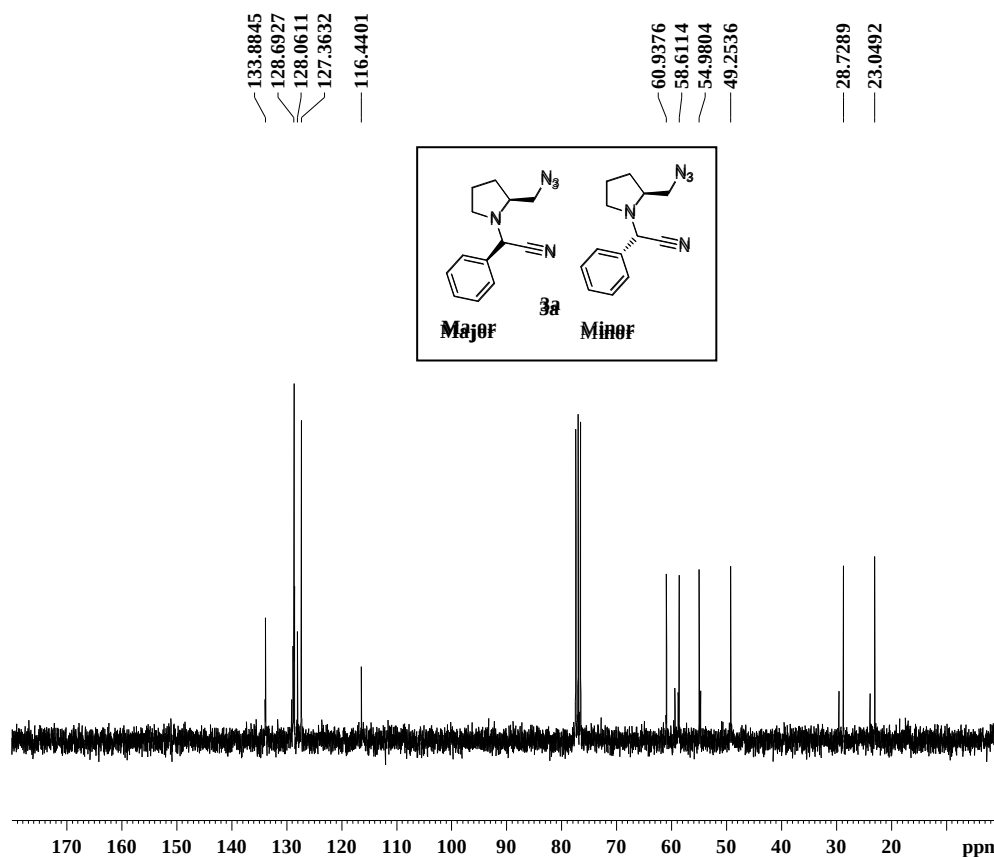


Current Data Parameters
NAME sm 250 ml water 2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130917
Time 17.48
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 287.4
DW 111.100 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1319508 MHz
F2 - Processing parameters
SI 16384
SF 300.1300006 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.969 ppm
FI 4182.50 Hz
FIP -1.013 ppm
F2 -303.90 Hz
PFMCM 0.74908 ppm
H2CM 224.83013 Hz



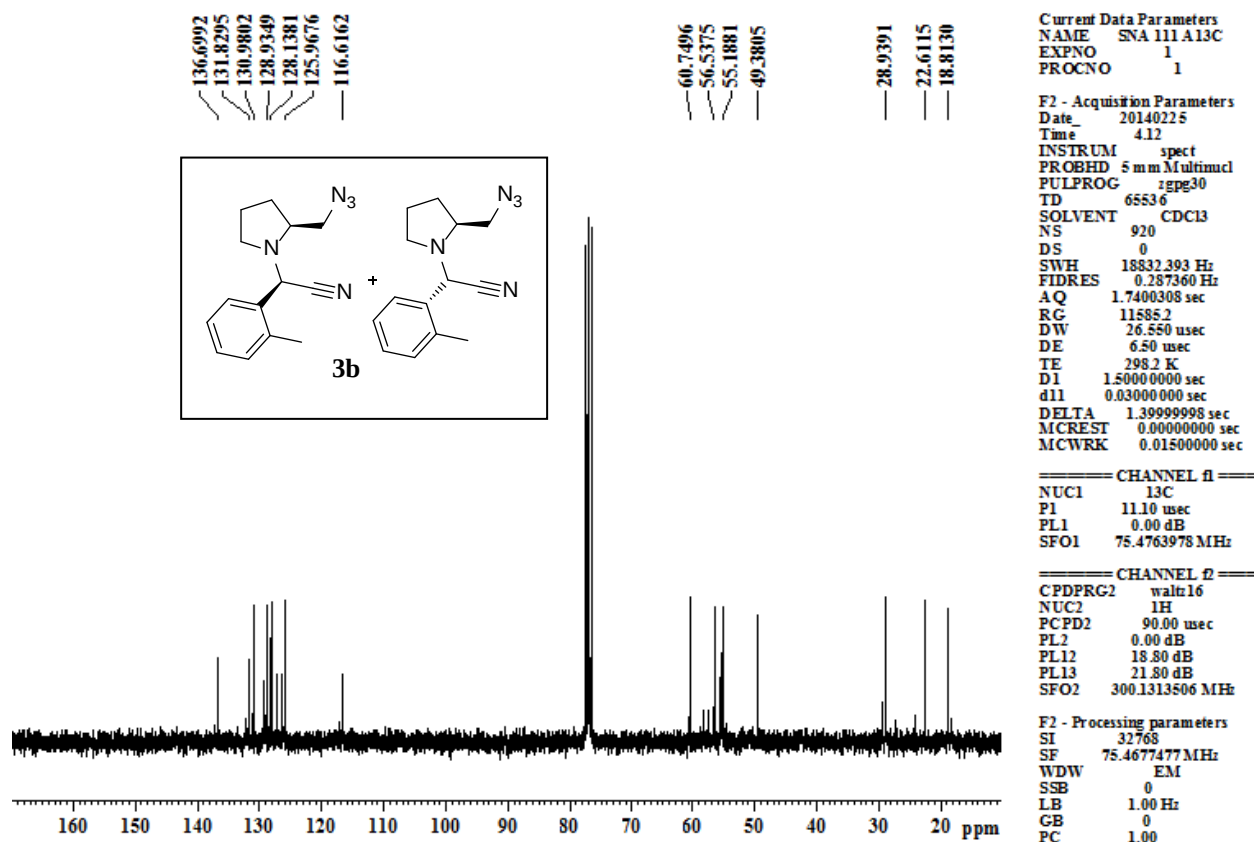
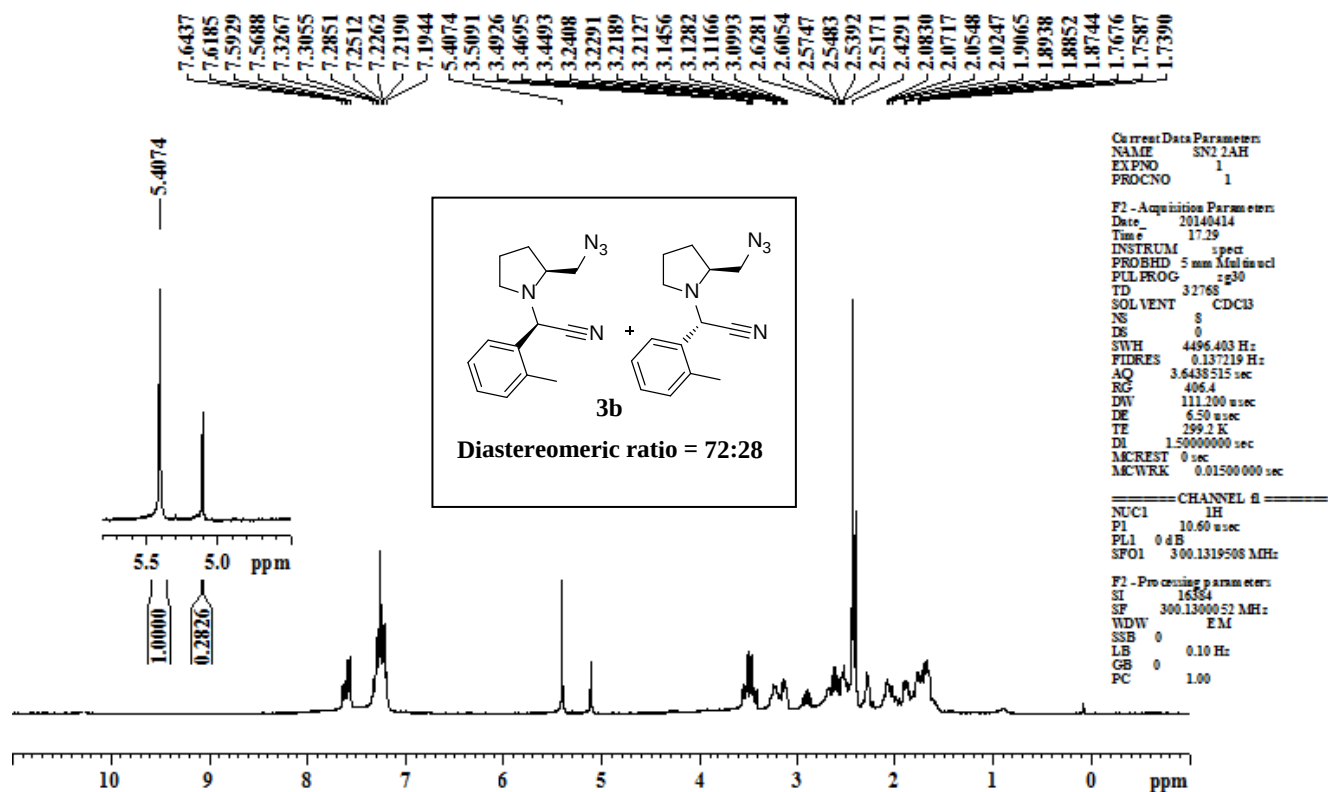
Current Data Parameters
NAME SNA aq KCN 67 13C
EXPNO 2
PROCNO 1

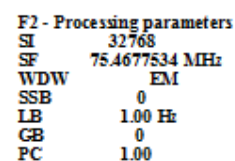
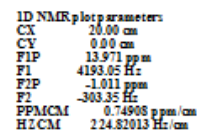
F2 - Acquisition Parameters
Date_ 20130920
Time 14.23
INSTRUM spect
PROBHD 5 mm Multinuc
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 13004
DW 26.550 usec
DE 6.50 usec
TE 300.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999999 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

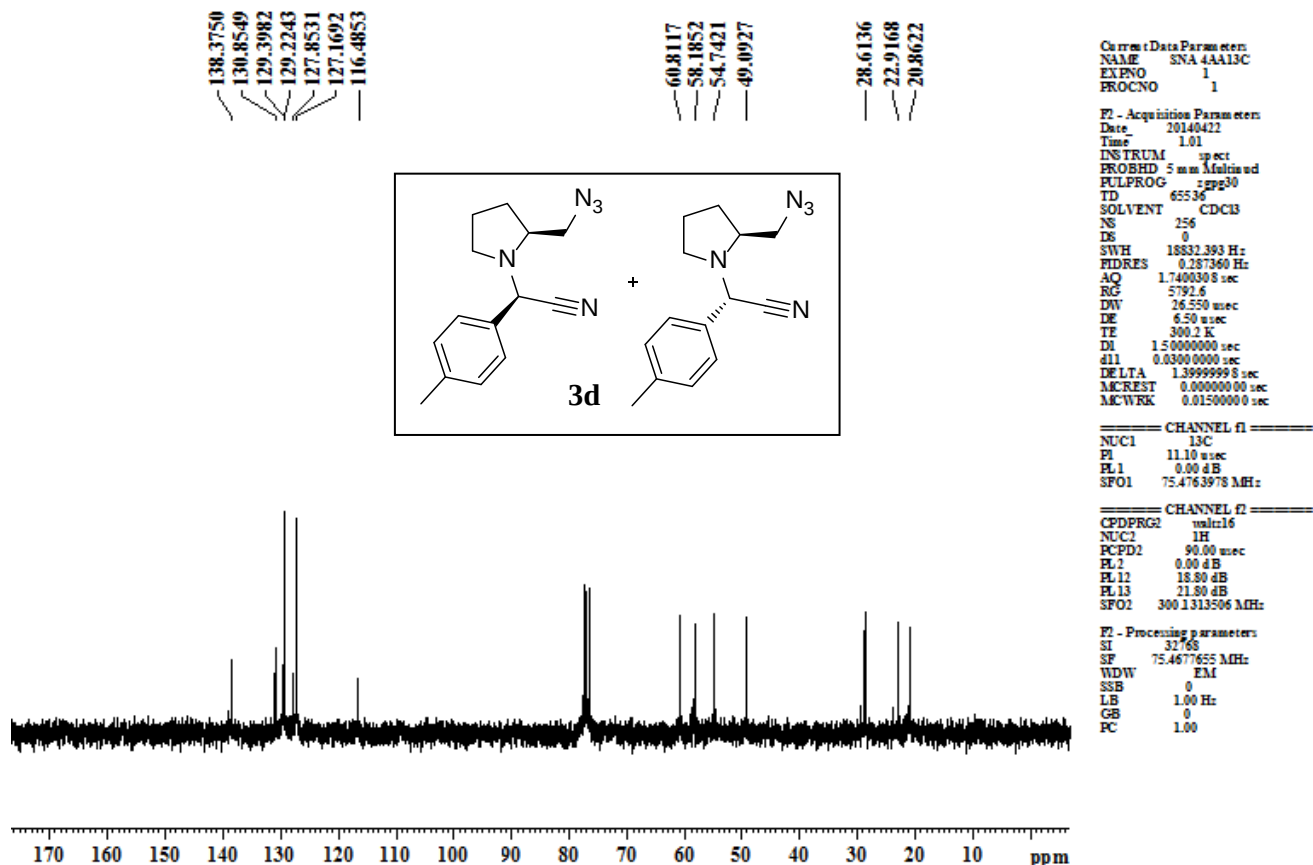
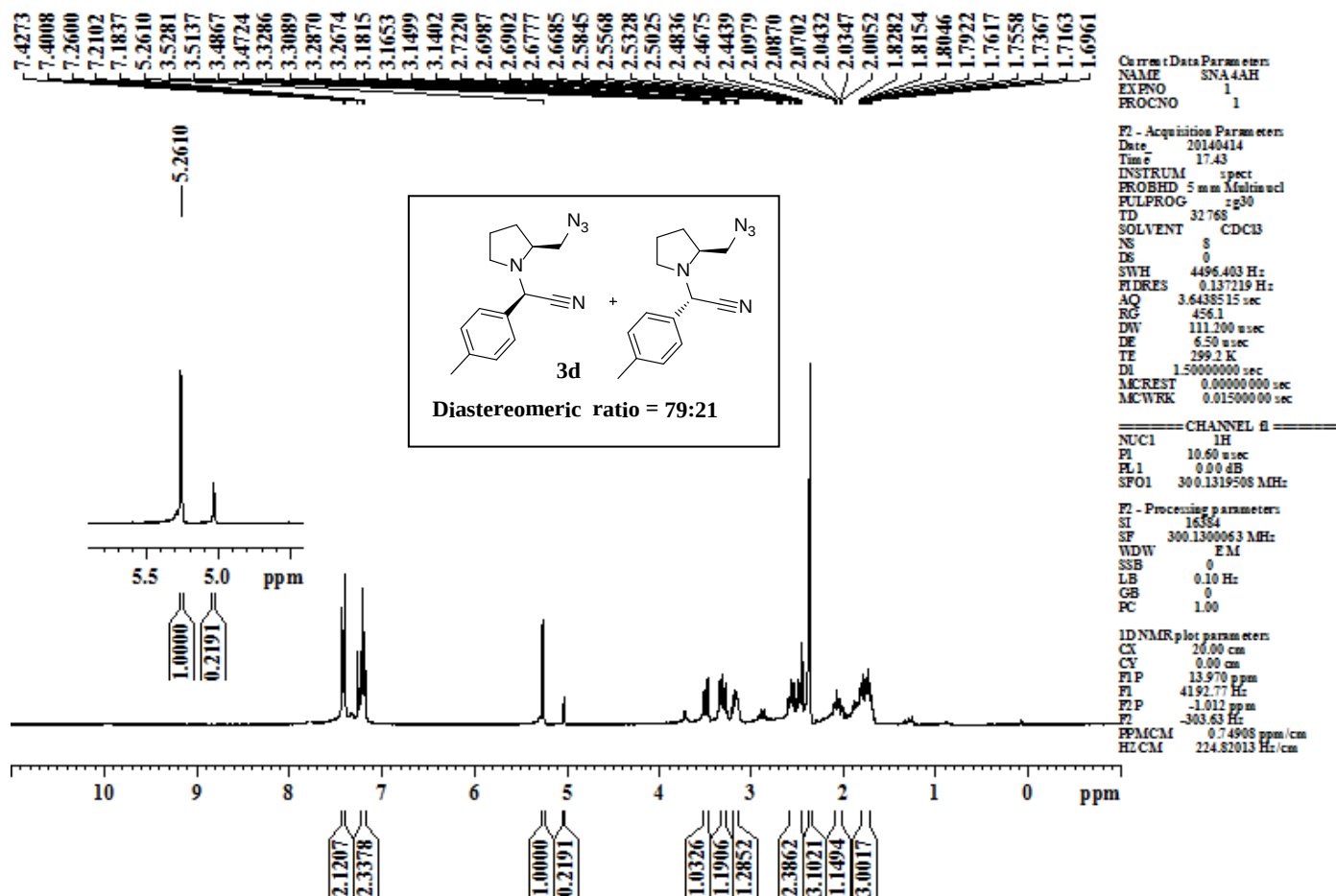
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

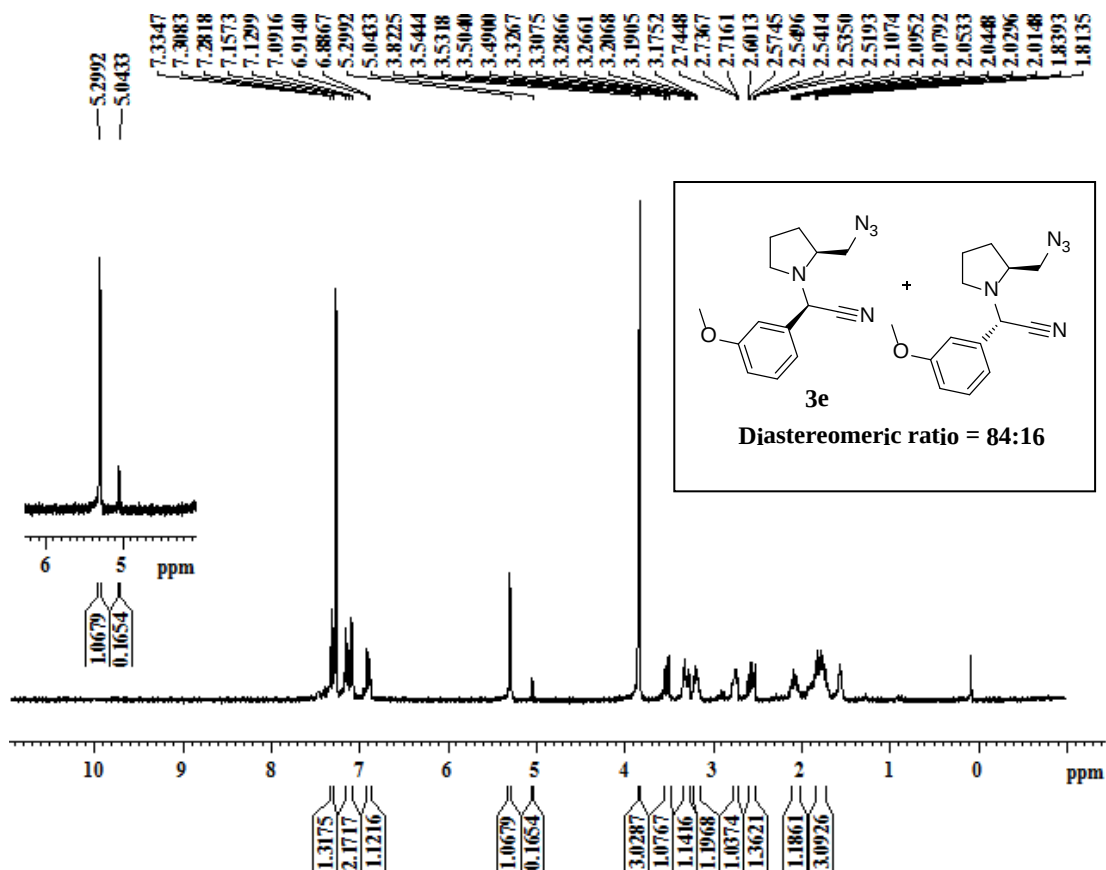
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00









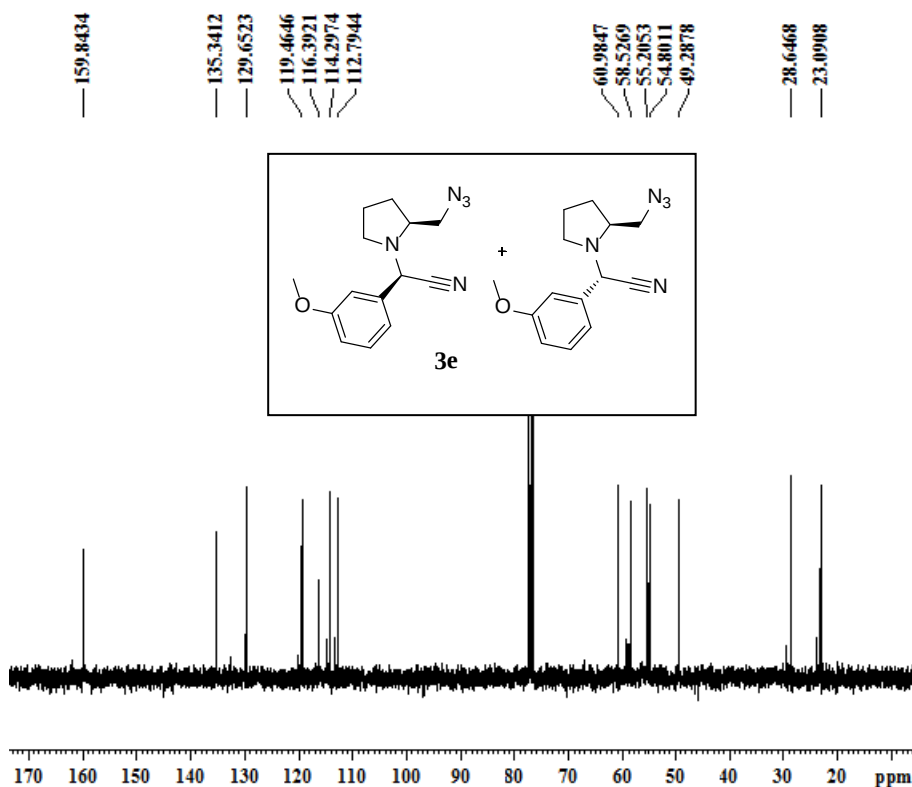
Current Data Parameters
NAME SNA128AH
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140228
Time 16.47
INSTRUM spect
PROBHD 5mm Multinuc
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 3448.2
DW 111.300 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1 =
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1315936 MHz

F2 - Processing parameters
SI 16384
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.971 ppm
F1 4193.02 Hz
F2 -1.011 ppm
F2 -303.35 Hz
PPHMC 0.74908 ppm
HZCM 224.82014 Hz



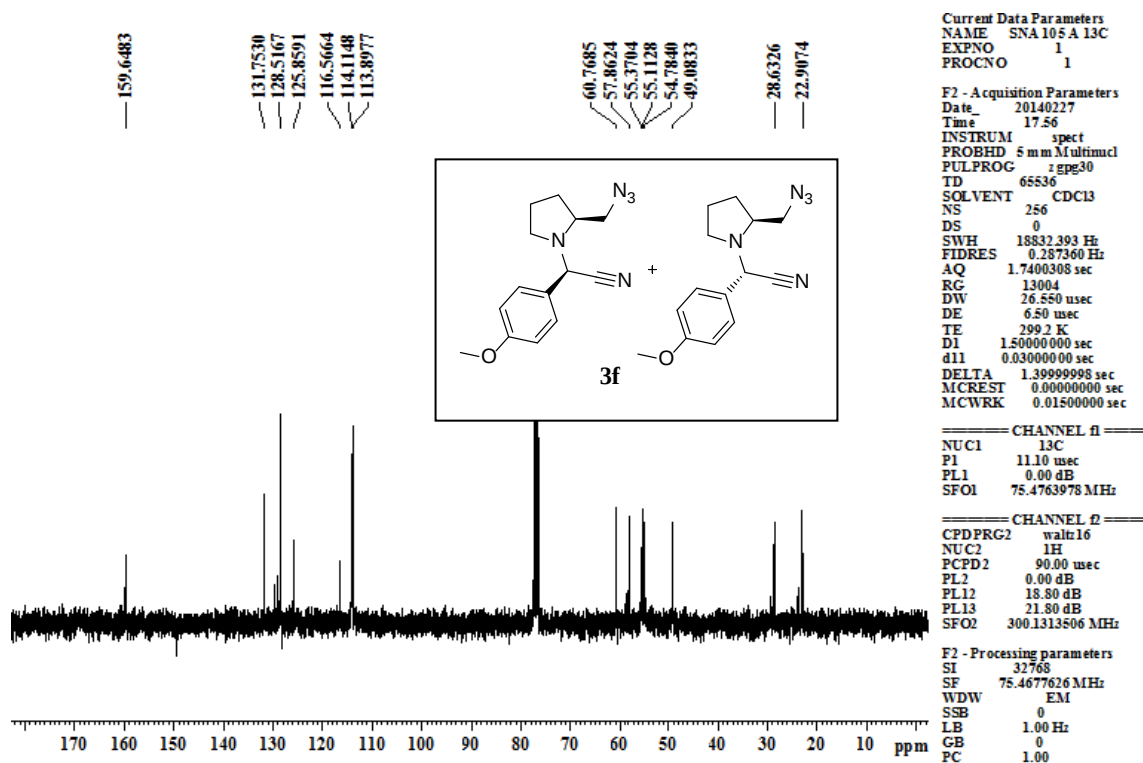
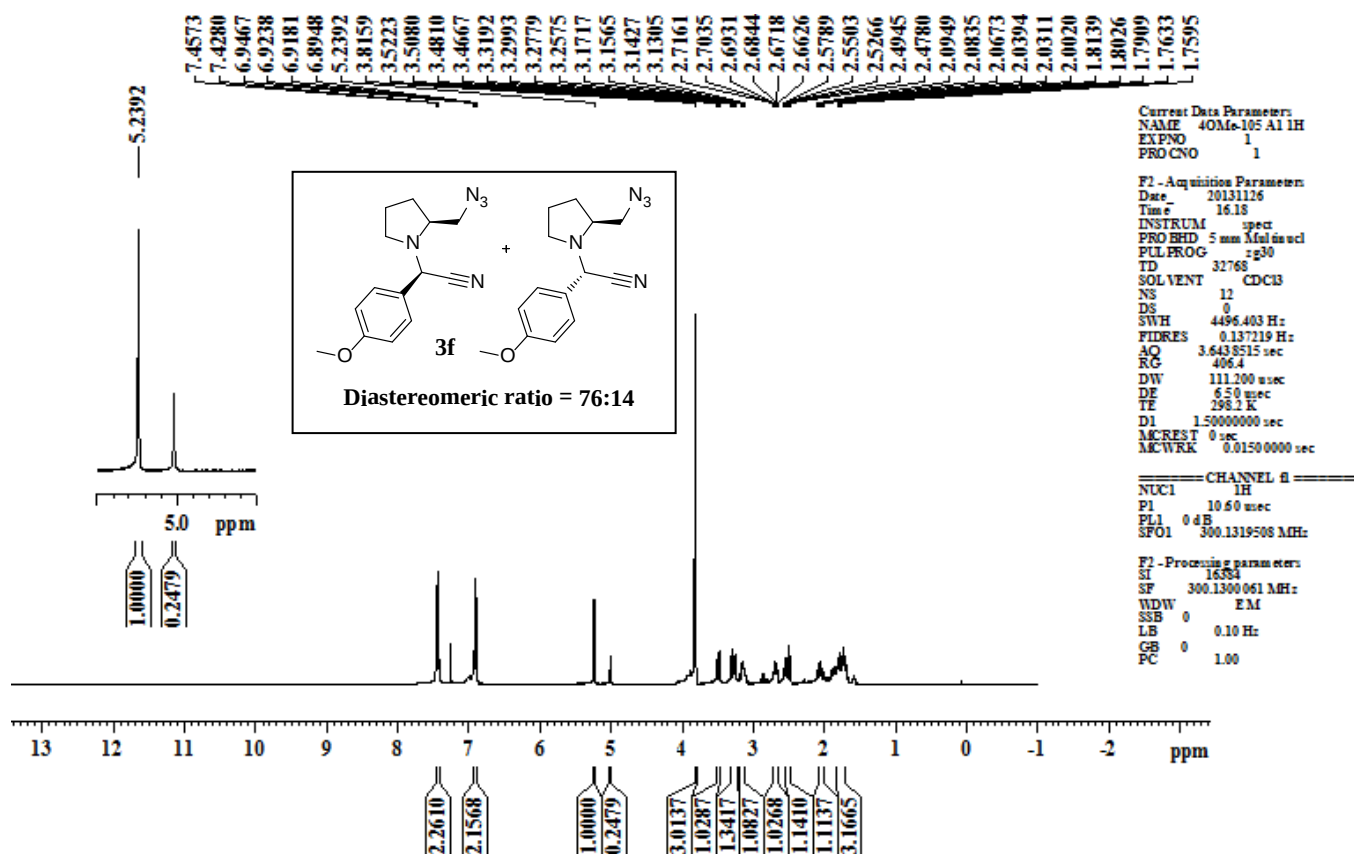
Current Data Parameters
NAME SNA128A13C
EXPNO 3
PROCNO 1

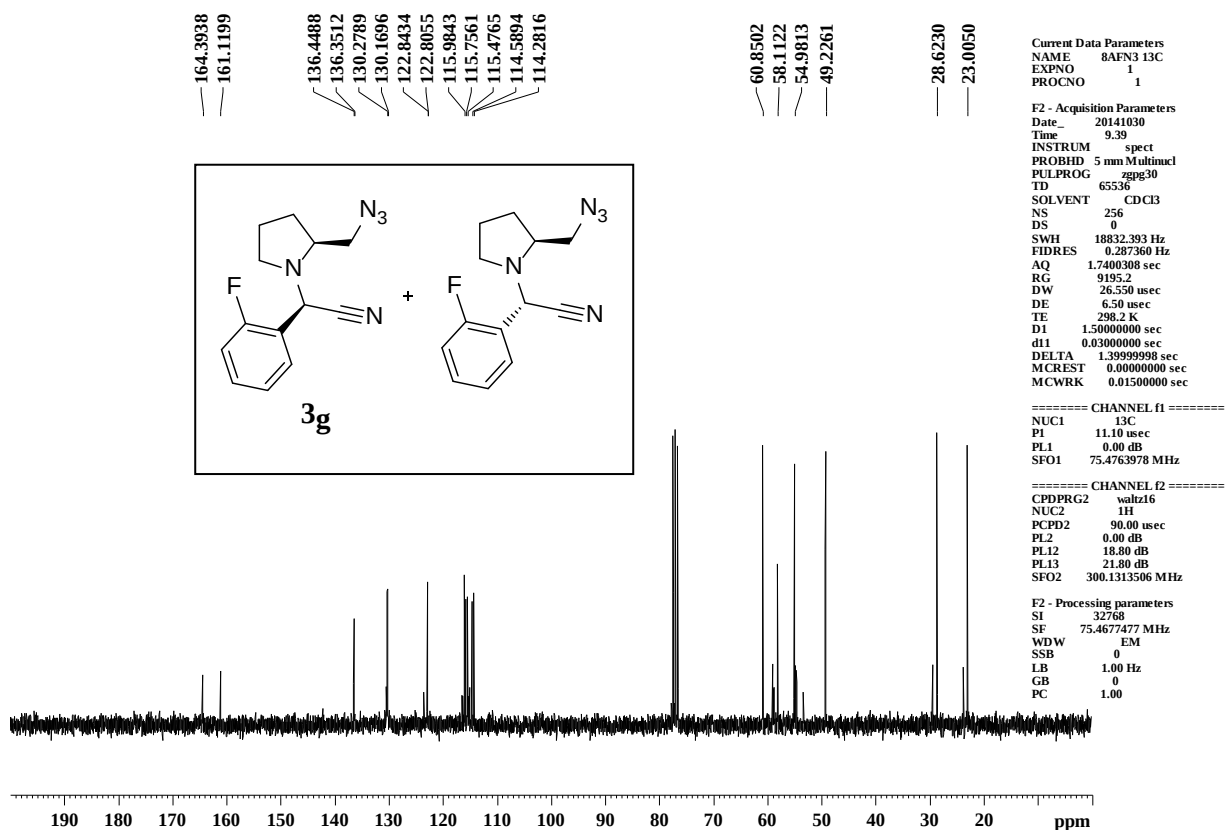
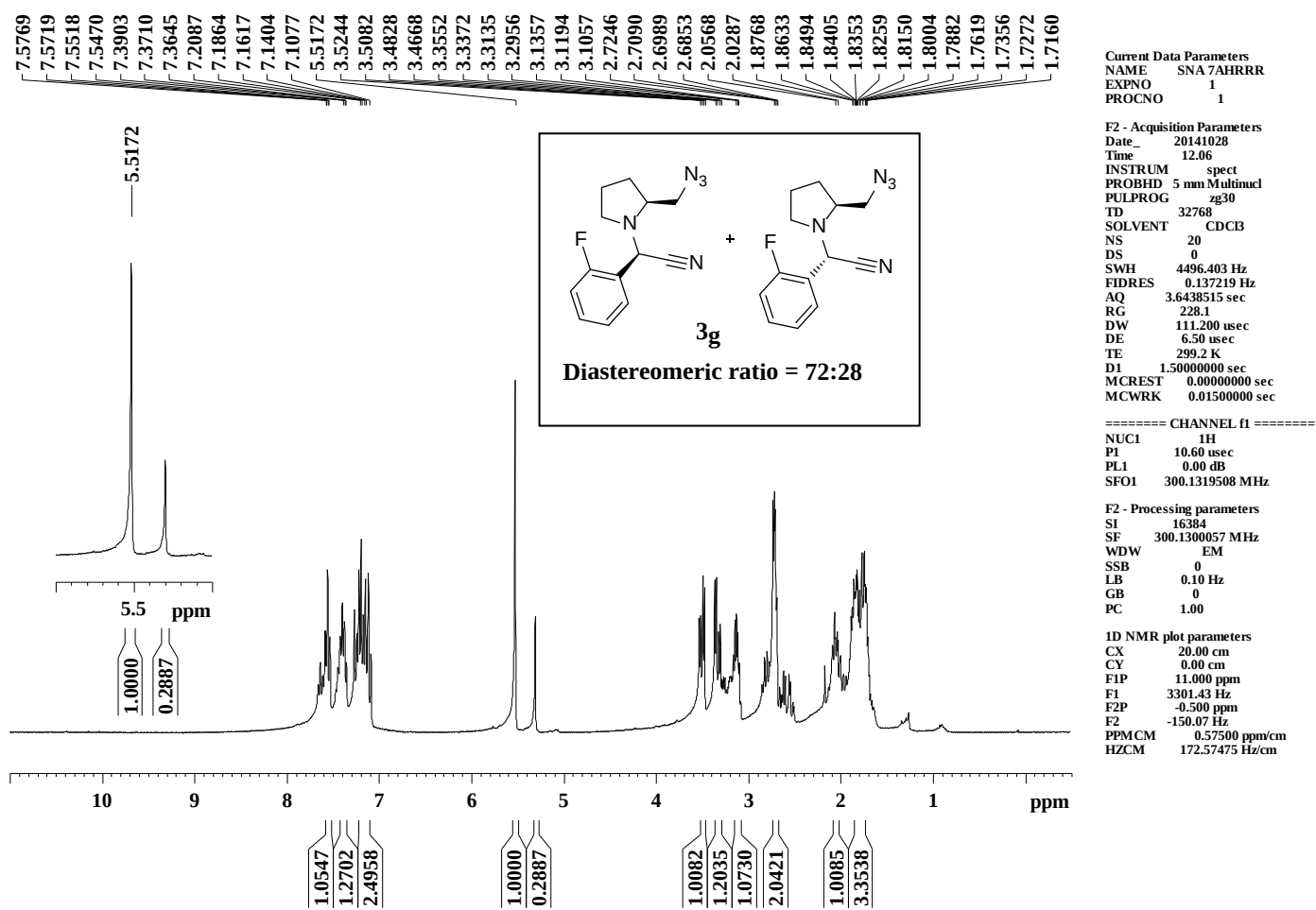
F2 - Acquisition Parameters
Date_ 20140228
Time 17.08
INSTRUM spect
PROBHD 5mm Multinuc
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

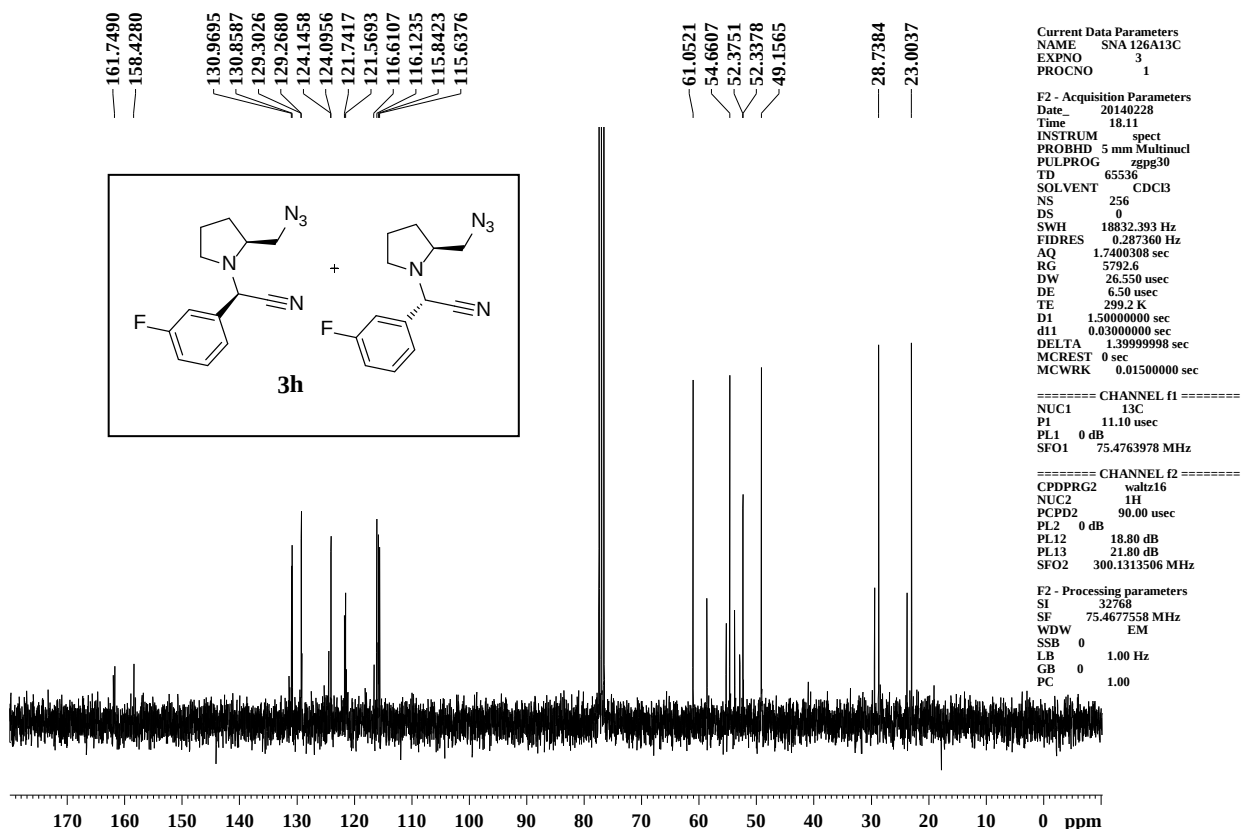
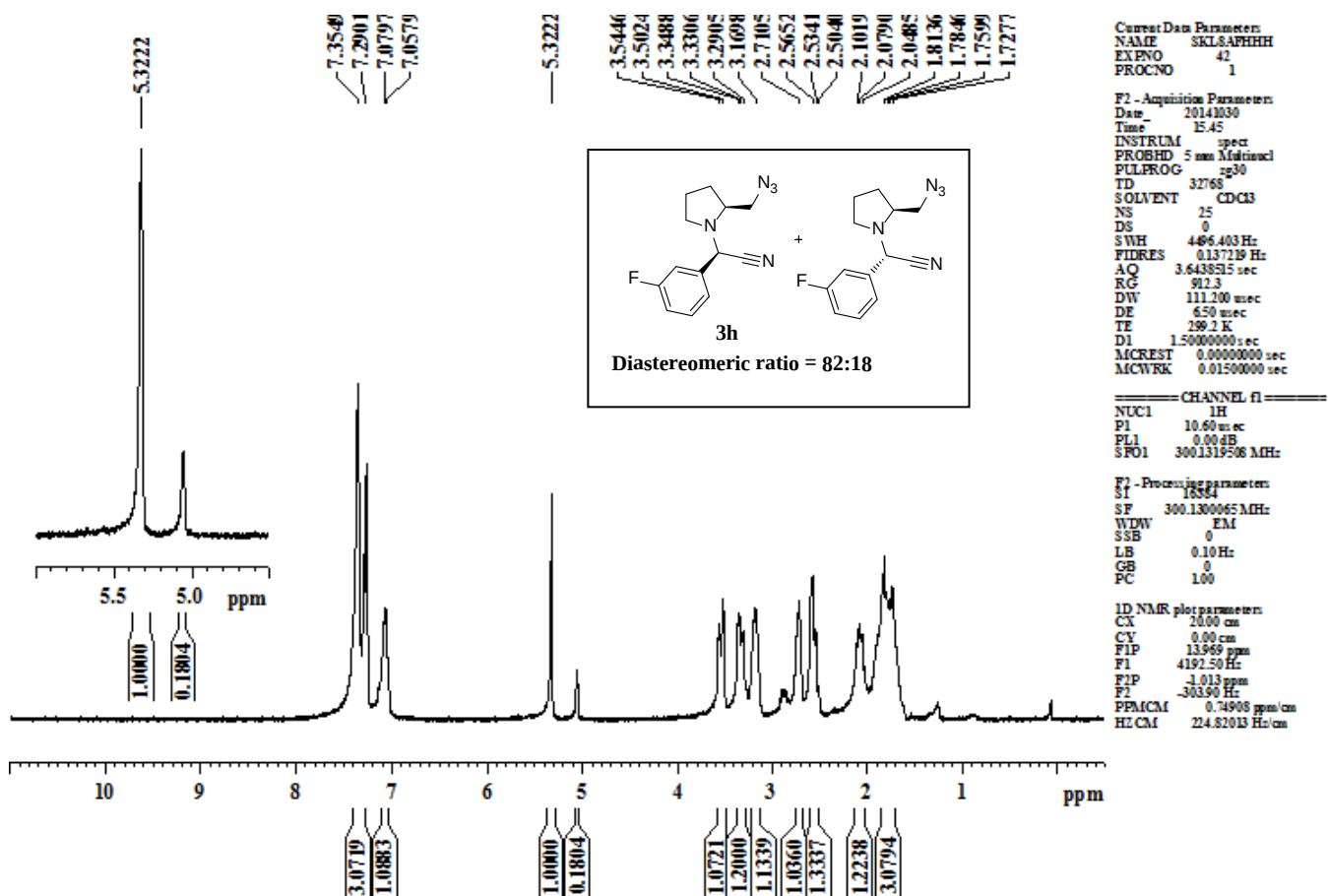
CHANNEL f1 =
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

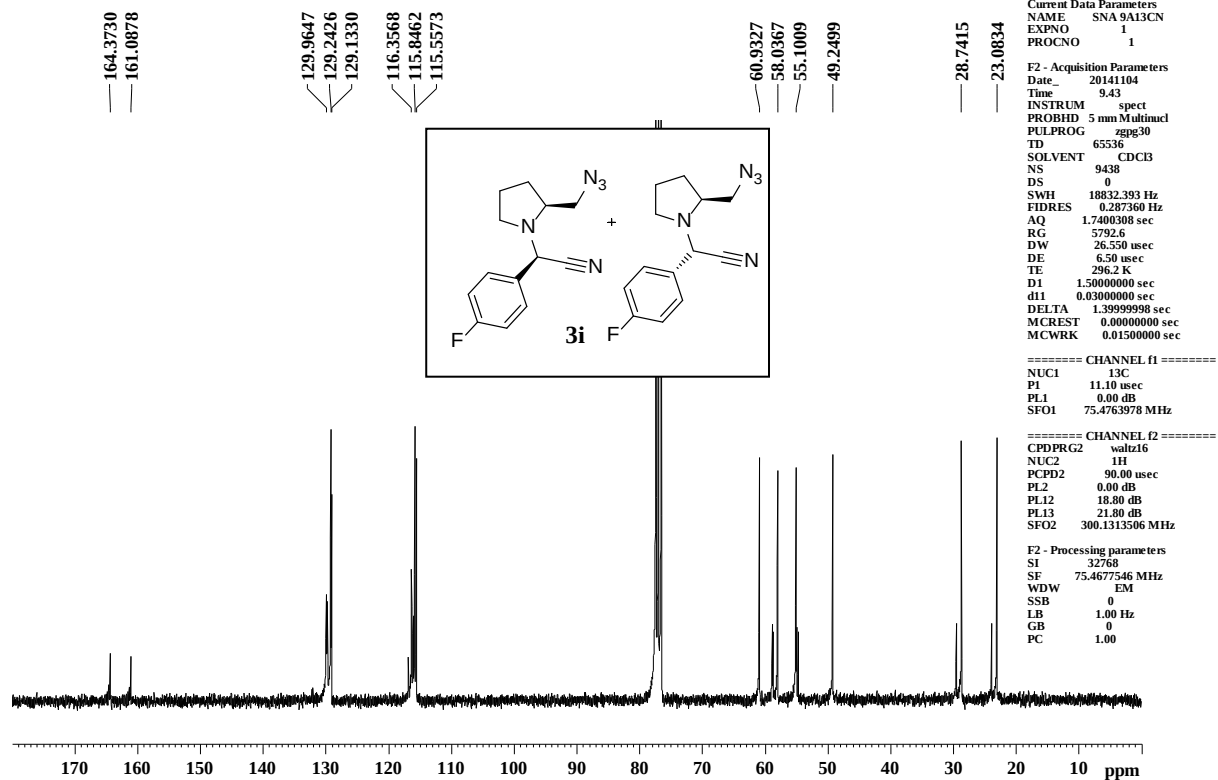
CHANNEL f2 =
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

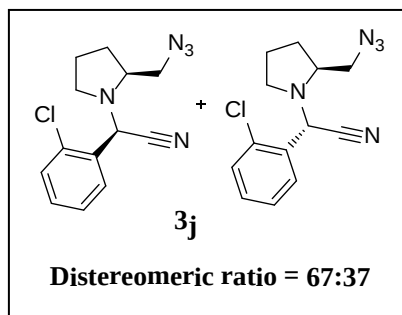
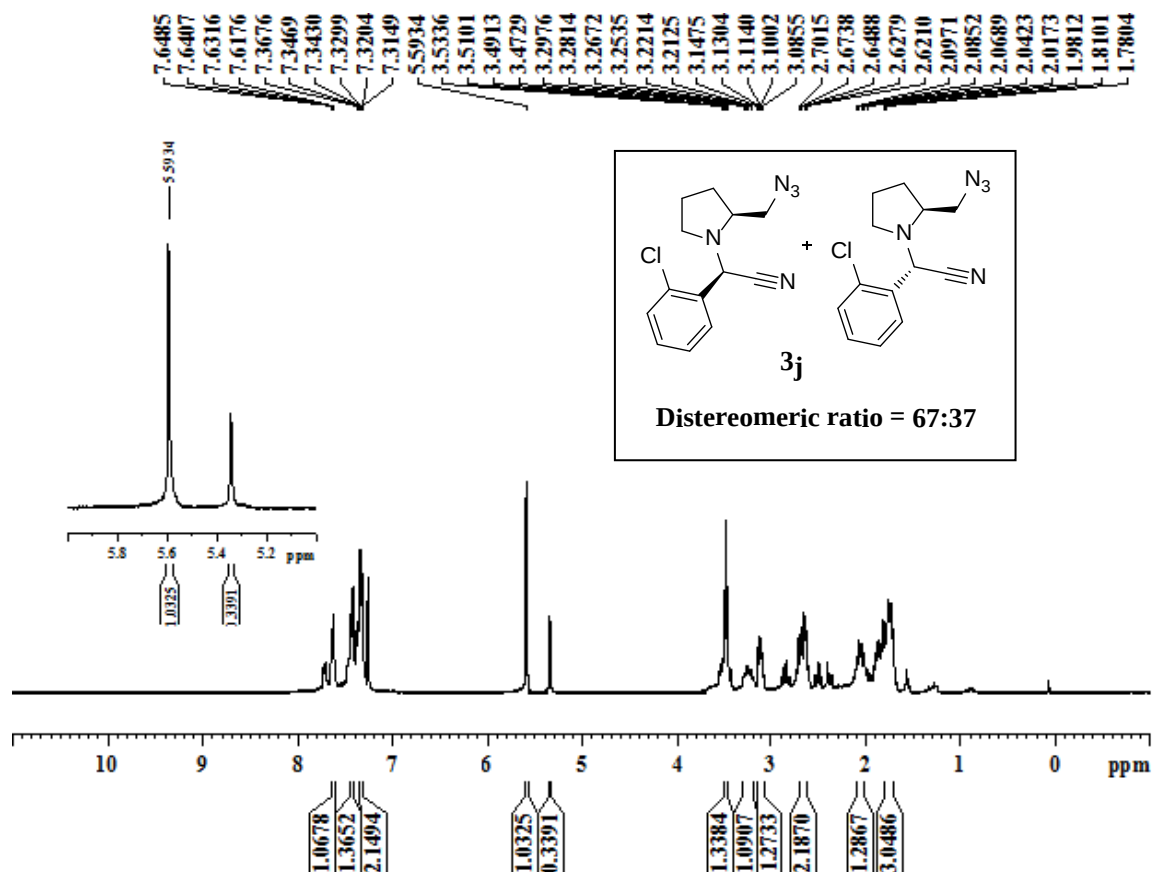
F2 - Processing parameters
SI 32768
SF 75.4677597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00











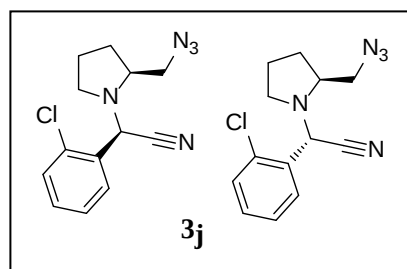
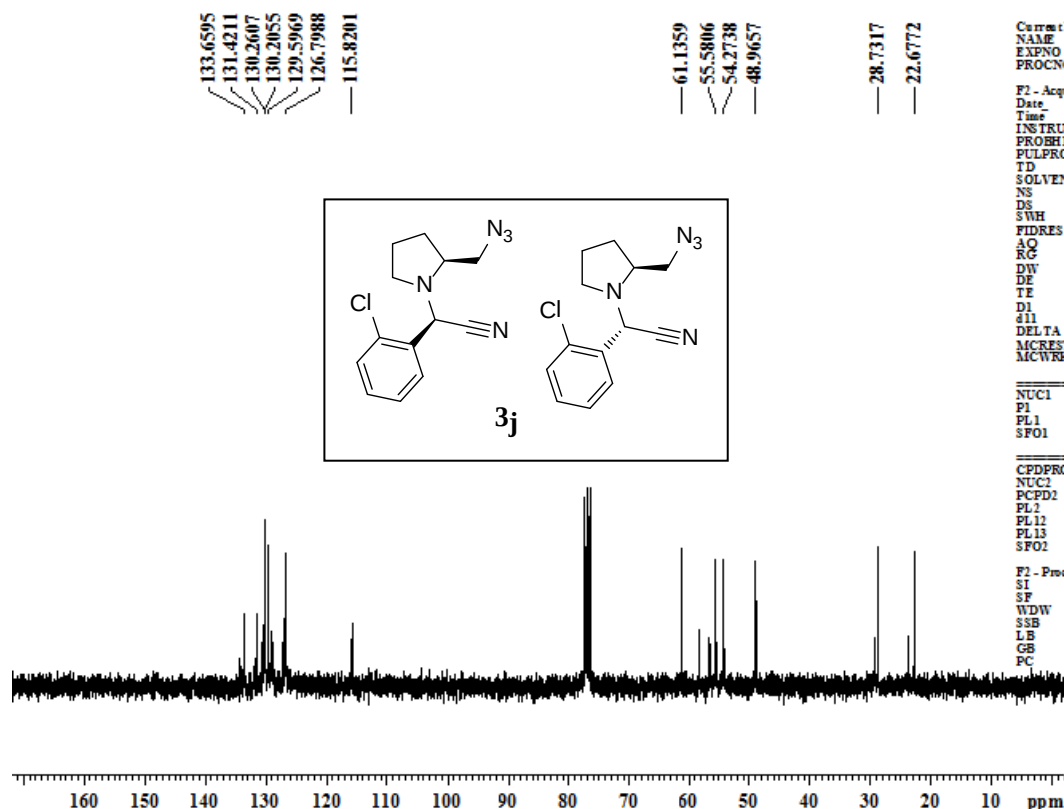
Current Data Parameters:
NAME SNA 10AH
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters:
Date_ 20140414
Time_ 17:37
INSTRUM spect
PROBHD 5 mm Maltinaucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 574.7
DW 111.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1315908 MHz

F2 - Processing parameters:
SI 16384
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters:
CX 20.00 cm
CY 0.00 cm
F1P 13.970 ppm
F1 4192.77 Hz
F2P -1.012 ppm
F2 -303.63 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm



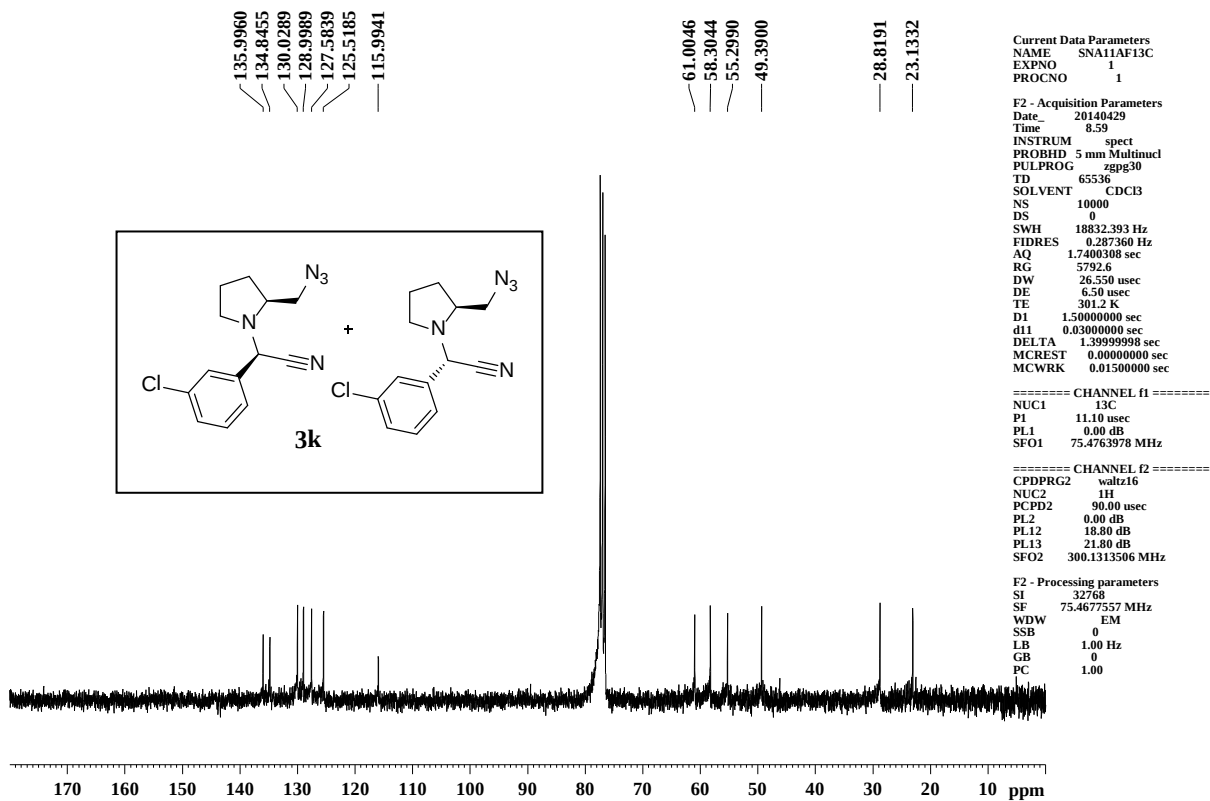
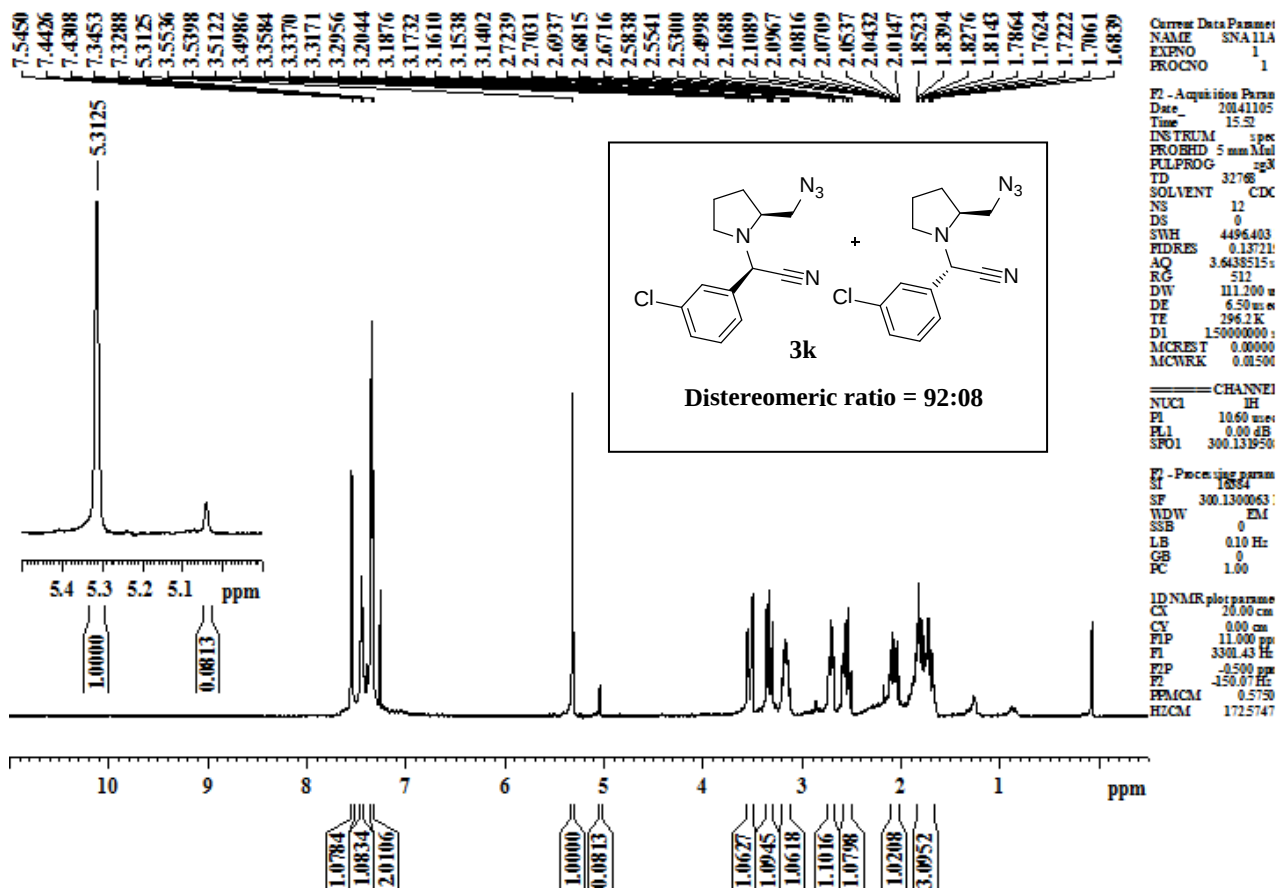
Current Data Parameters:
NAME SNA 10AH13C
EXPNO 1
PROCNO 1

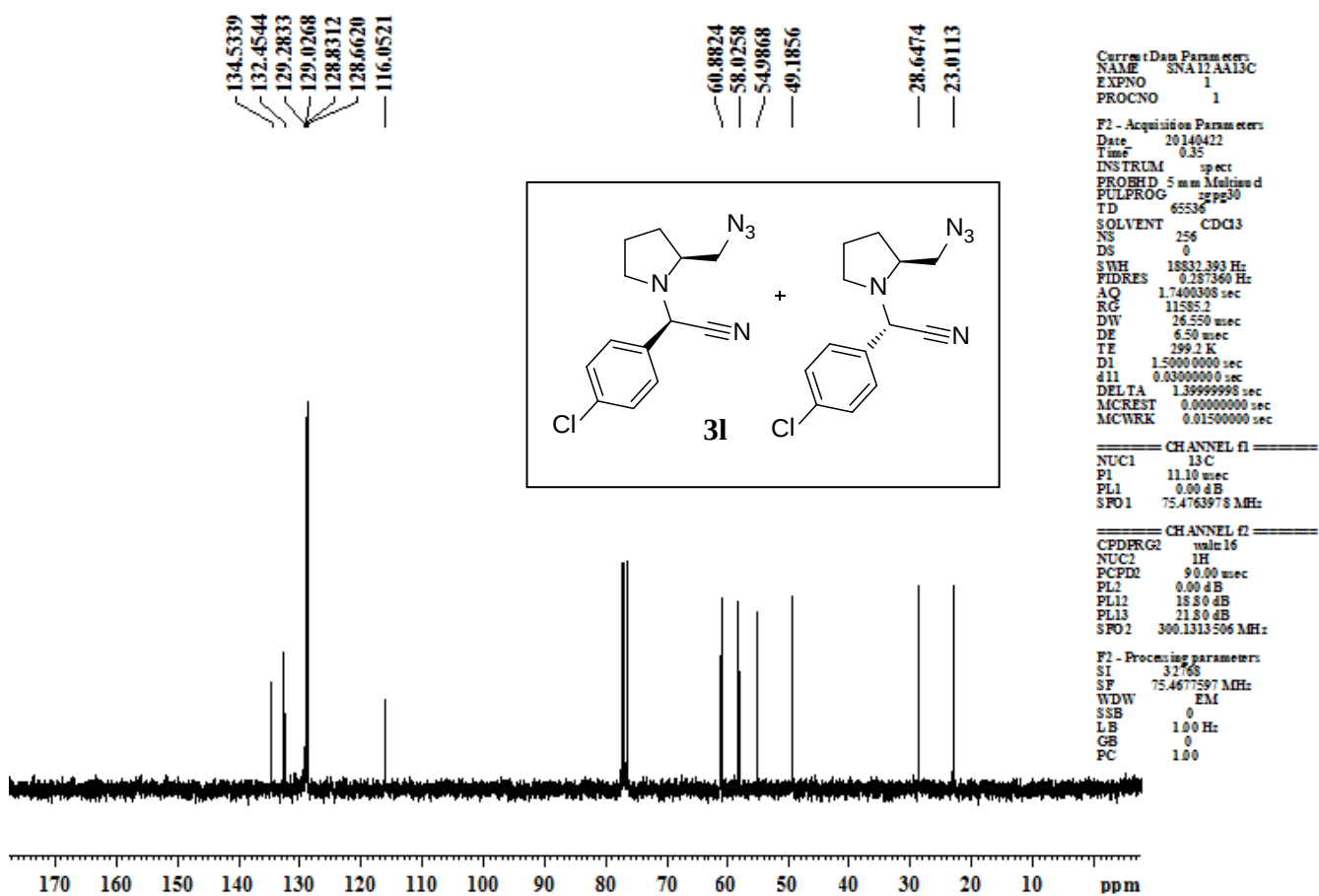
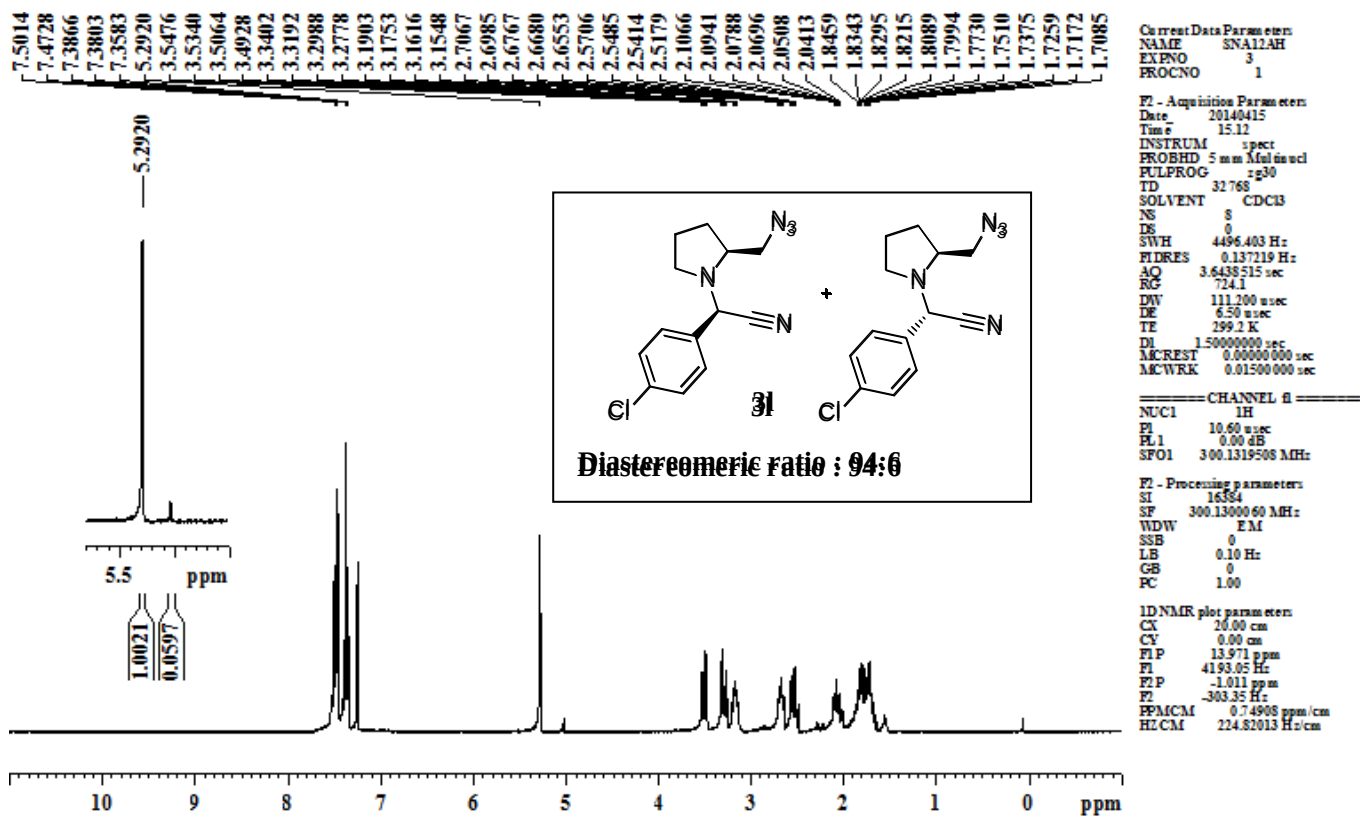
F2 - Acquisition Parameters:
Date_ 20140422
Time_ 1:19
INSTRUM spect
PROBHD 5 mm Maltinaucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 18832.393 Hz
FIDRES 0.187360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 300.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999999 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

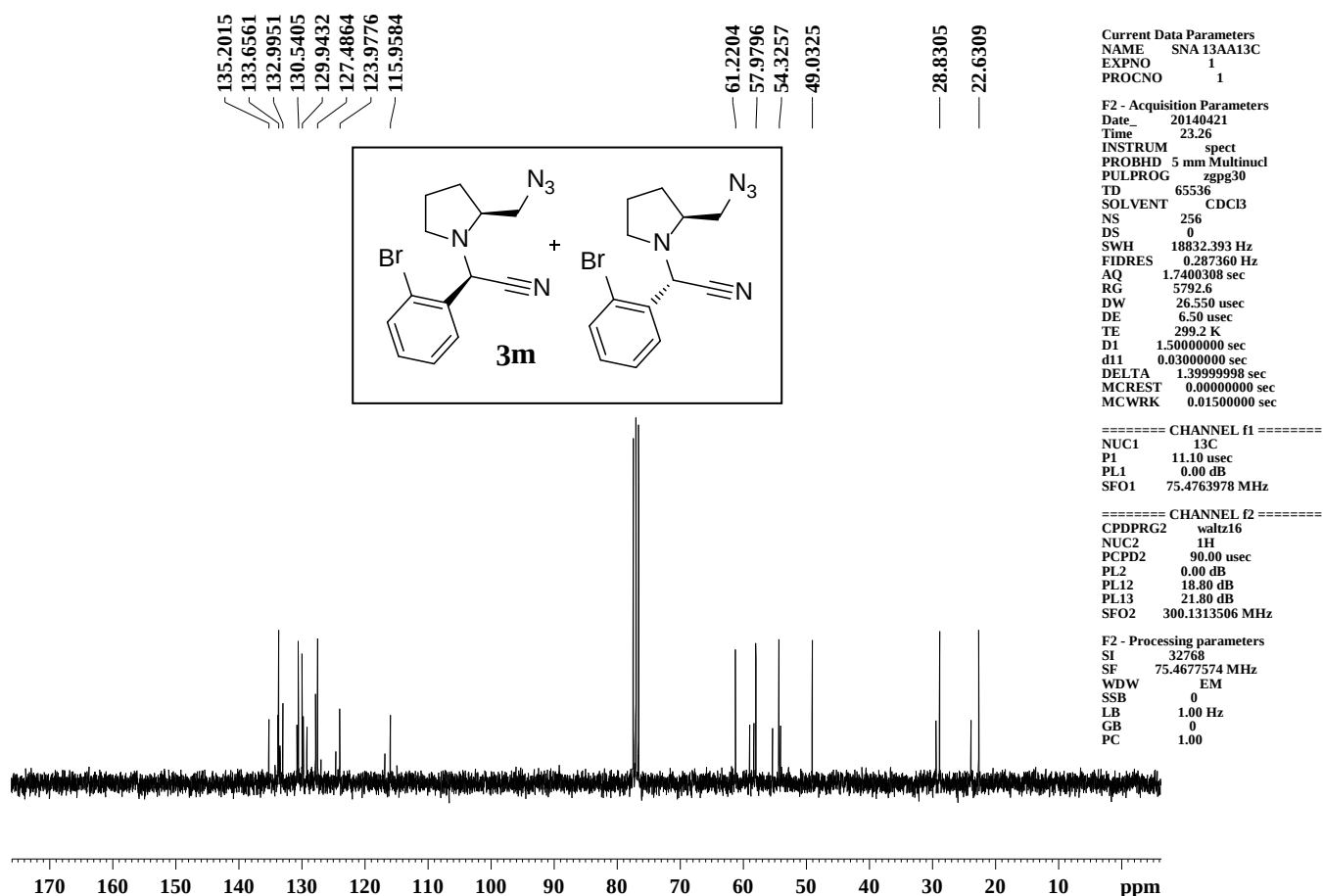
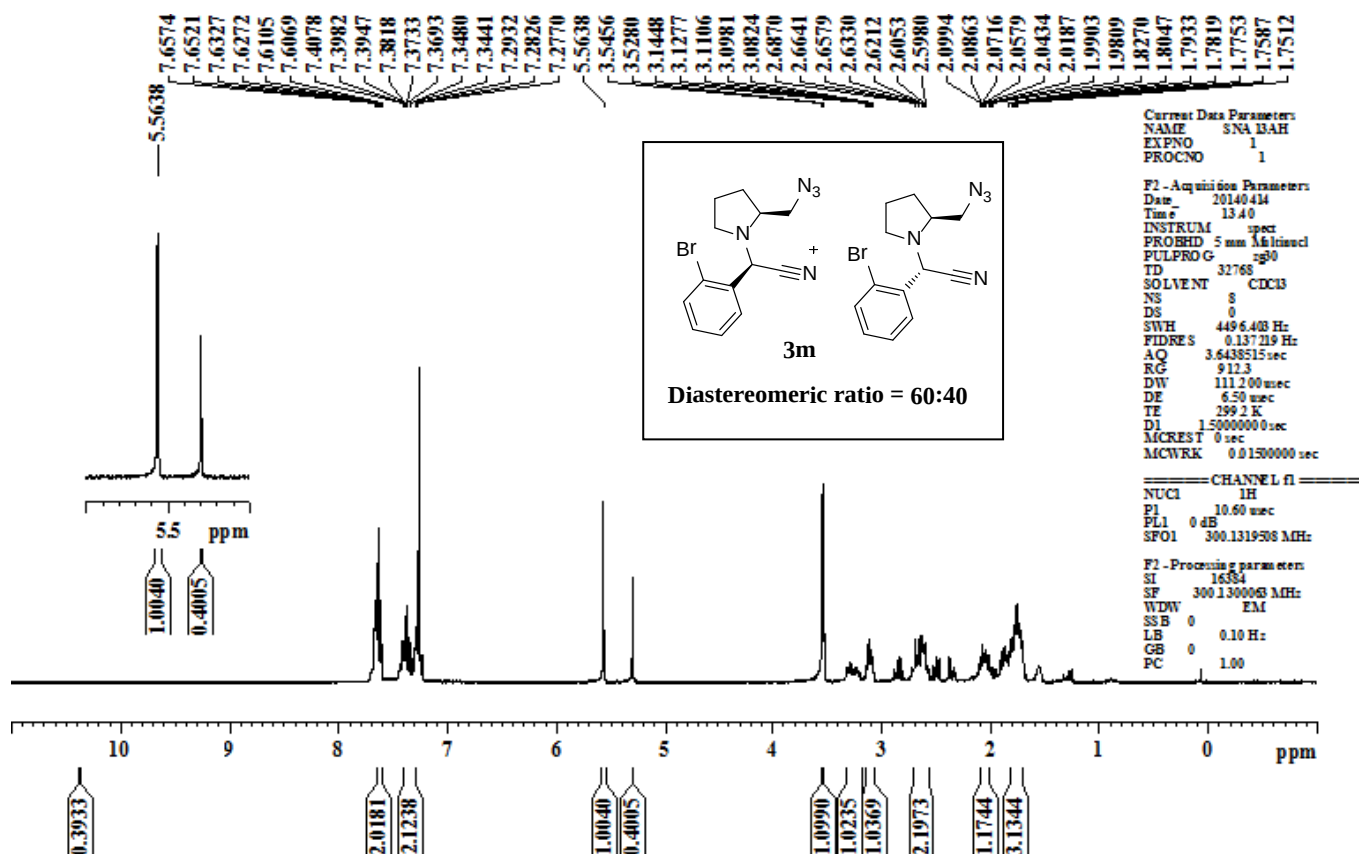
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

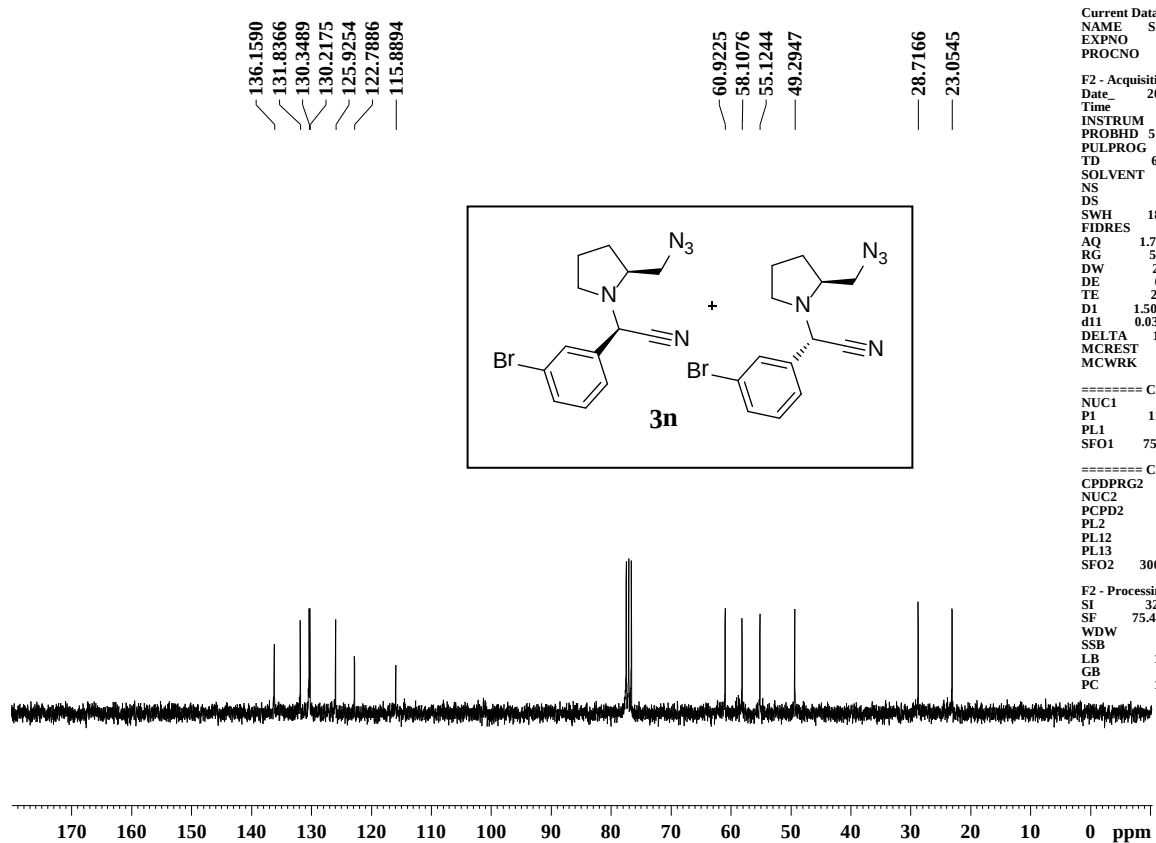
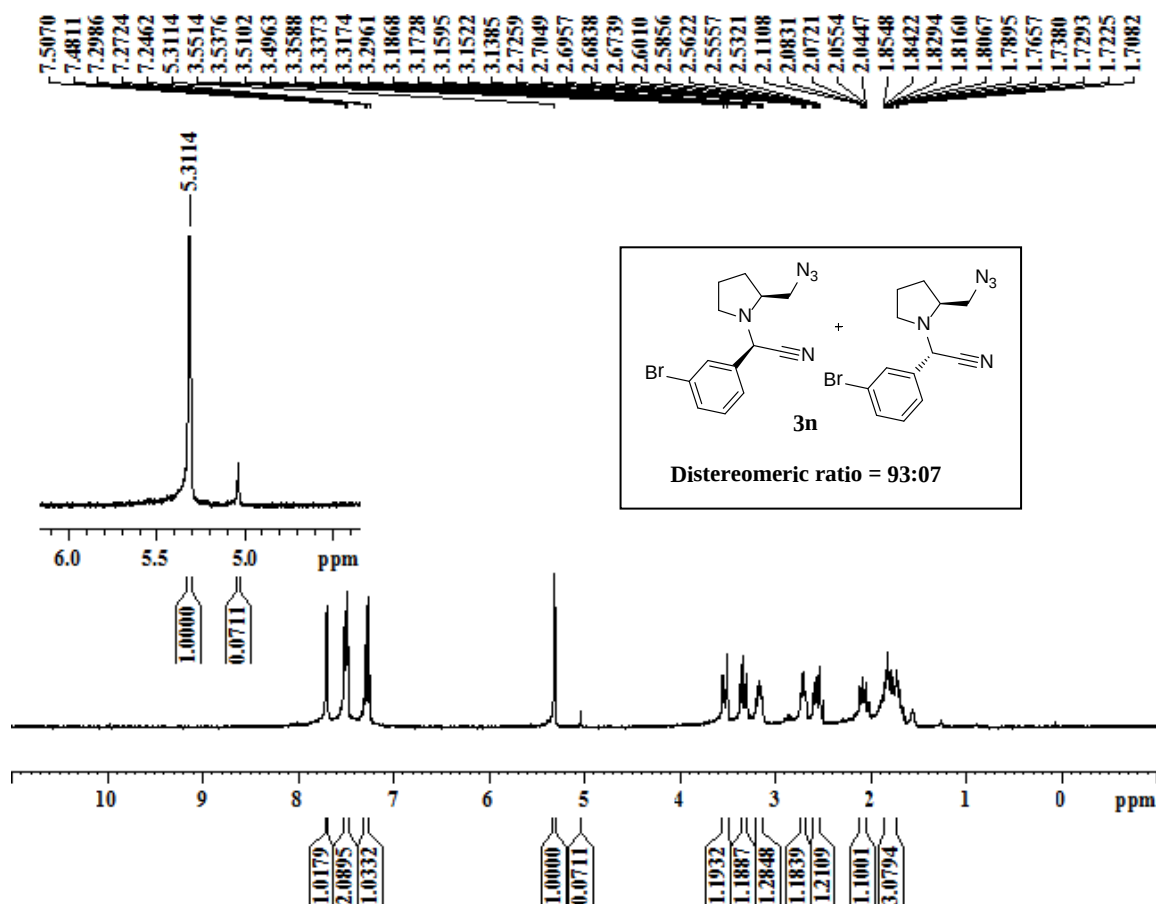
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1315906 MHz

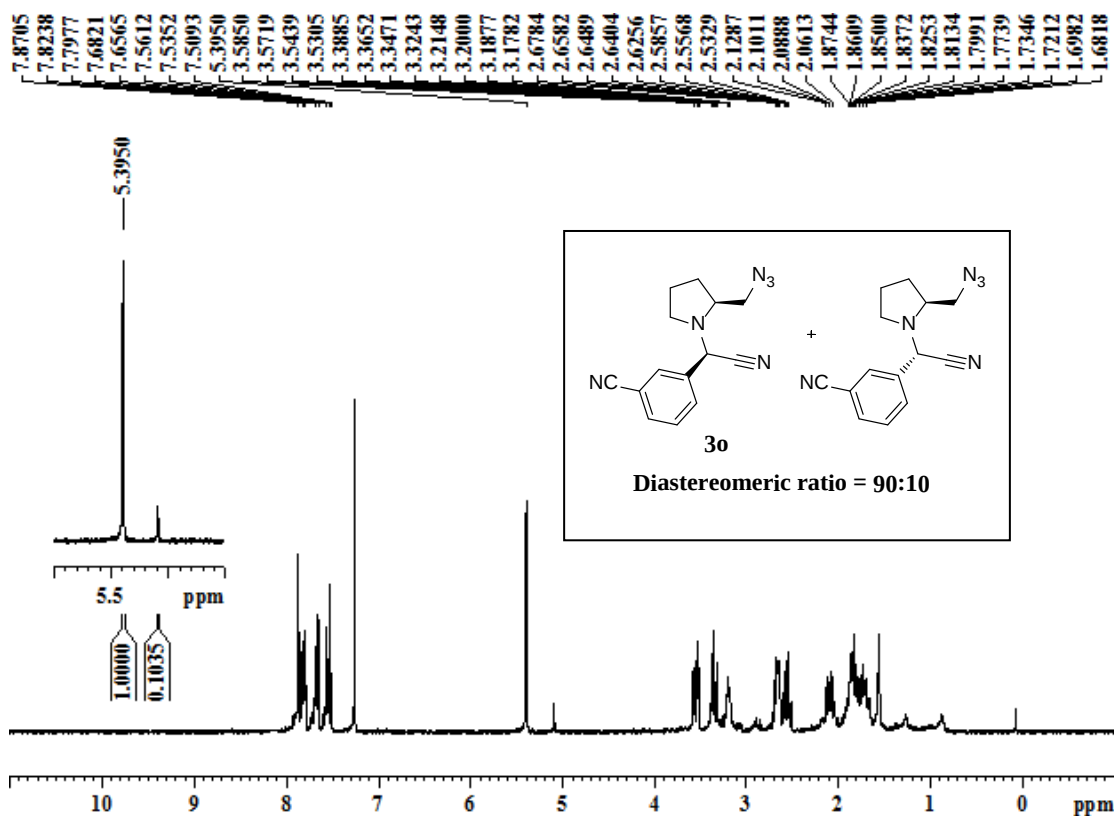
F2 - Processing parameters:
SI 32768
SF 75.4677649 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00









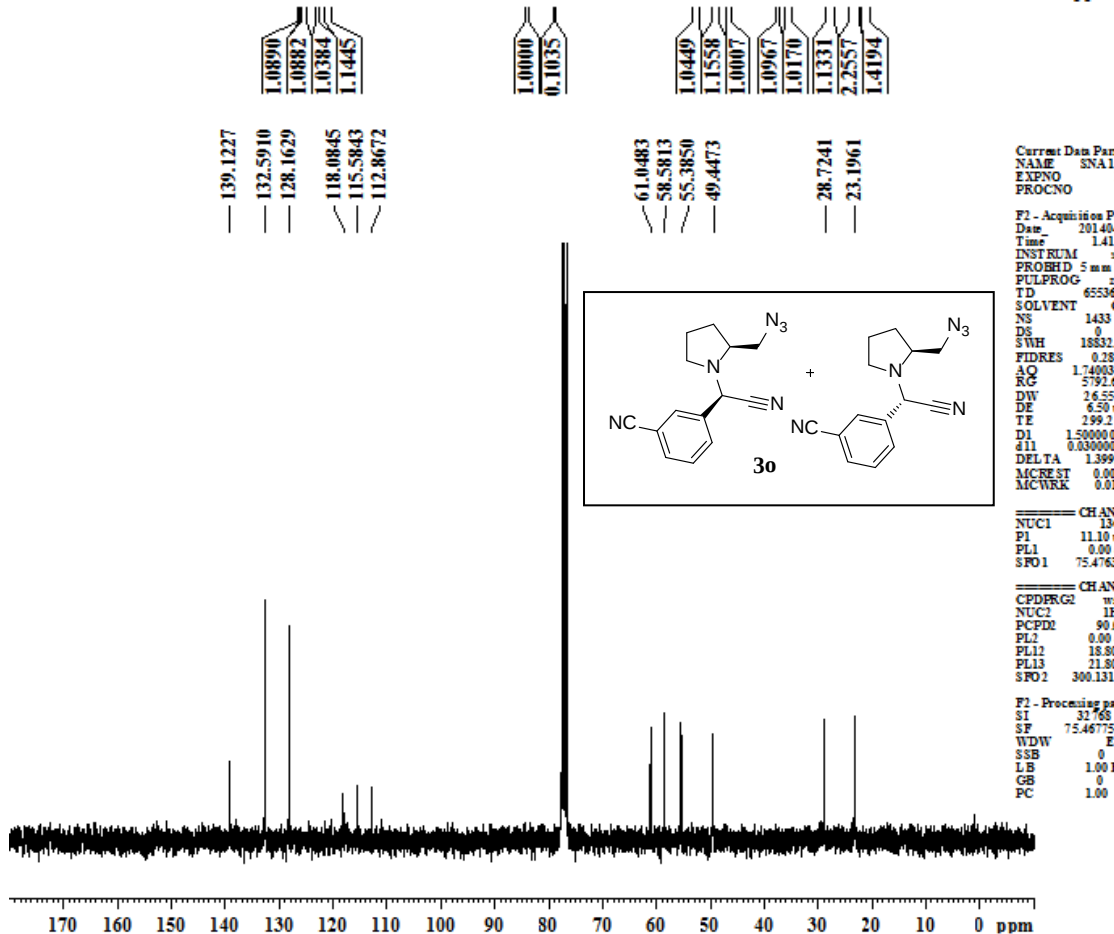


Current Data Parameters
NAME SNA15AH
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140414
Time 14.02
INSTRUM spect
PROBHD 5 mm Maltinocl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 1024
DW 111.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.5000000 sec
MCREST 0 sec
MCWKK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



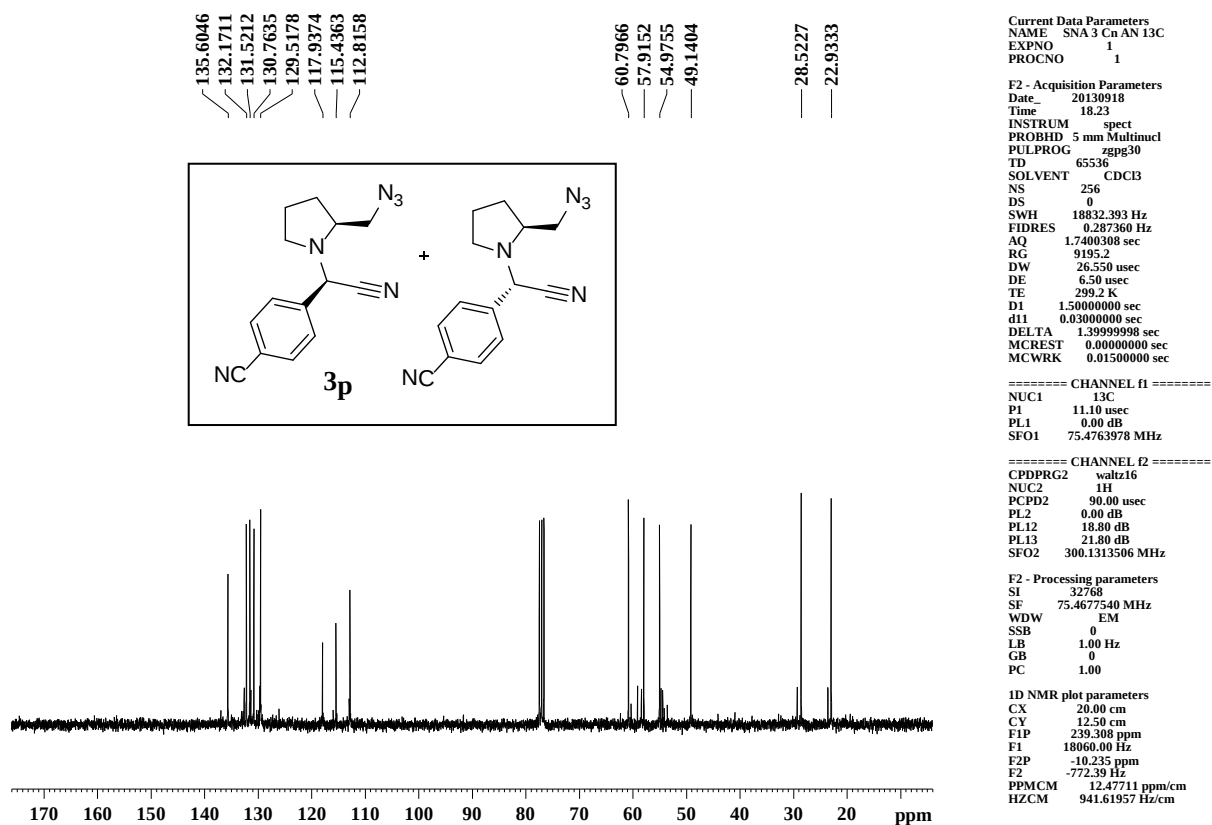
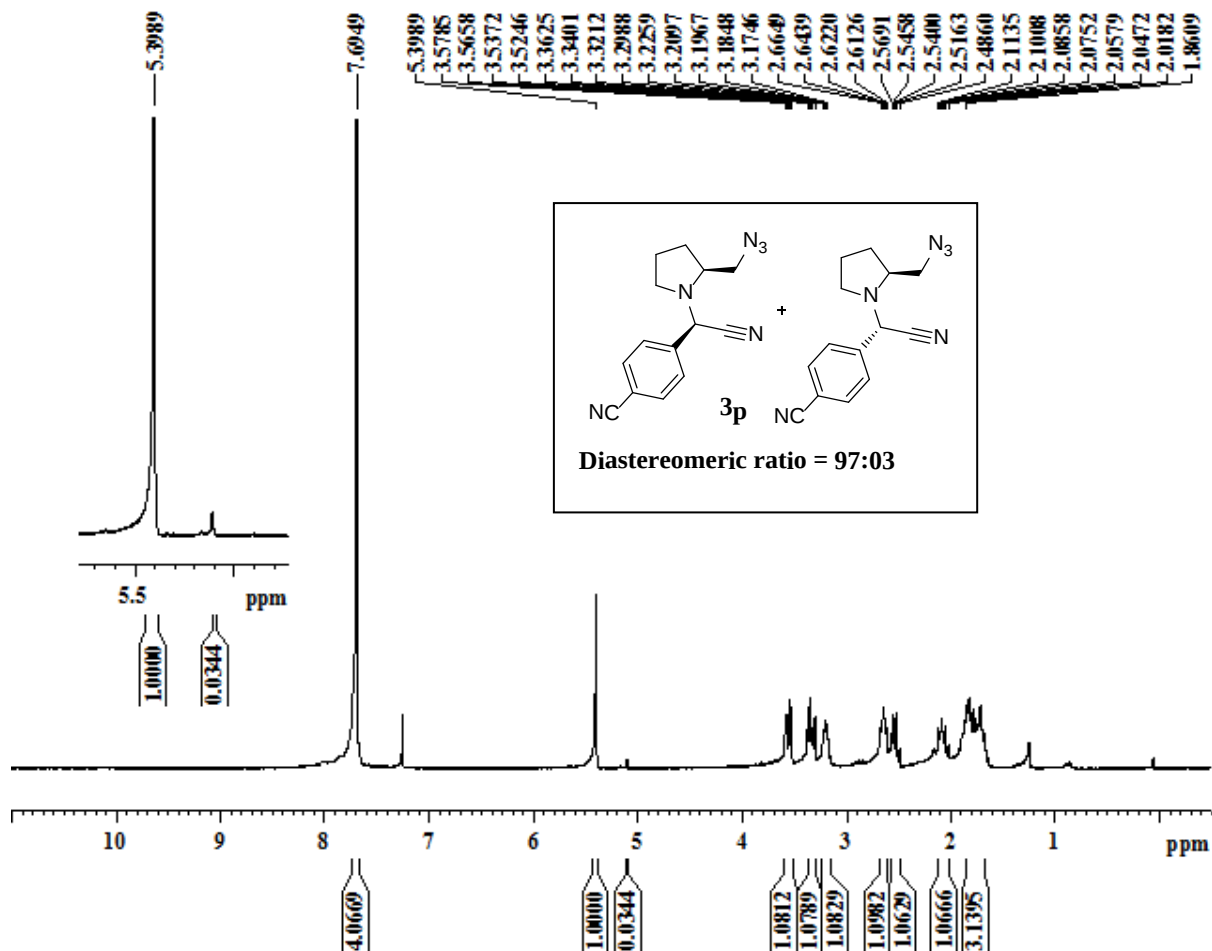
Current Data Parameters
NAME SNA16AAL3C
EXPNO 1
PROCNO 1

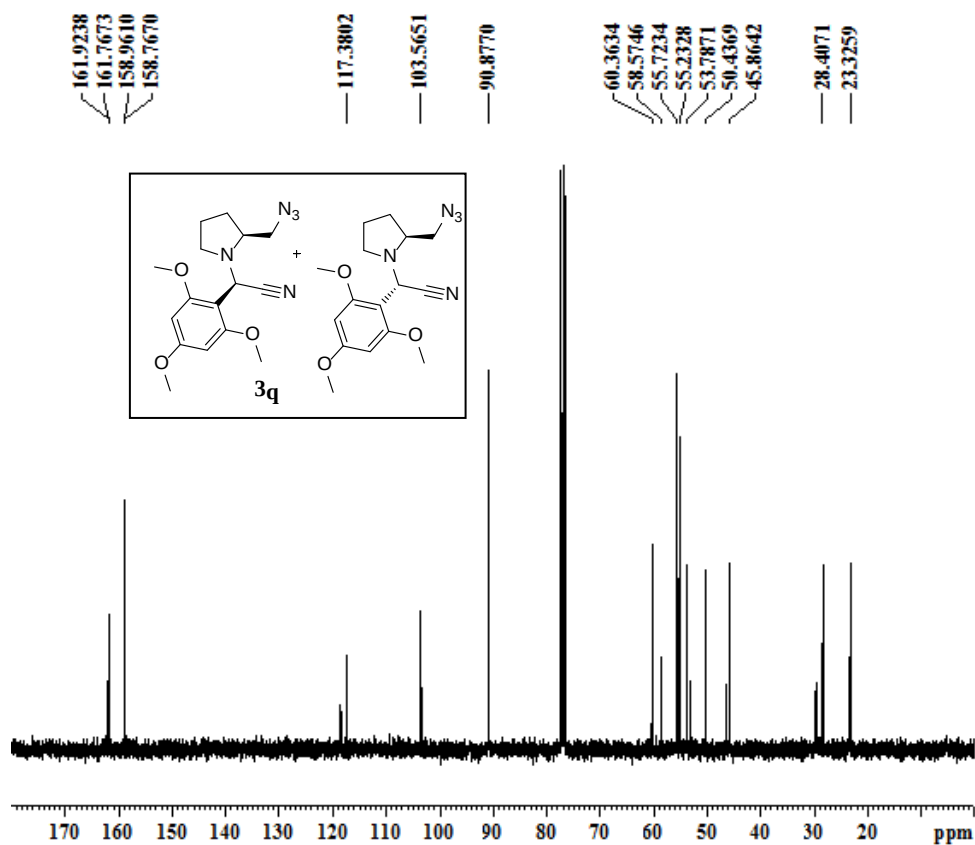
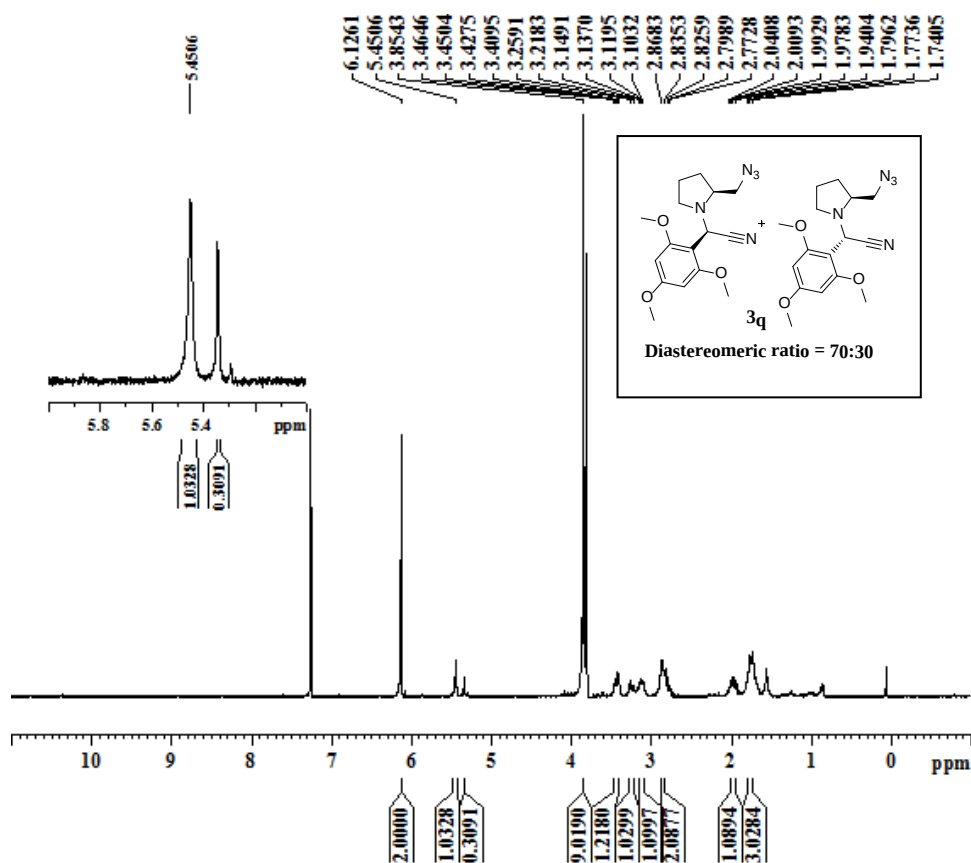
F2 - Acquisition Parameters
Date_ 20140422
Time 1.41
INSTRUM spect
PROBHD 5 mm Maltinocl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1433
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7408308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.5000000 sec
d11 0.0300000 sec
DELTA 1.39999999 sec
MCREST 0.0000000 sec
MCWKK 0.0150000 sec

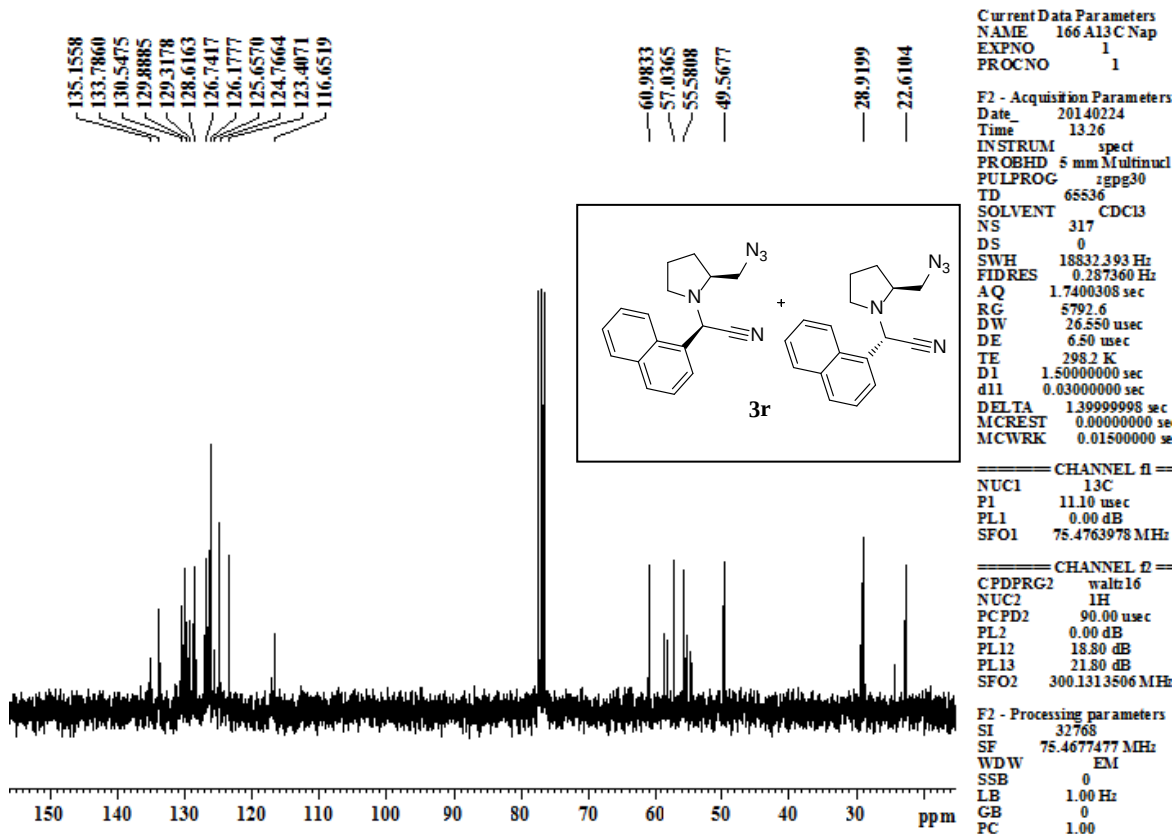
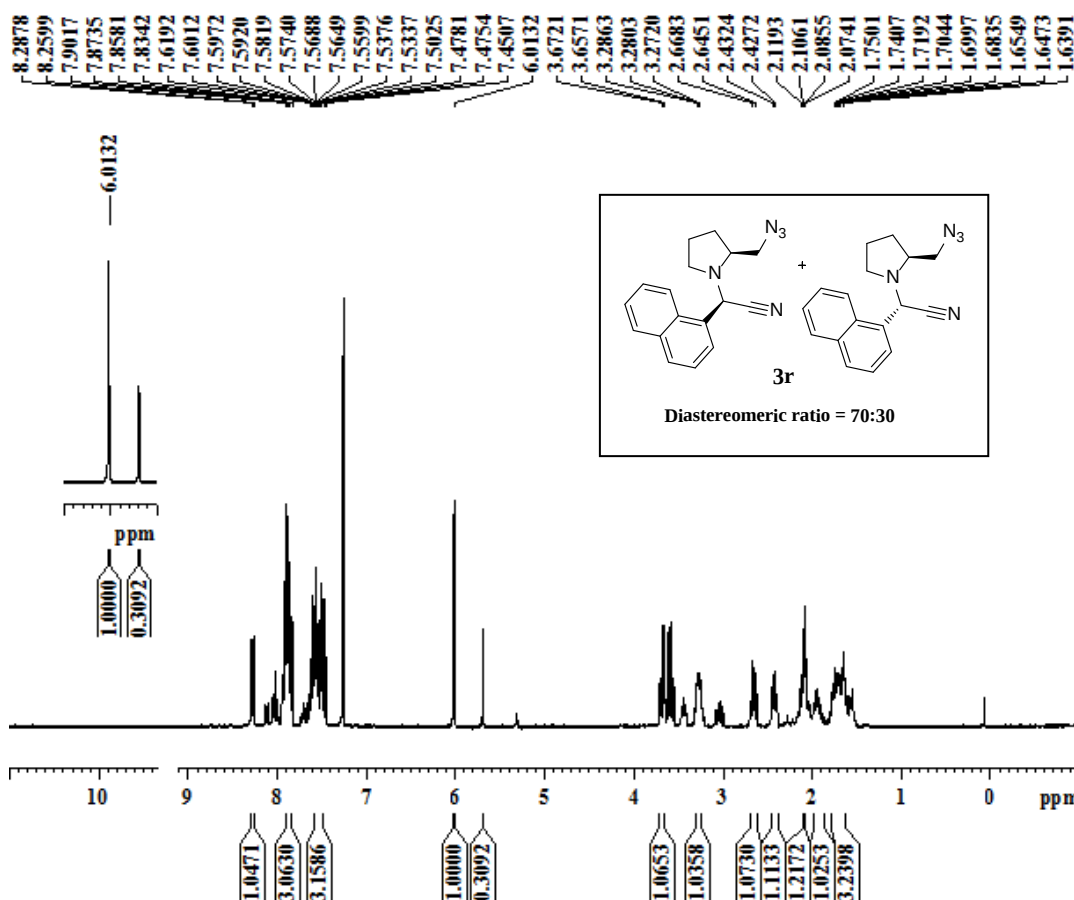
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

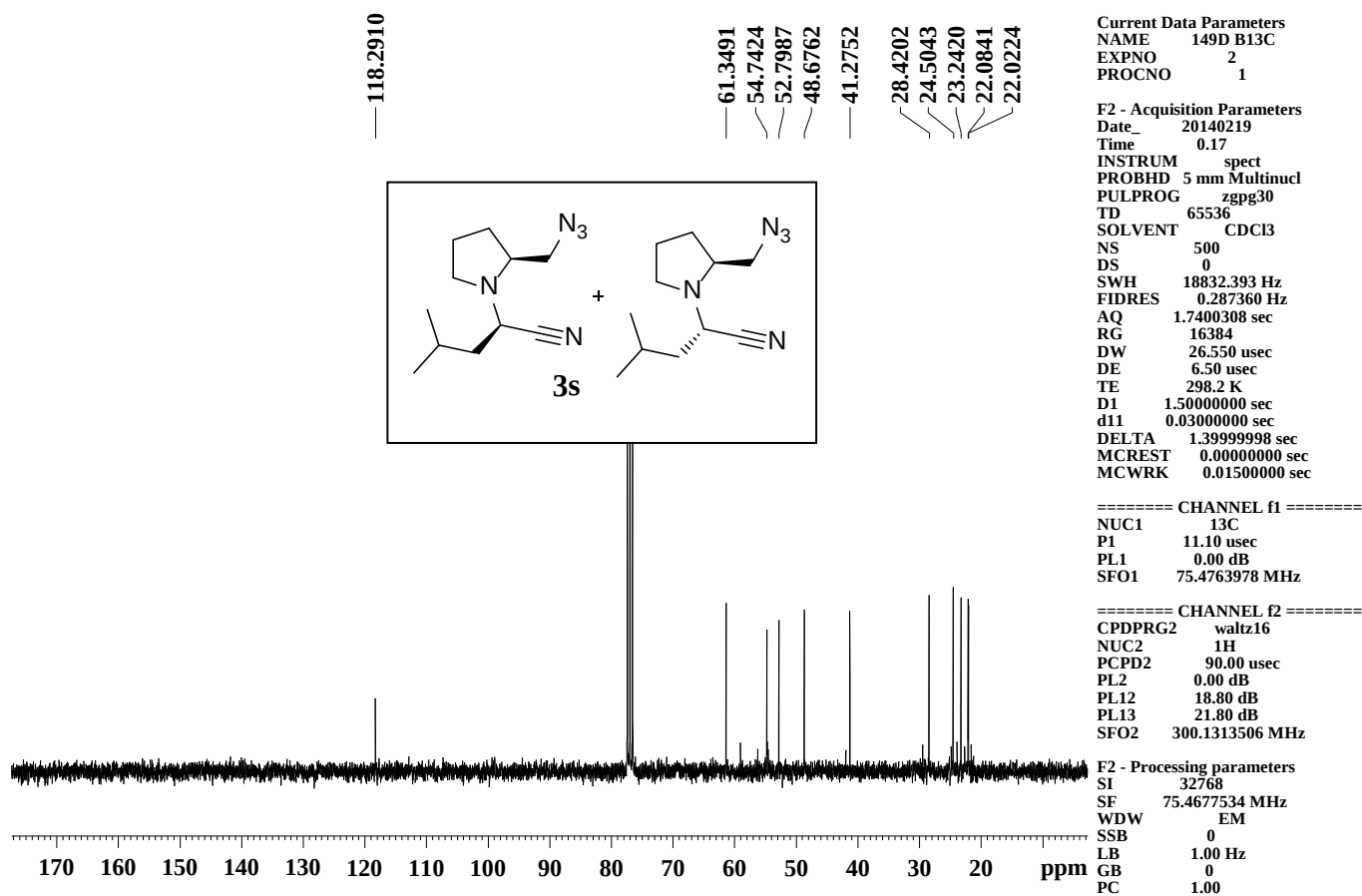
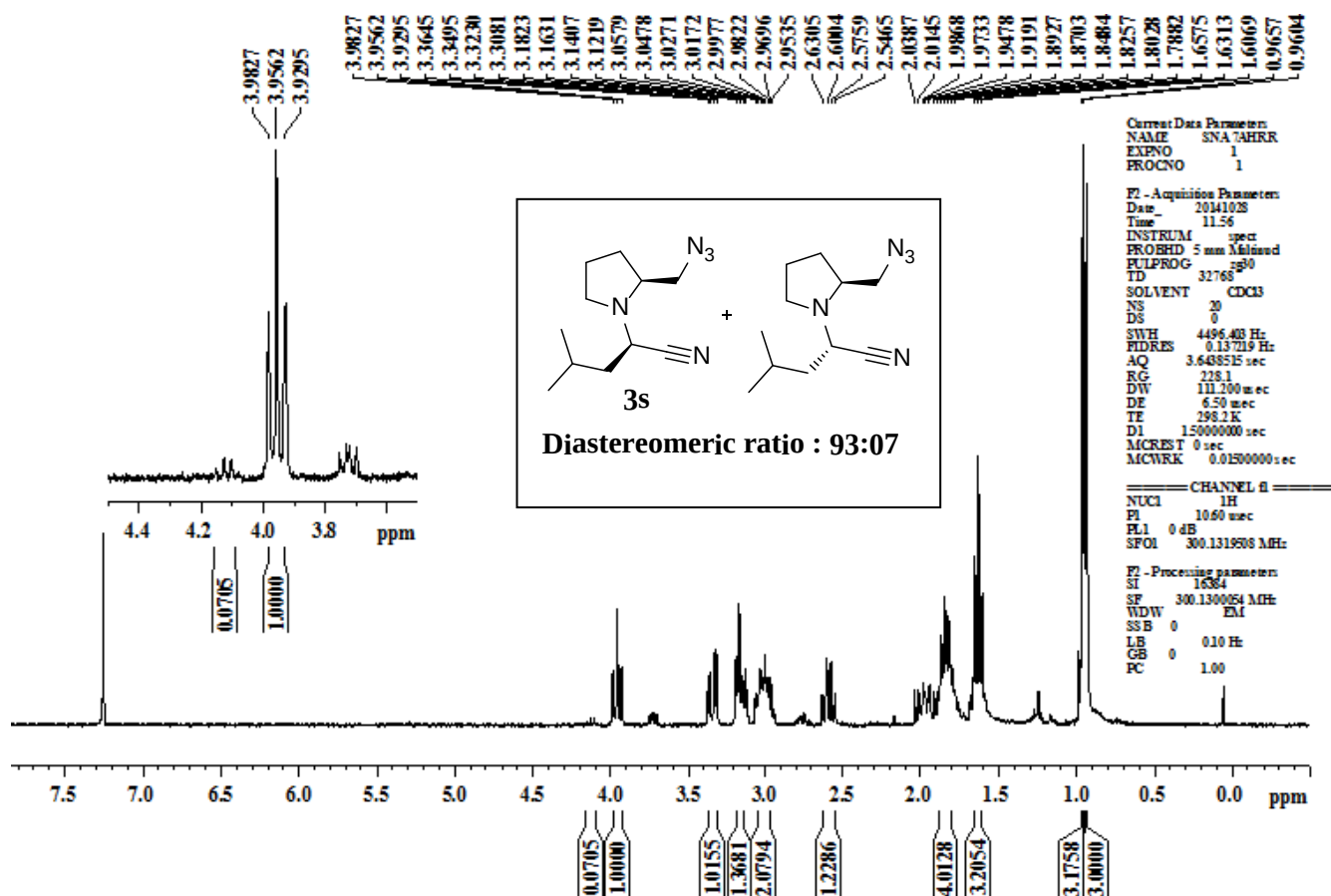
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

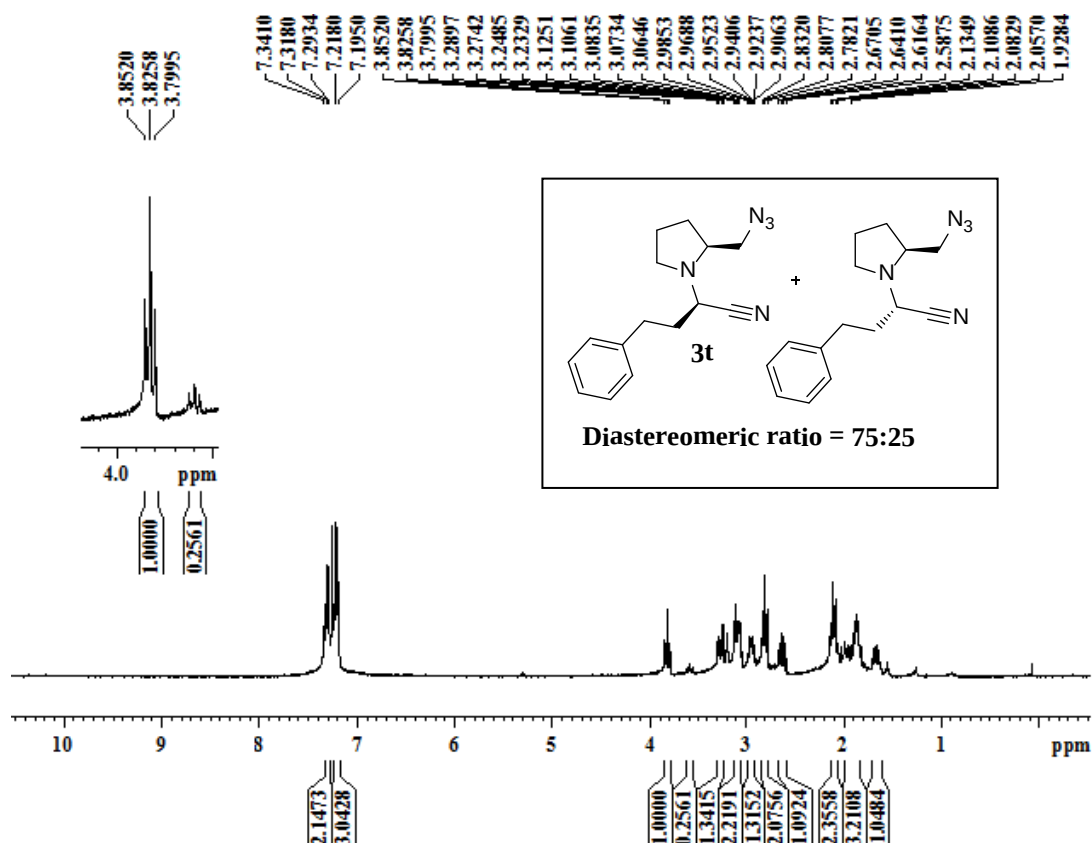
F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00









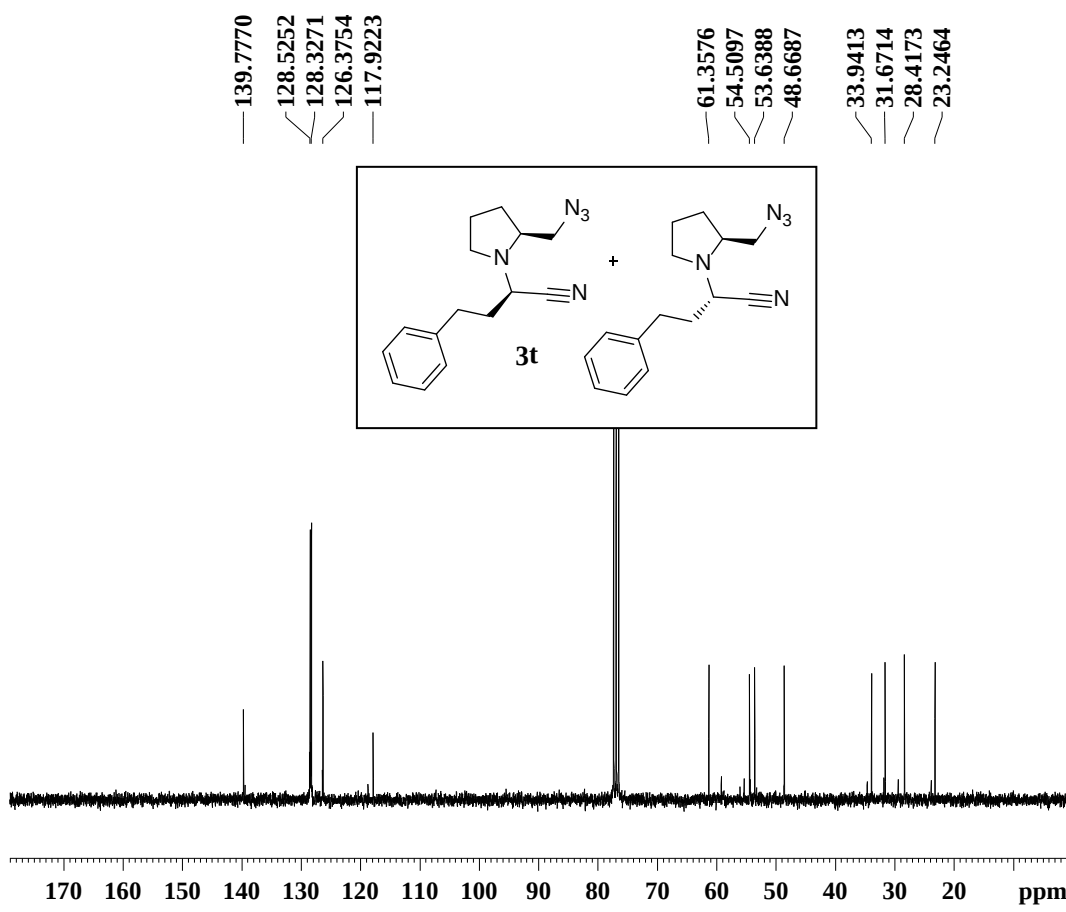


Current Data Parameters
NAME SNI20AH
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140415
Time 14.59
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 645.1
DW 111.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0.15000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.0 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.130063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



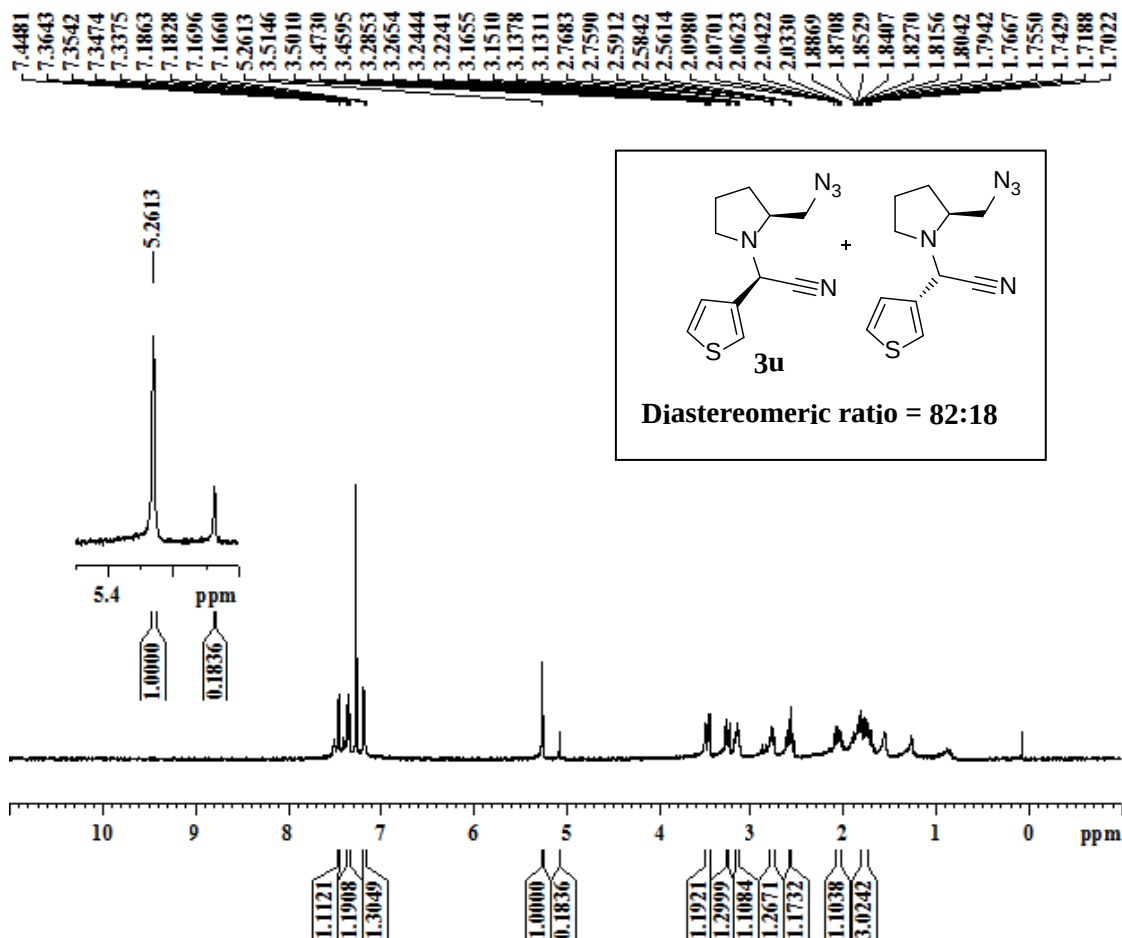
Current Data Parameters
NAME SNA 170 A13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140225
Time 3.12
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 875
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677563 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

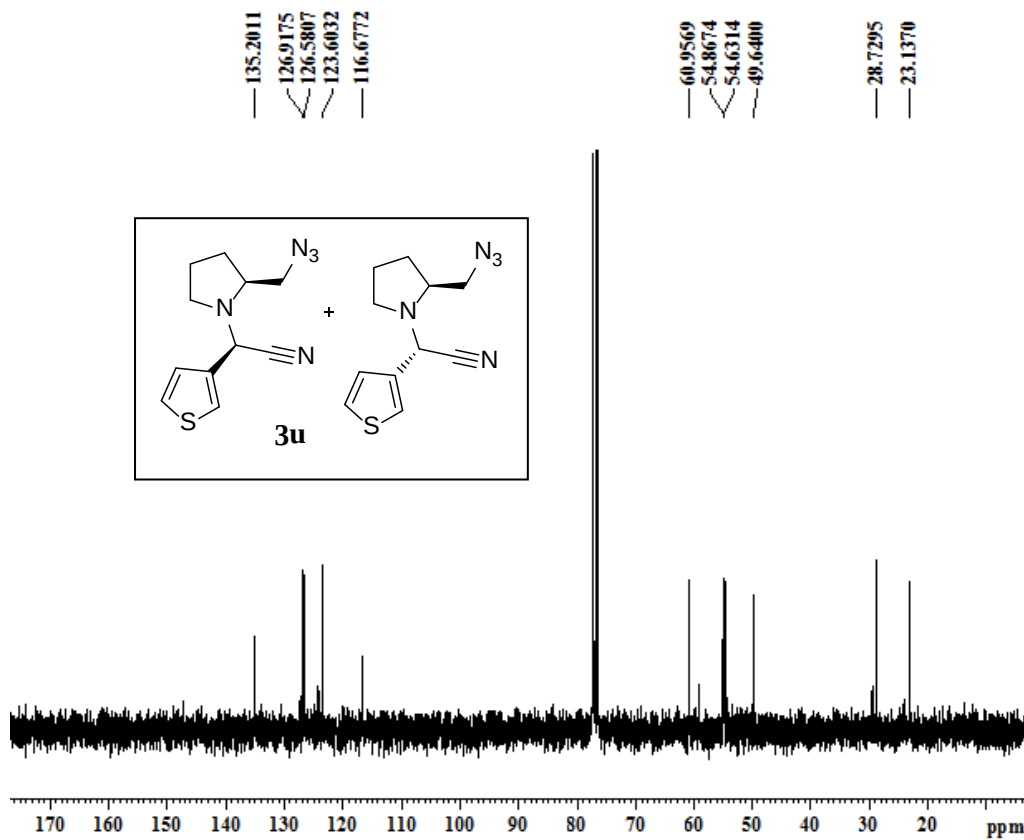


Current Data Parameters
NAME SNA11AH
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140415
Time 15.23
INSTRUM spect
PROBHD 5 mm Multispec
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 1149.4
DW 111.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
PL 10.60 usec
PL1 0.00 dB
SFO1 300.131508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.971 ppm
FI 4193.05 Hz
F1 -1.011 ppm
F2 -303.35 Hz
PPMCM 0.74908 ppm/cm
H1 CM 224.82013 Hz/cm



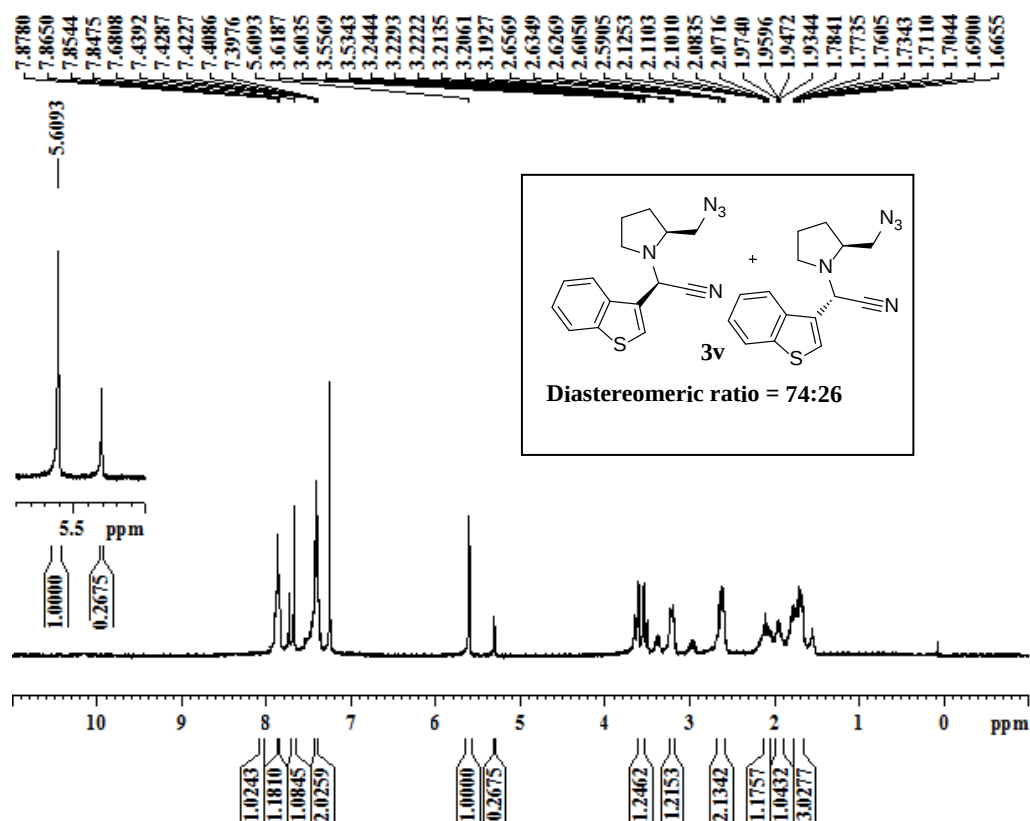
Current Data Parameters
NAME SNA 144 A13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140226
Time 0.37
INSTRUM spect
PROBHD 5 mm Multispec
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999999 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
PL 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



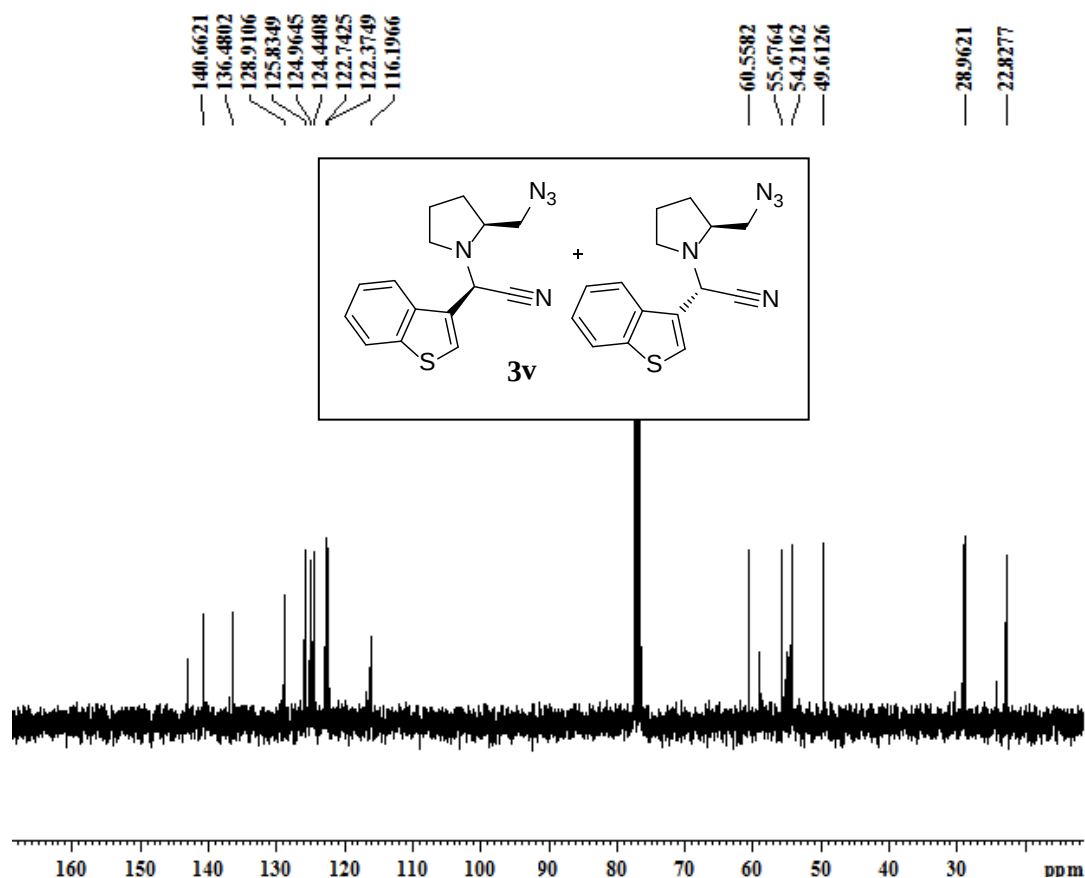
Current Data Parameters
NAME SNA12AH
EXPNO 3
PROCNO 1

F1 - Acquisition Parameters
Date_ 20140415
Time 15.17
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 912.3
DW 111.700 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.131508 MHz

F1 - Processing parameters
SI 16384
SF 300.130065 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.969 ppm
FI 4192.50 Hz
FIP -1.013 ppm
F1 -303.90 Hz
F2 0.74908 ppm/cm
HZ CM 224.82013 Hz/cm



Current Data Parameters
NAME SNA153A13C
EXPNO 3
PROCNO 1

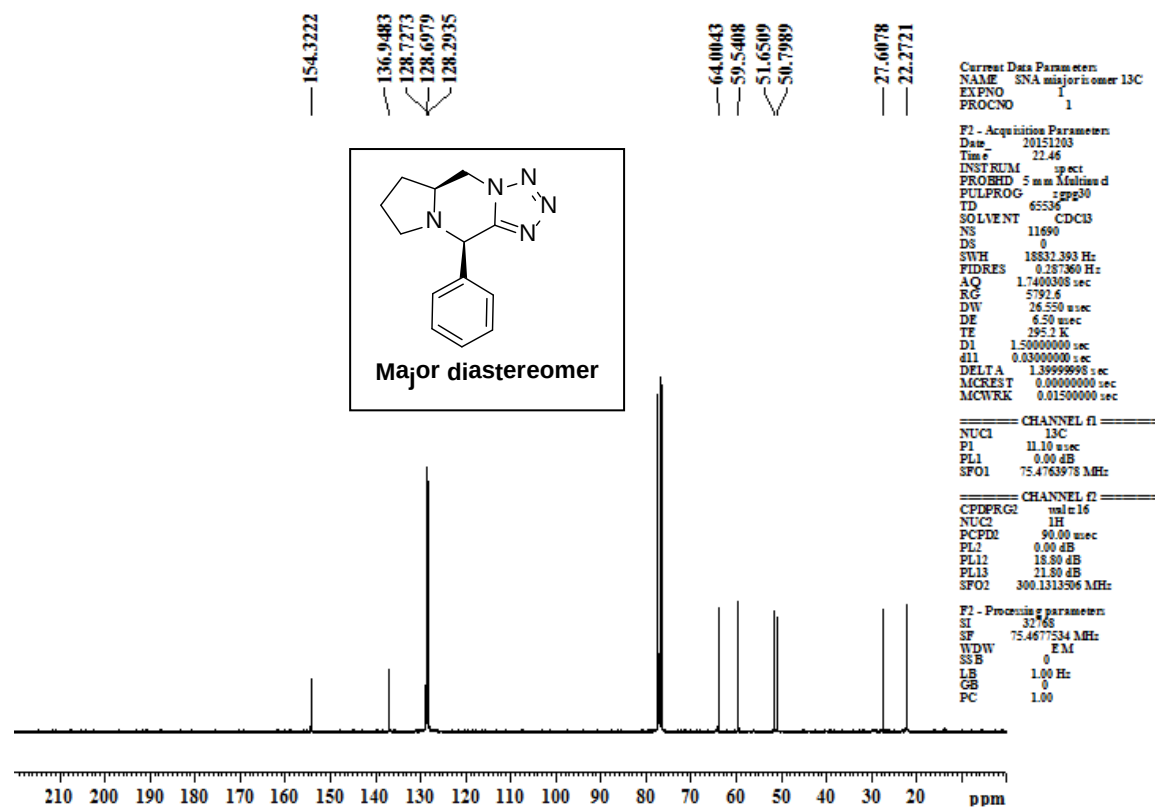
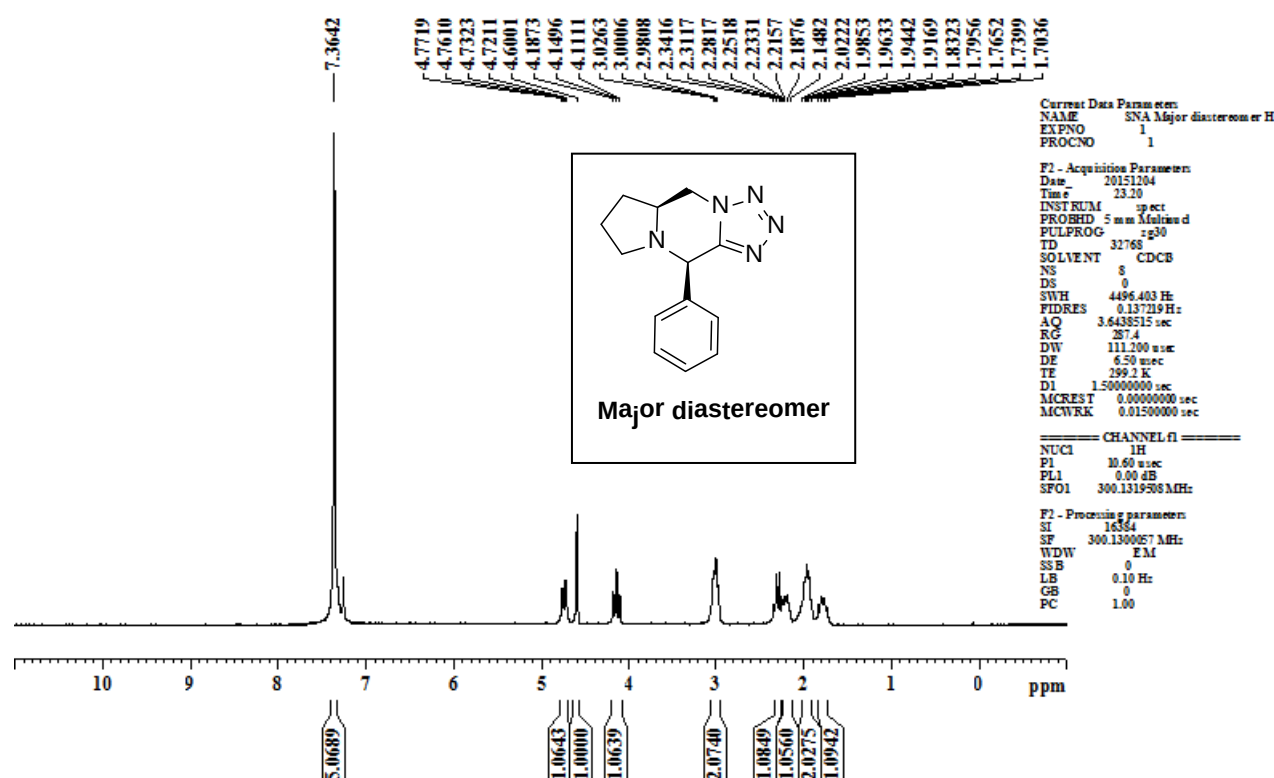
F1 - Acquisition Parameters
Date_ 20140228
Time 18.31
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 18832.393 Hz
FIDRES 0.187360 Hz
AQ 1.7400308 sec
RG 20642.5
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999999 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

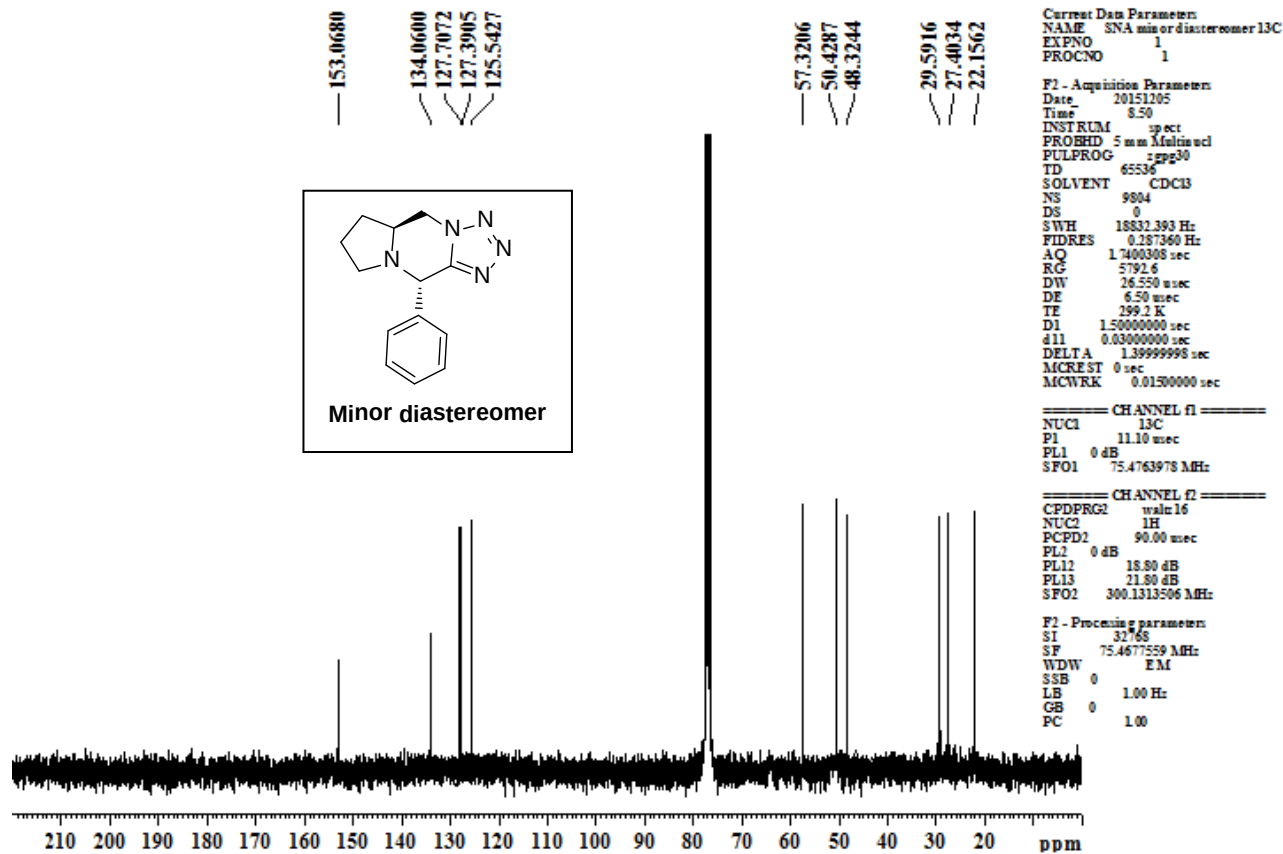
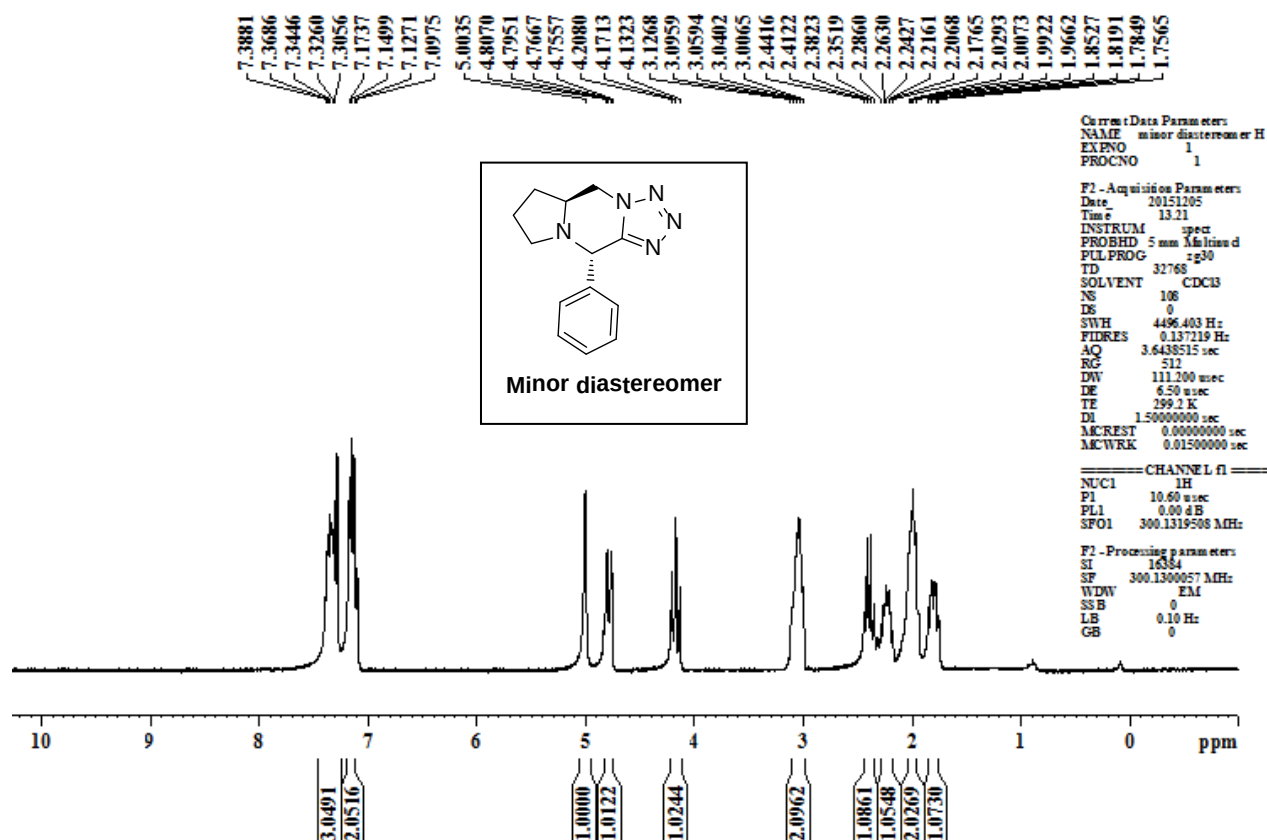
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

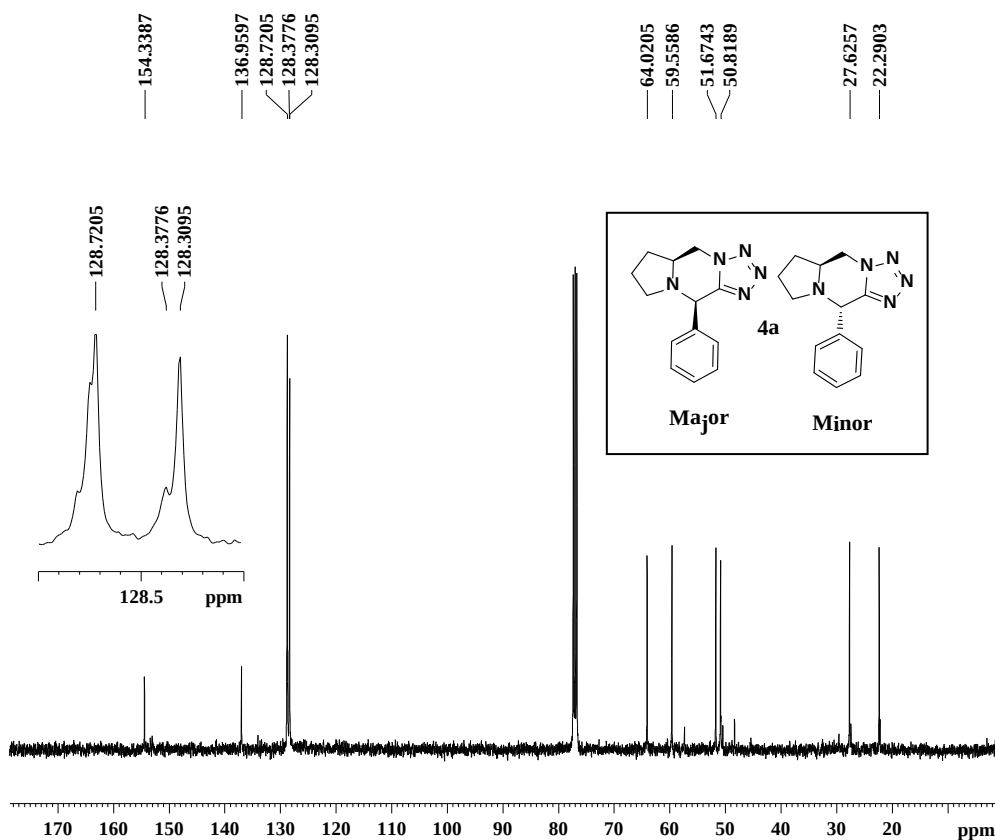
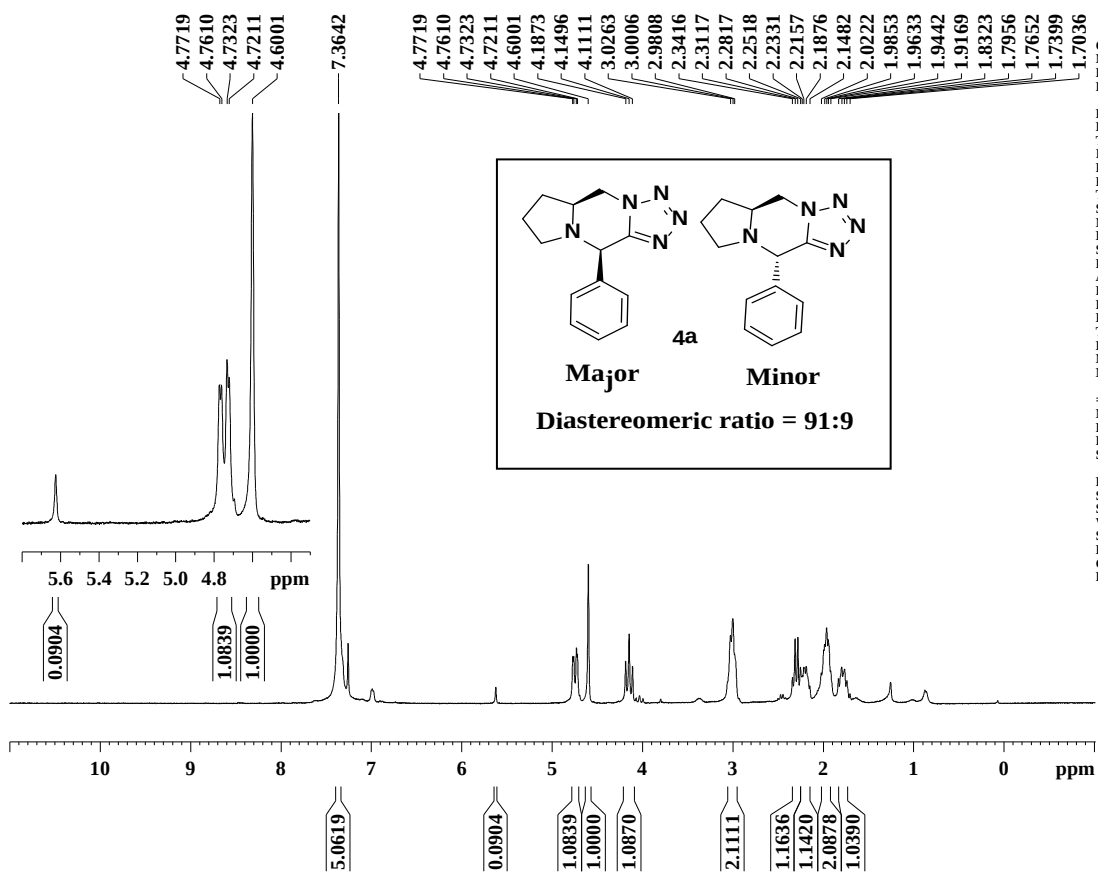
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

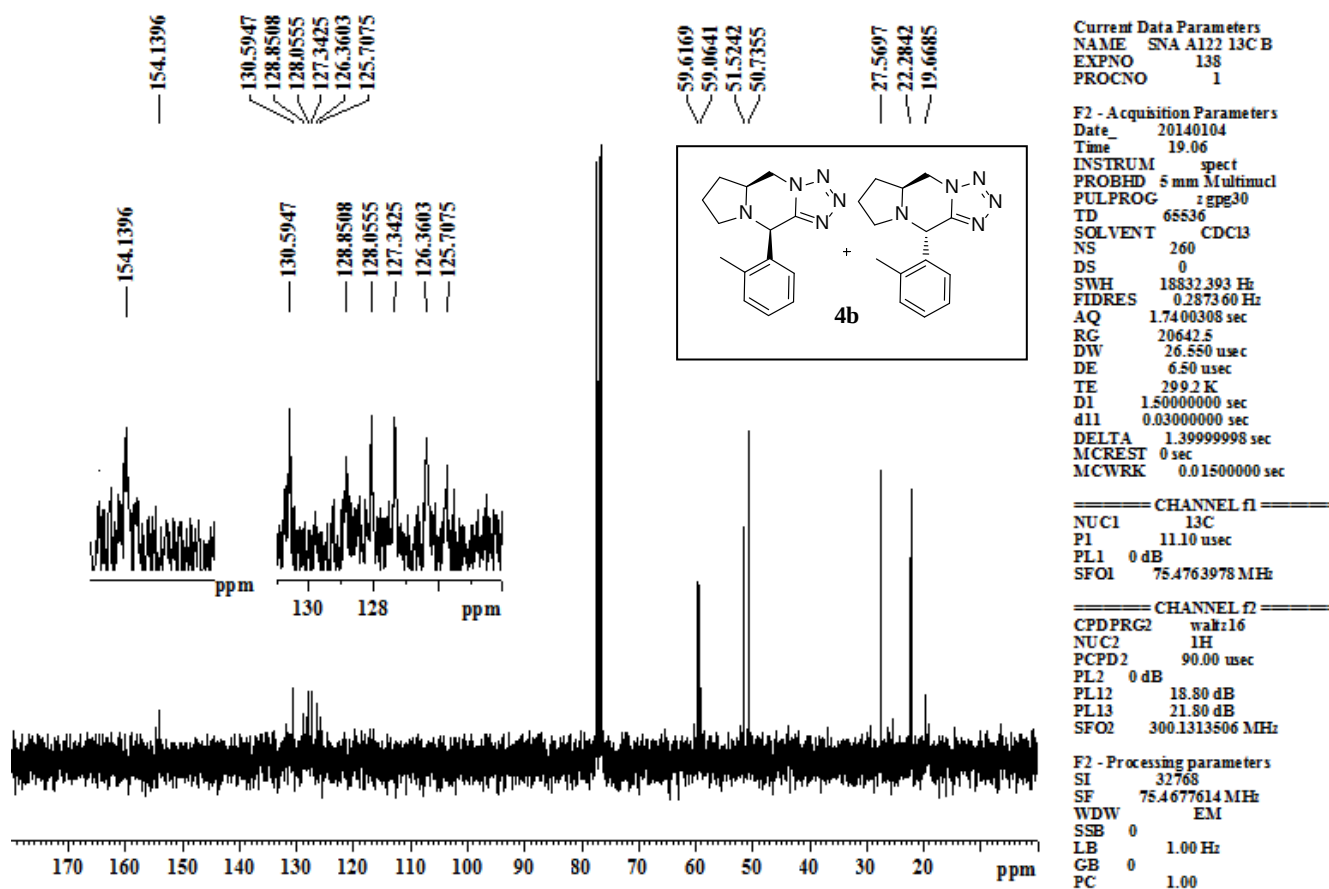
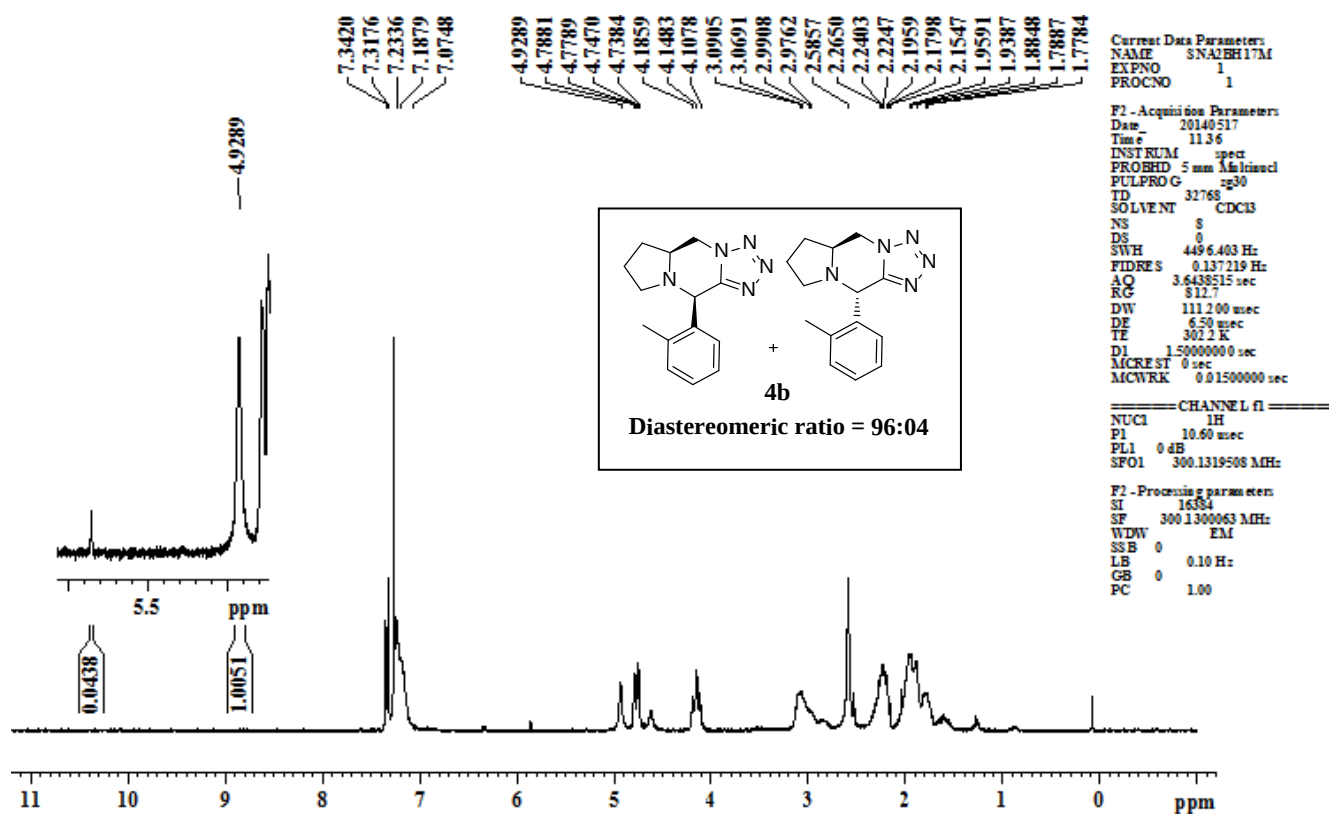
F2 - Processing parameters
SI 32768
SF 75.4677597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

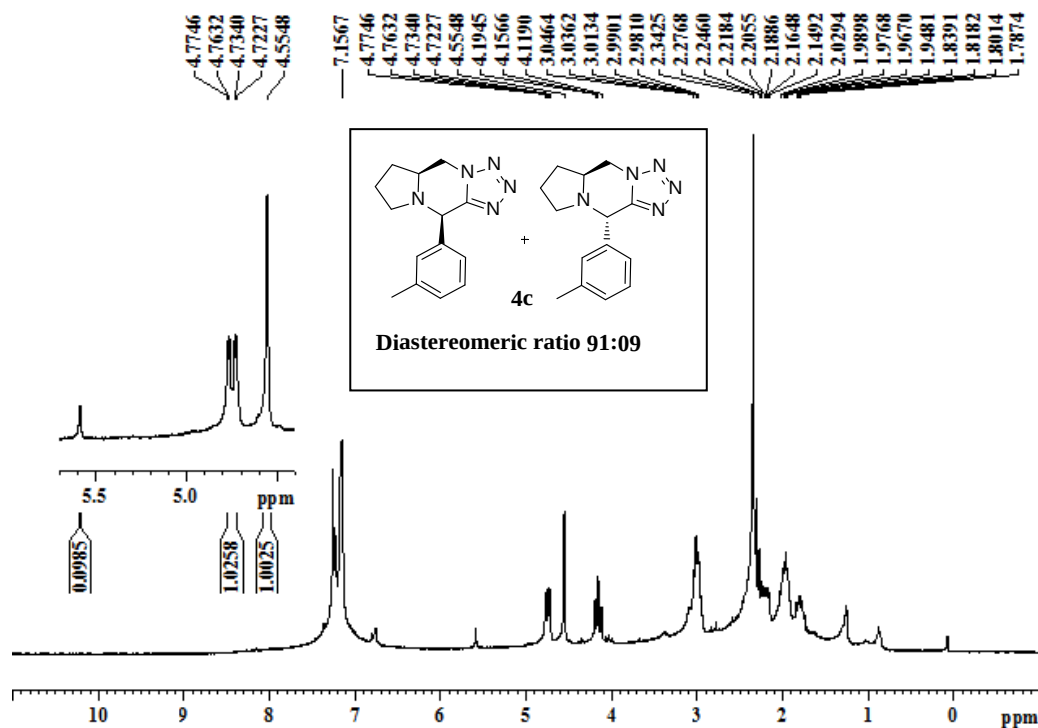
^1H , ^{13}C , Spectra of tricyclic fused tetrazoles









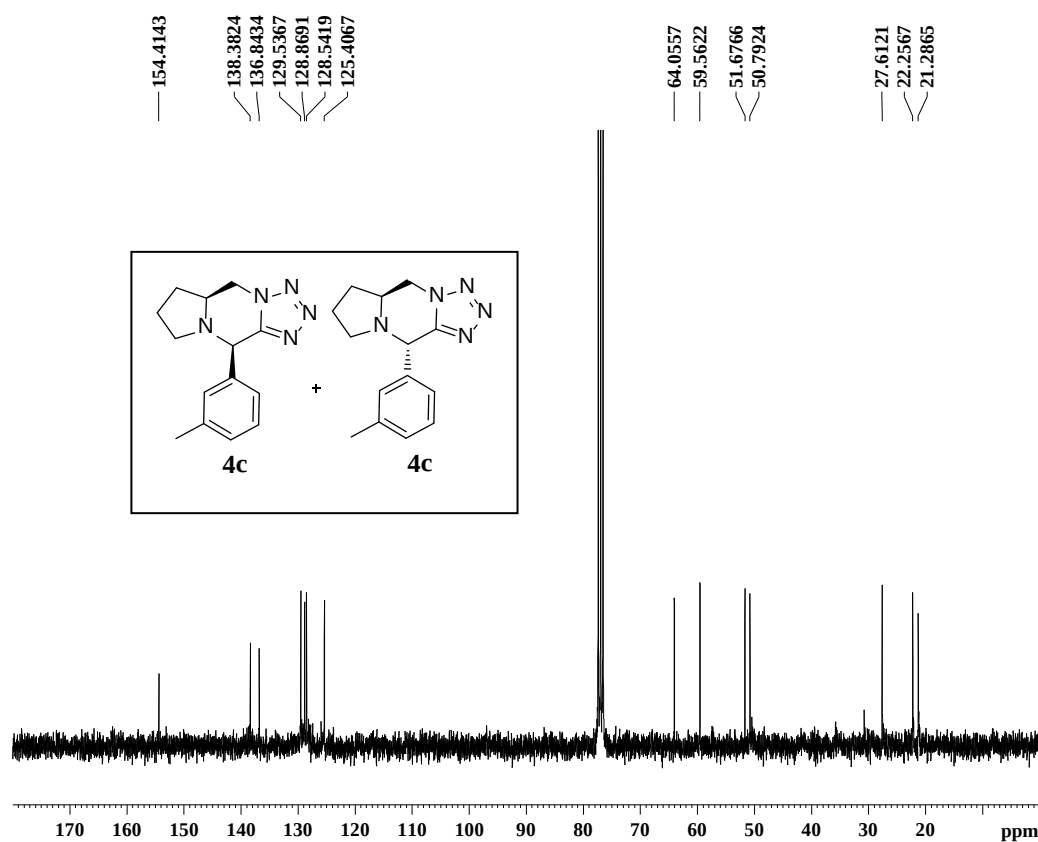


Current Data Parameters
NAME SNA3BHD13
EXPNO 1
PROCNO 1

F1 - Acquisition Parameters
Date_ 20140521
Time 14.20
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 85
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 574.7
DW 111.200 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0 dB
SFO1 300.1319508 MHz

F1 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



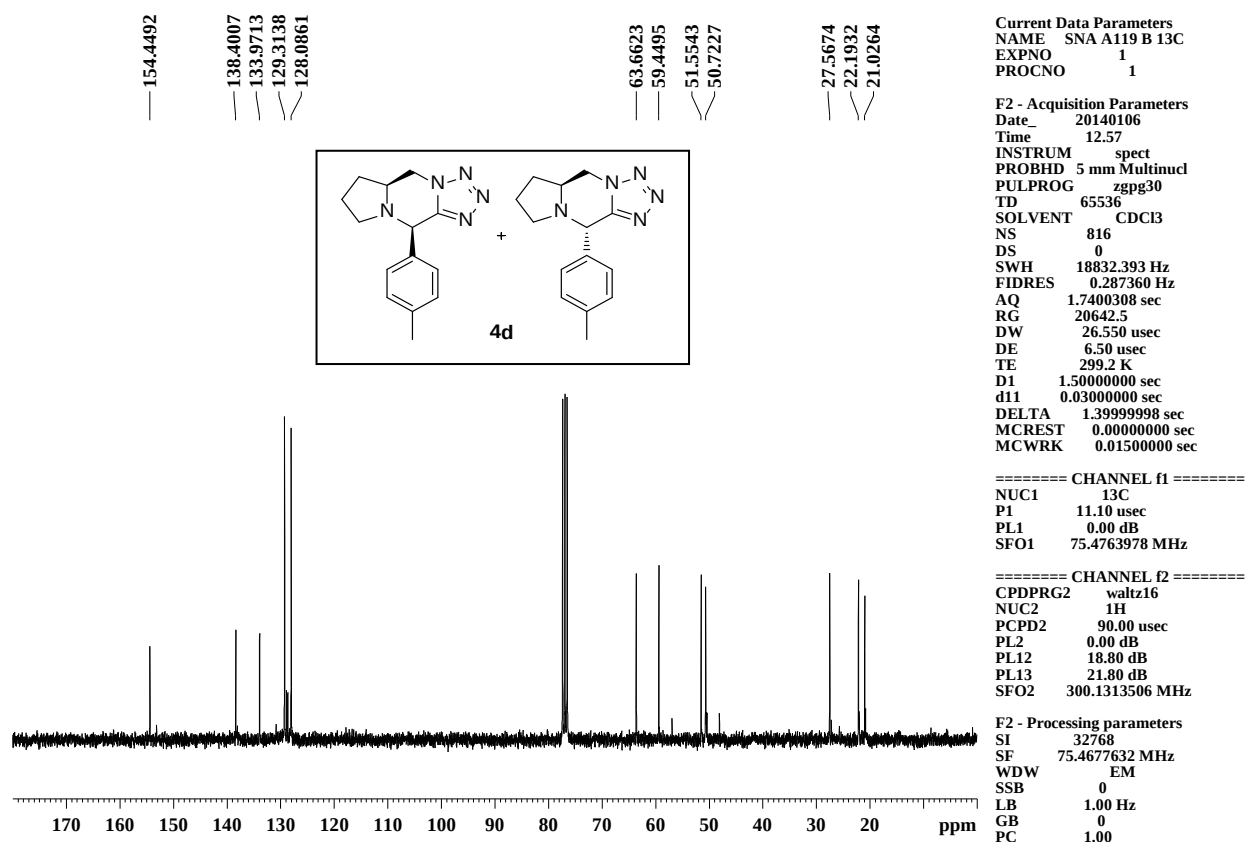
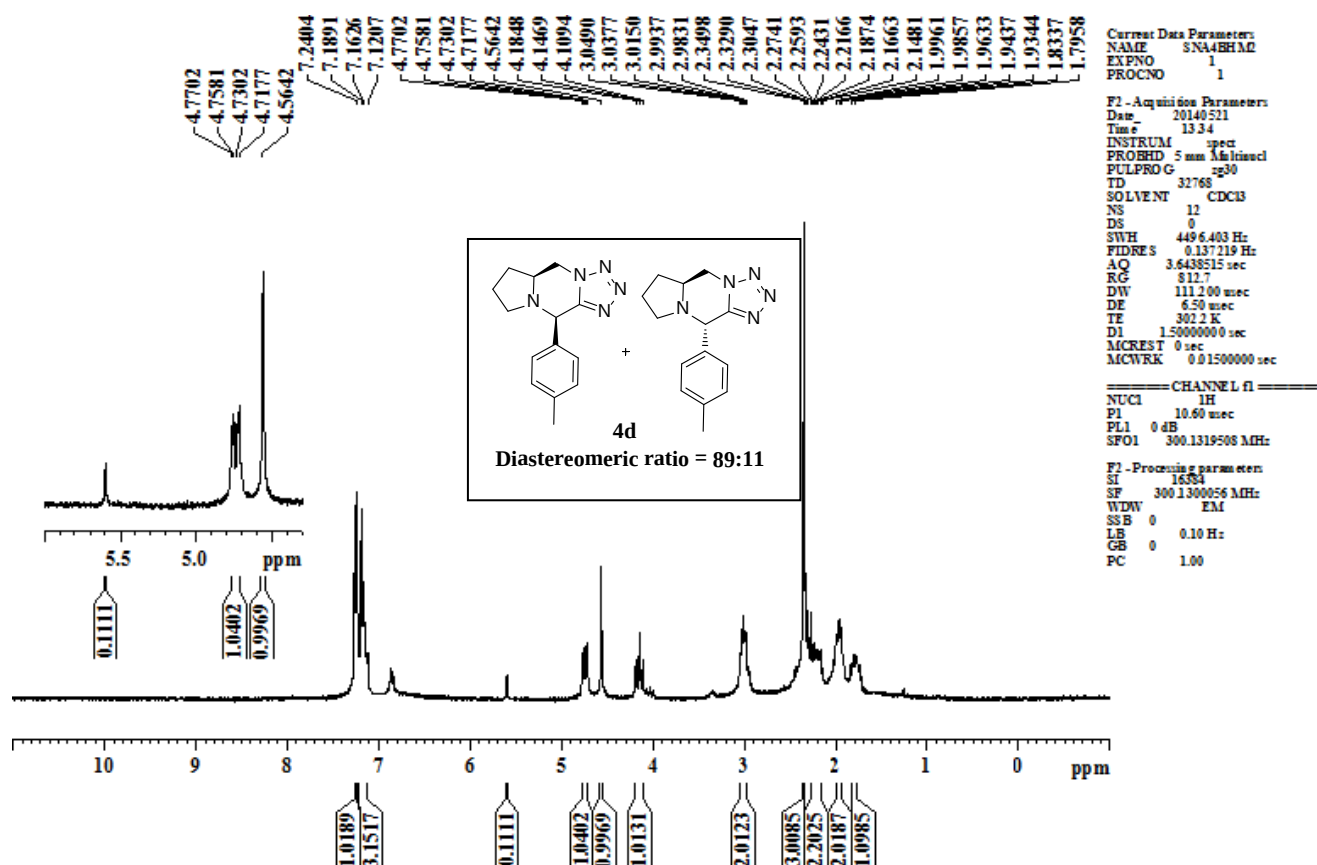
Current Data Parameters
NAME SNA A146 B13C
EXPNO 4
PROCNO 1

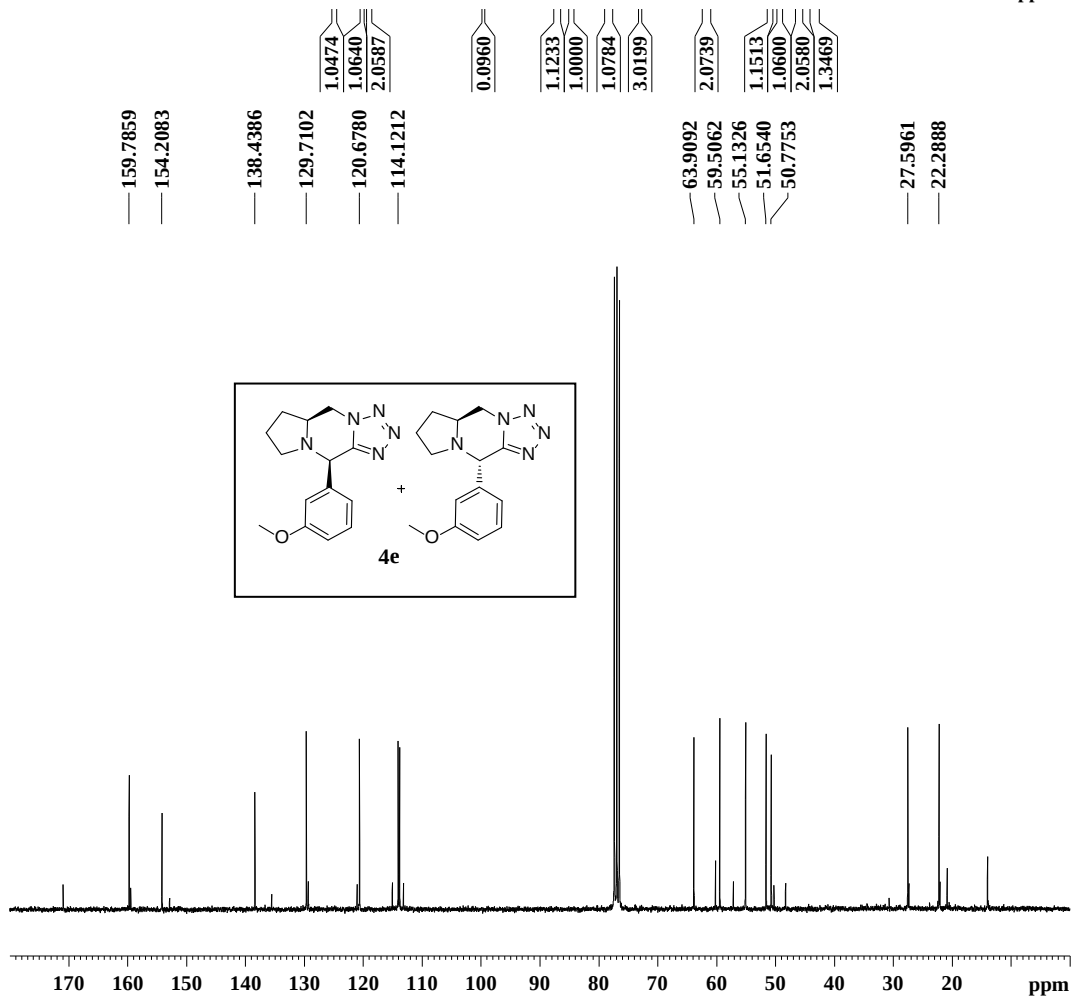
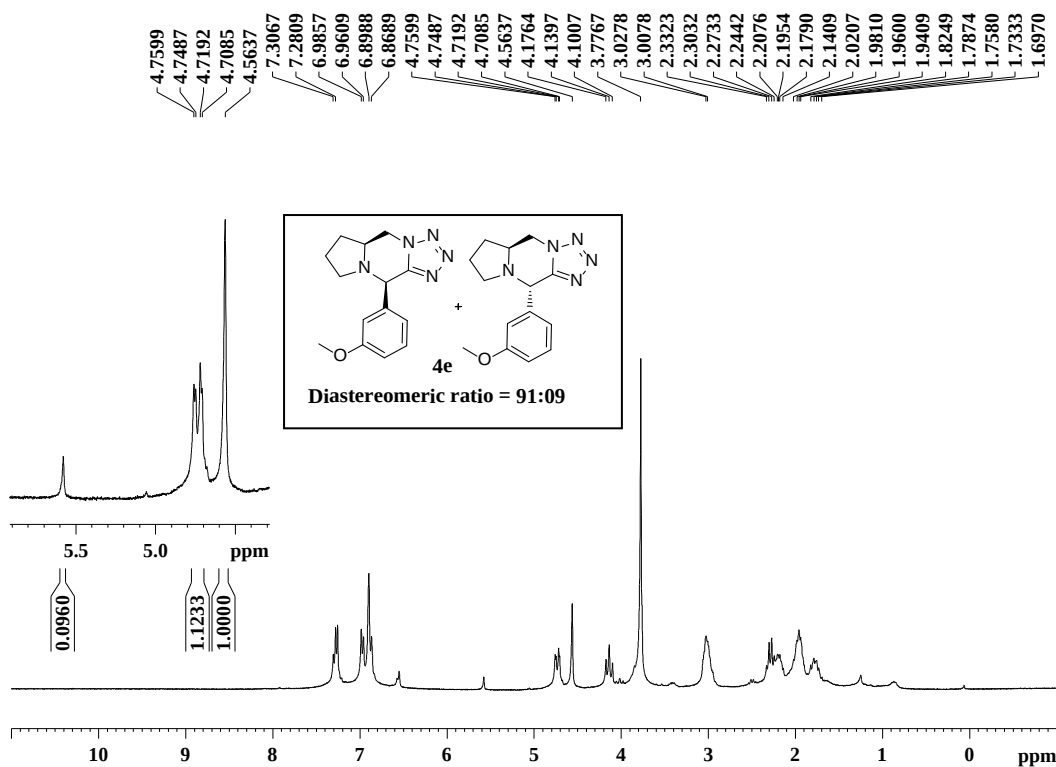
F2 - Acquisition Parameters
Date_ 20140108
Time 10.53
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1310
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

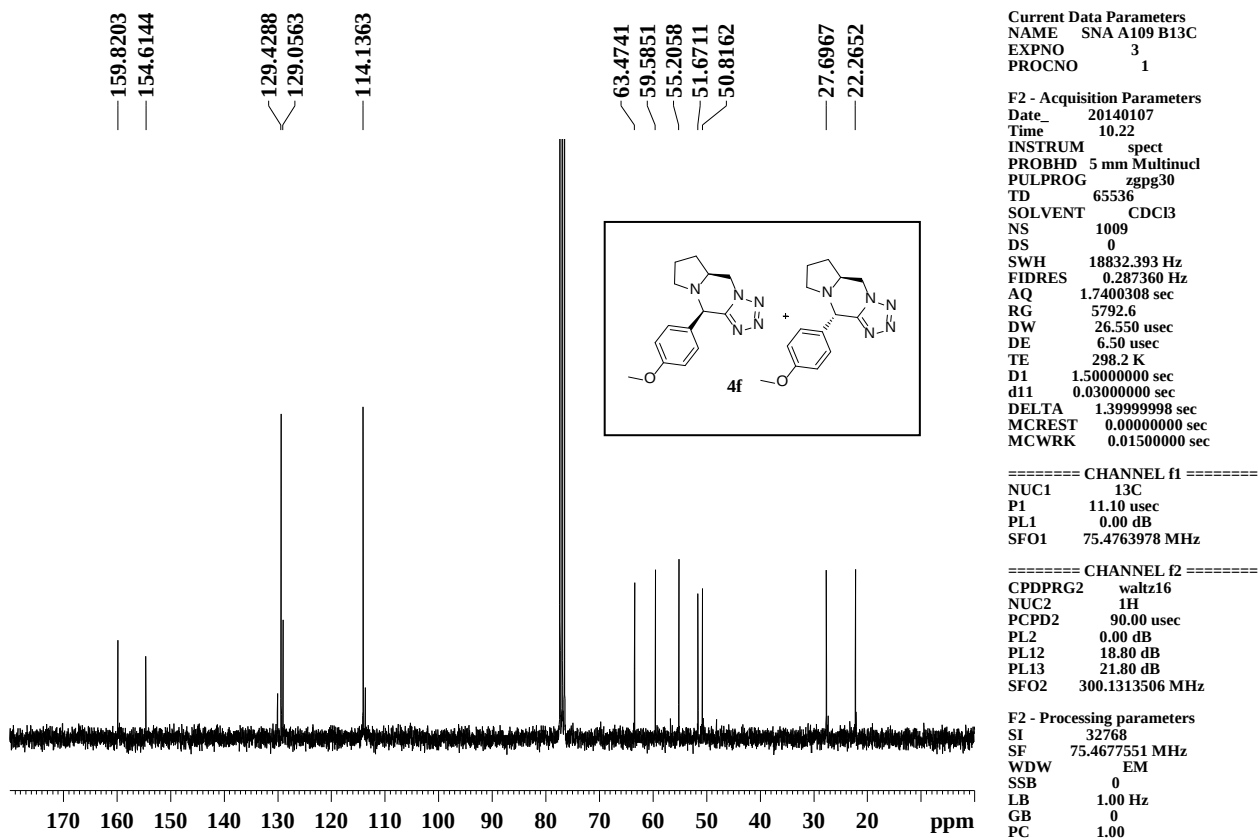
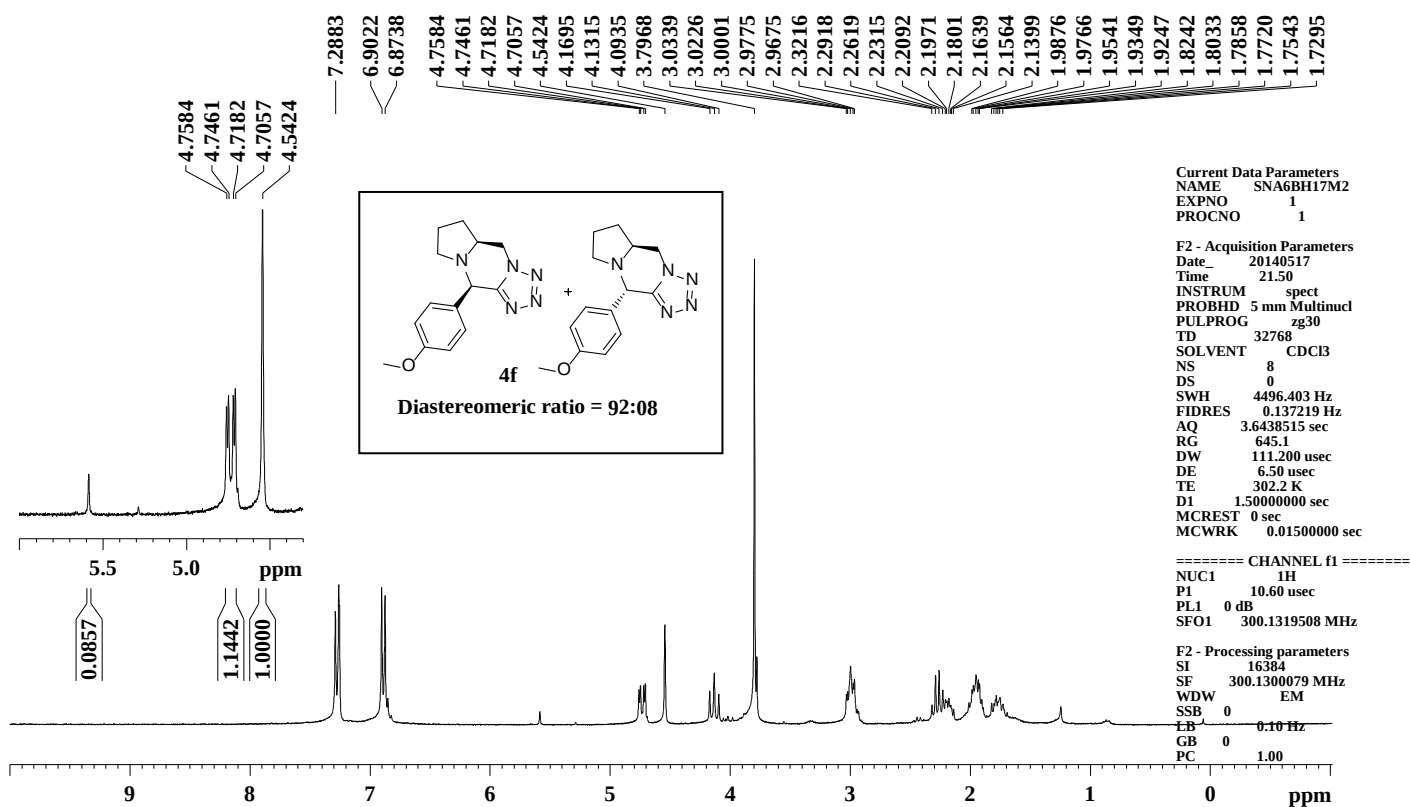
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

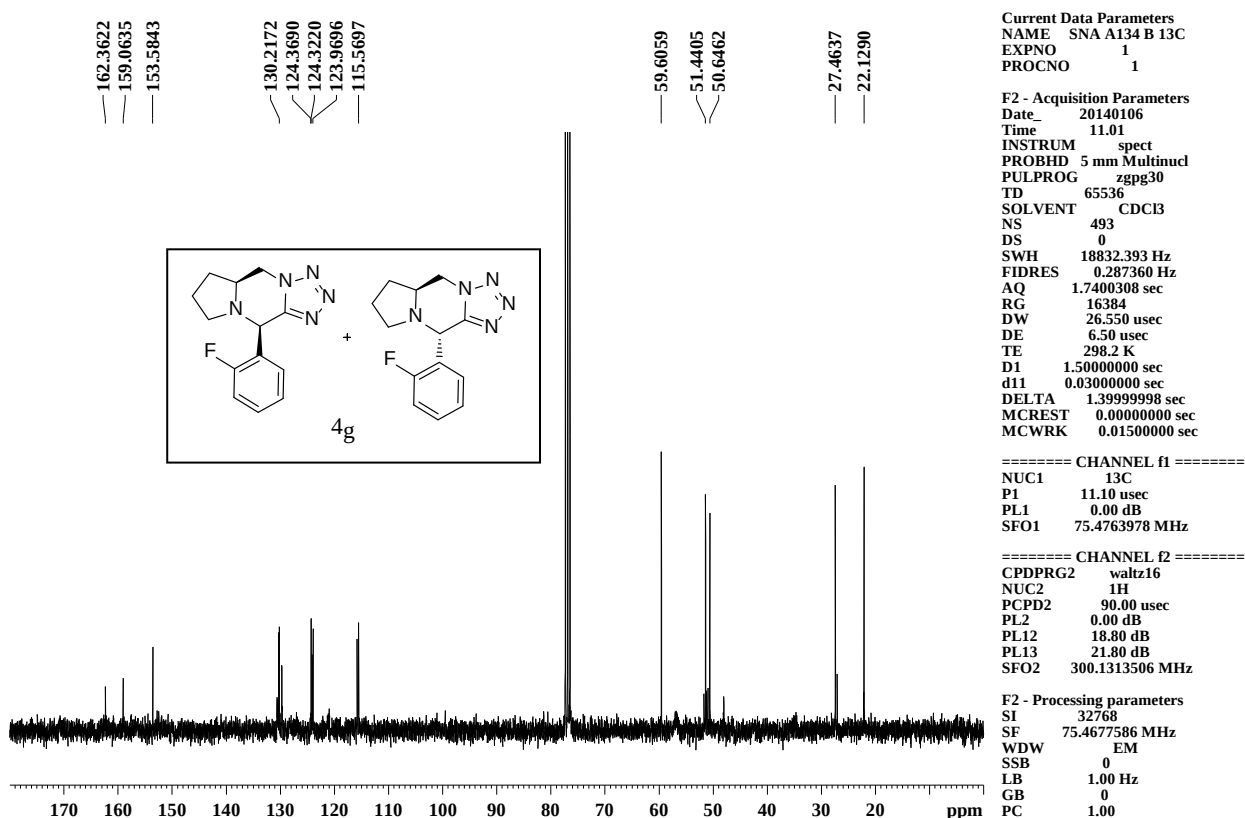
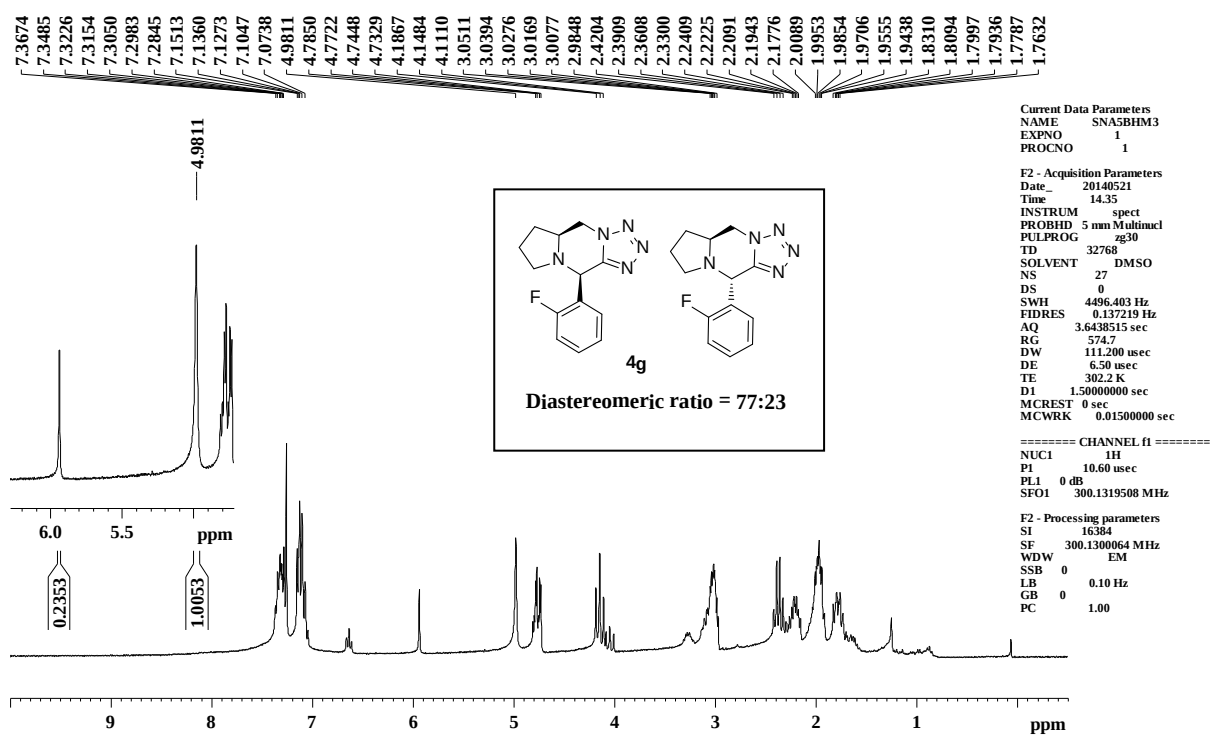
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

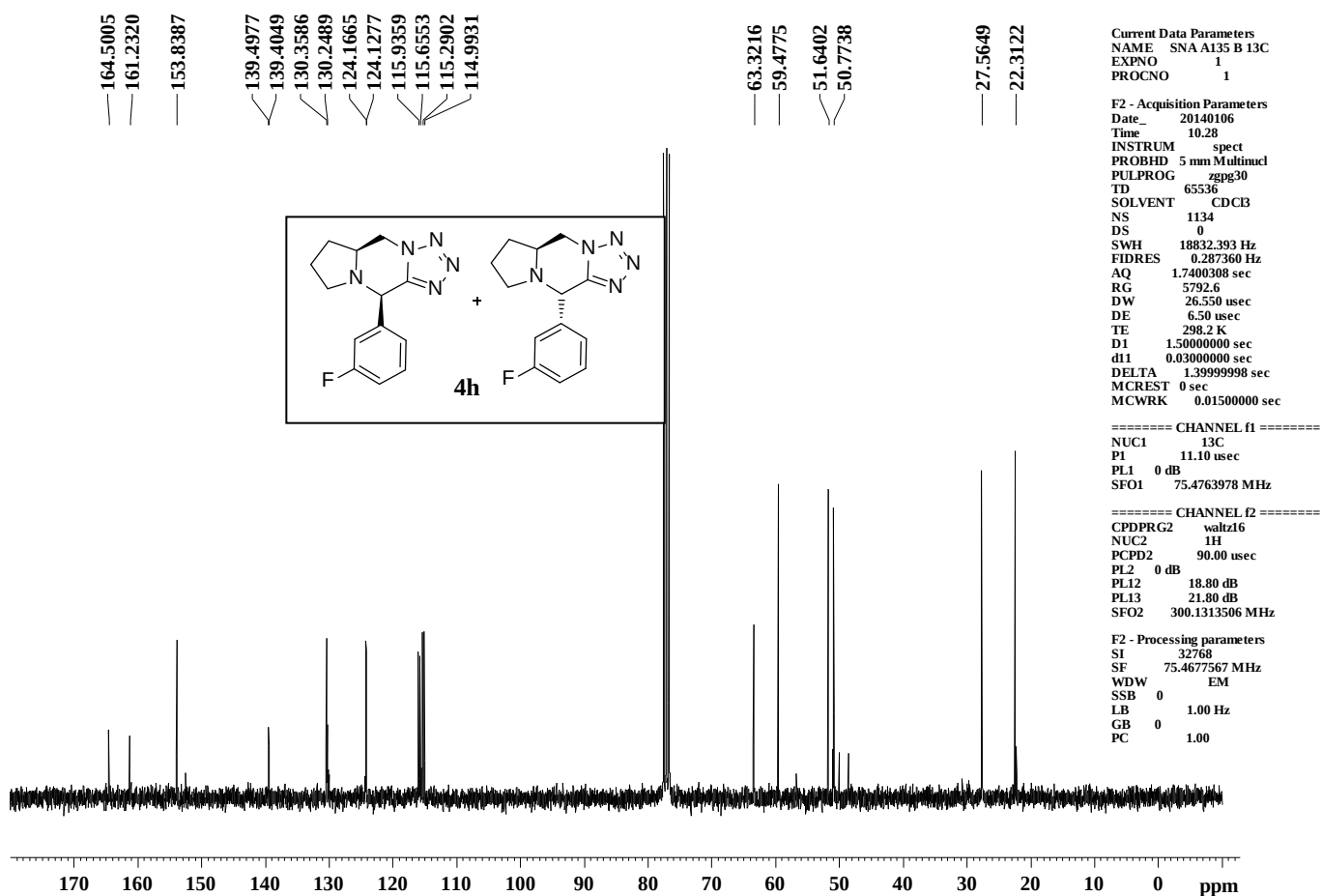
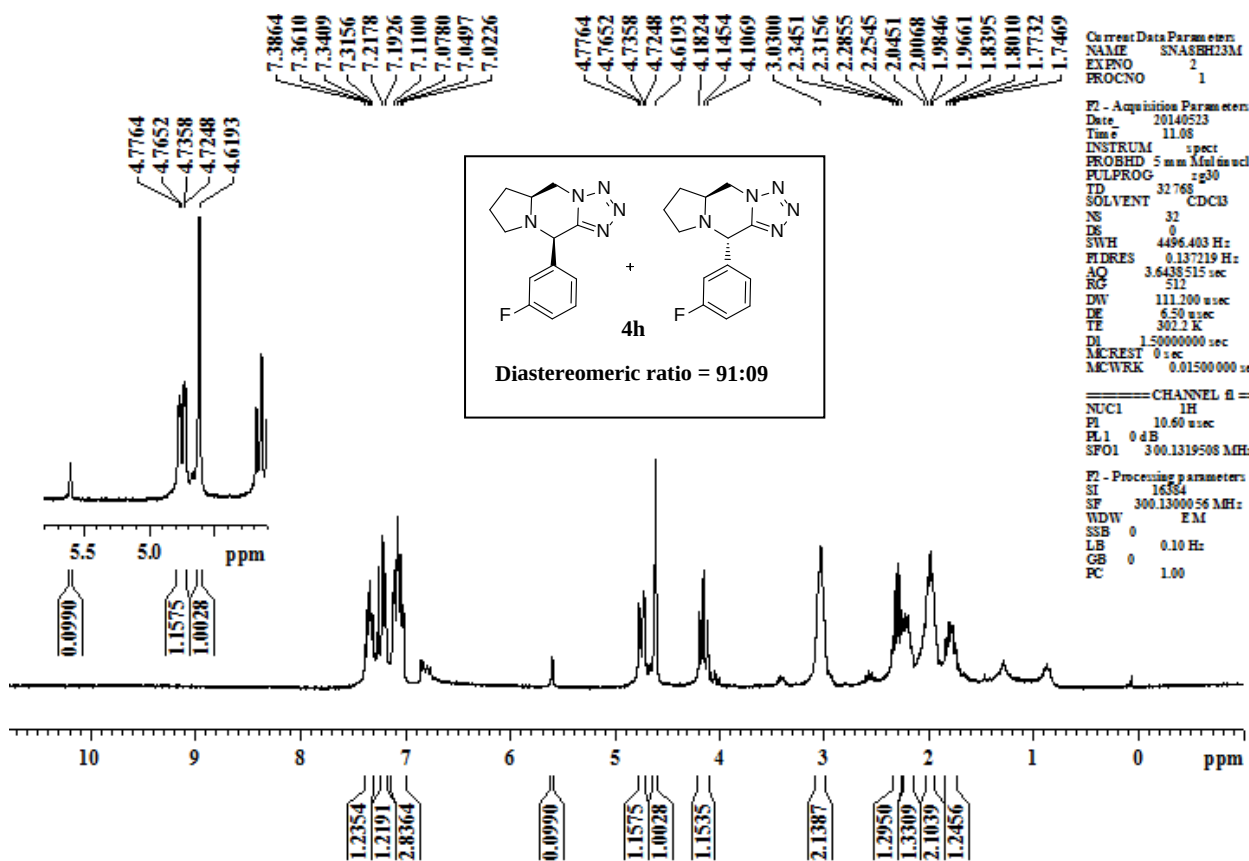
F2 - Processing parameters
SI 32768
SF 75.4677574 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

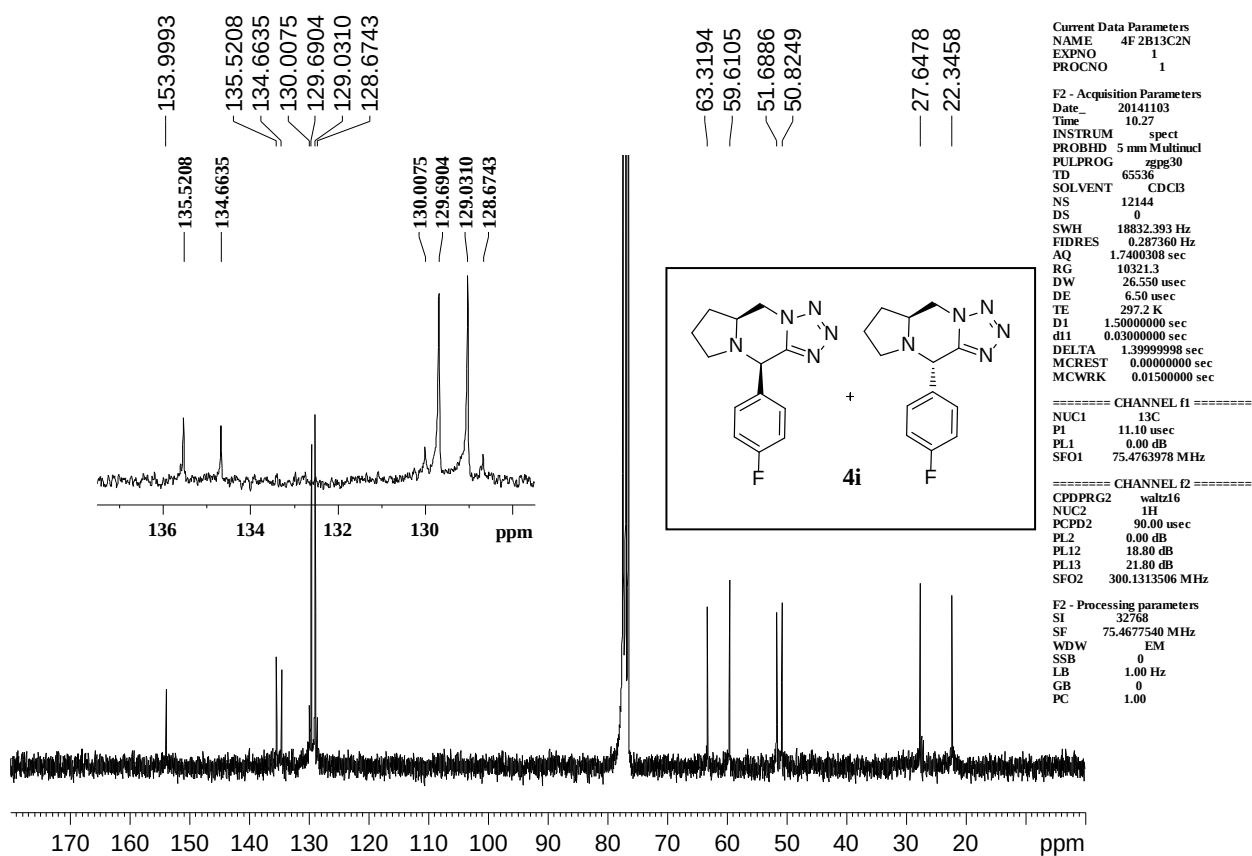
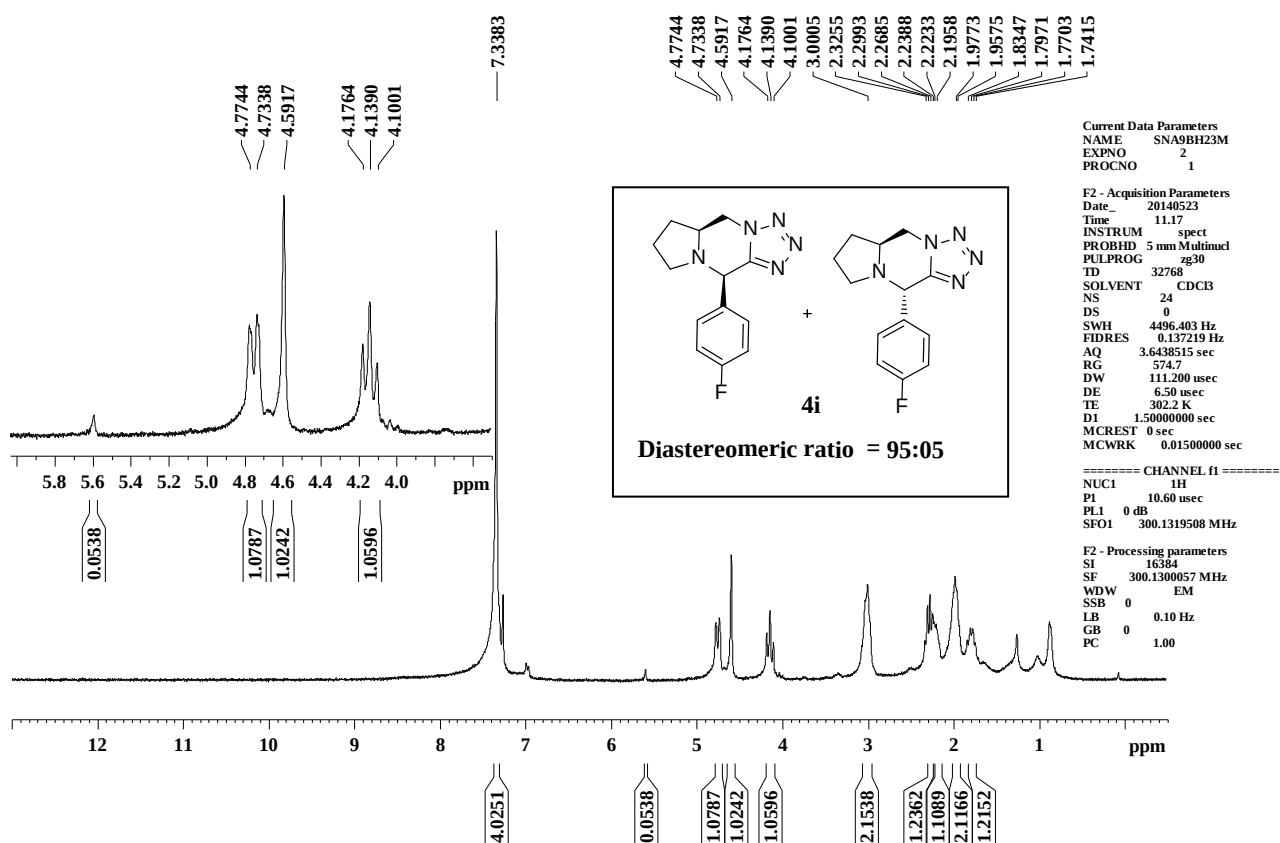


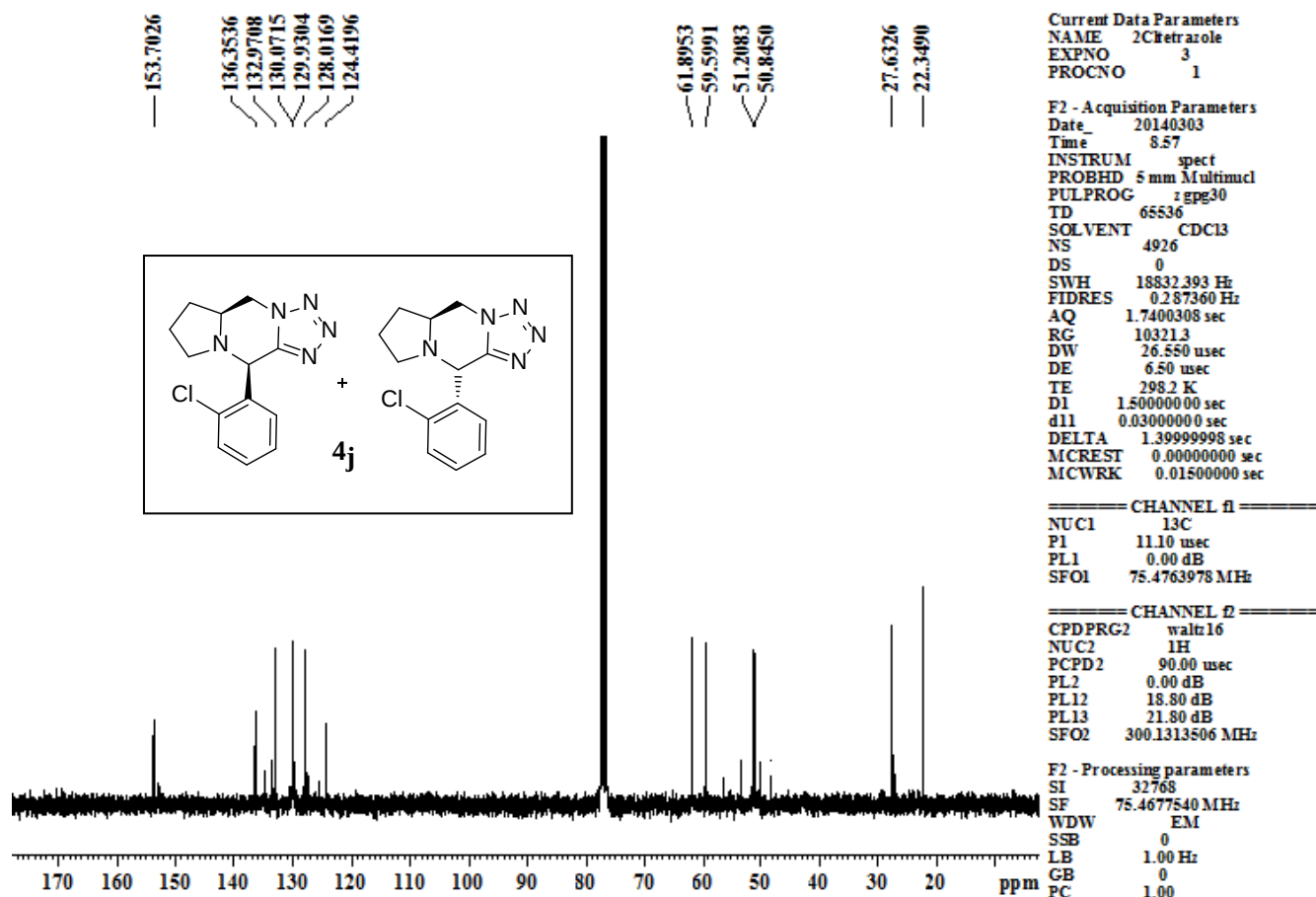
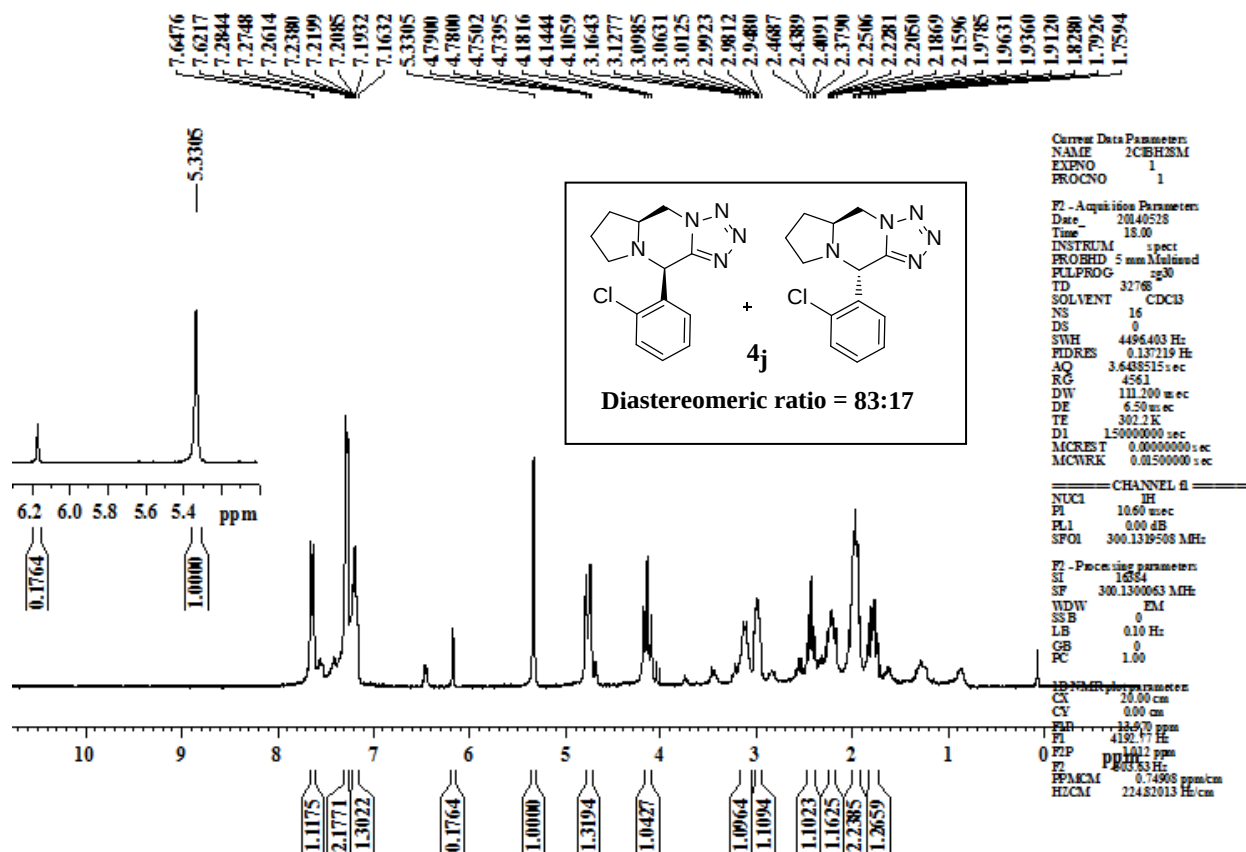


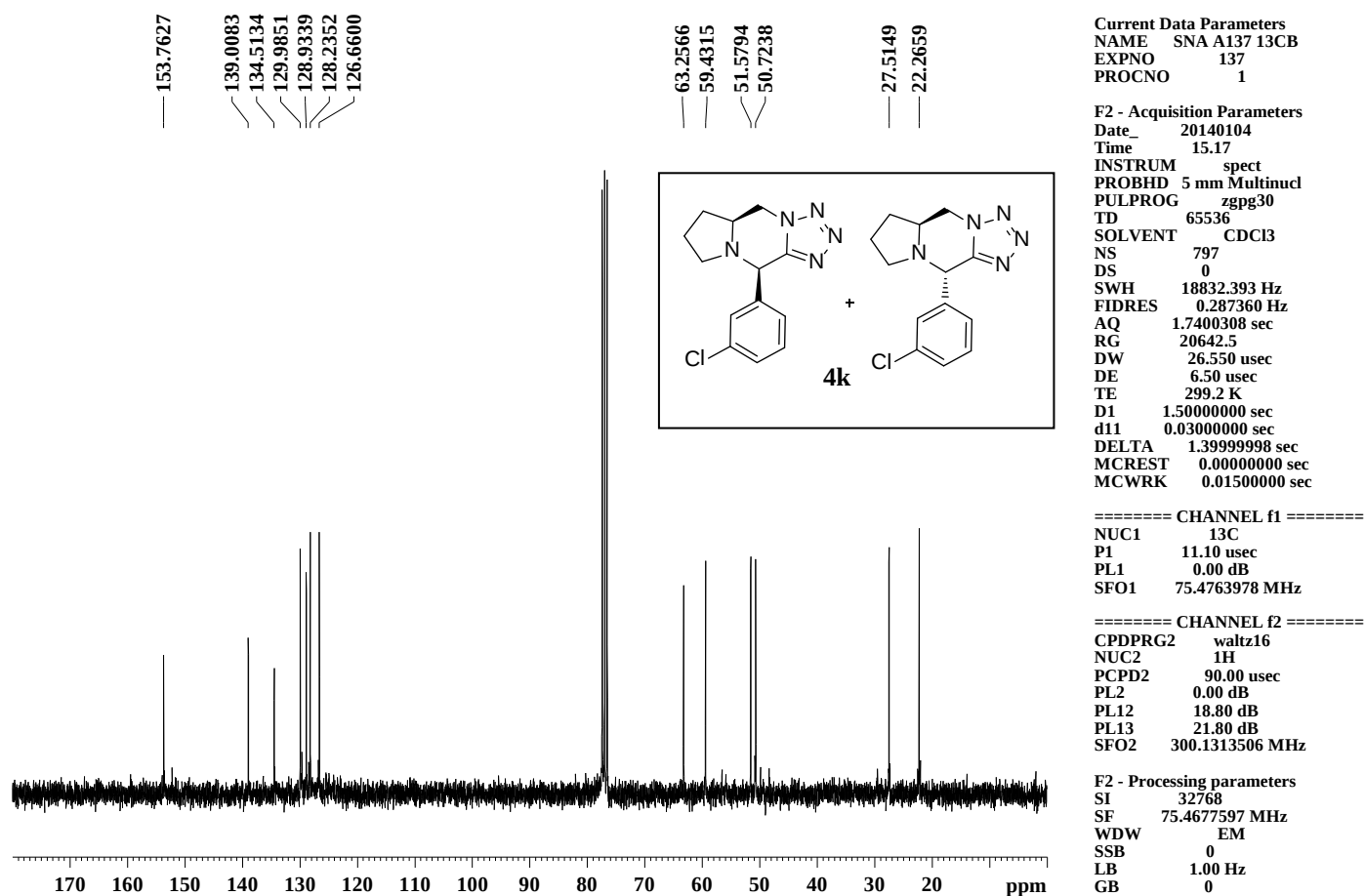
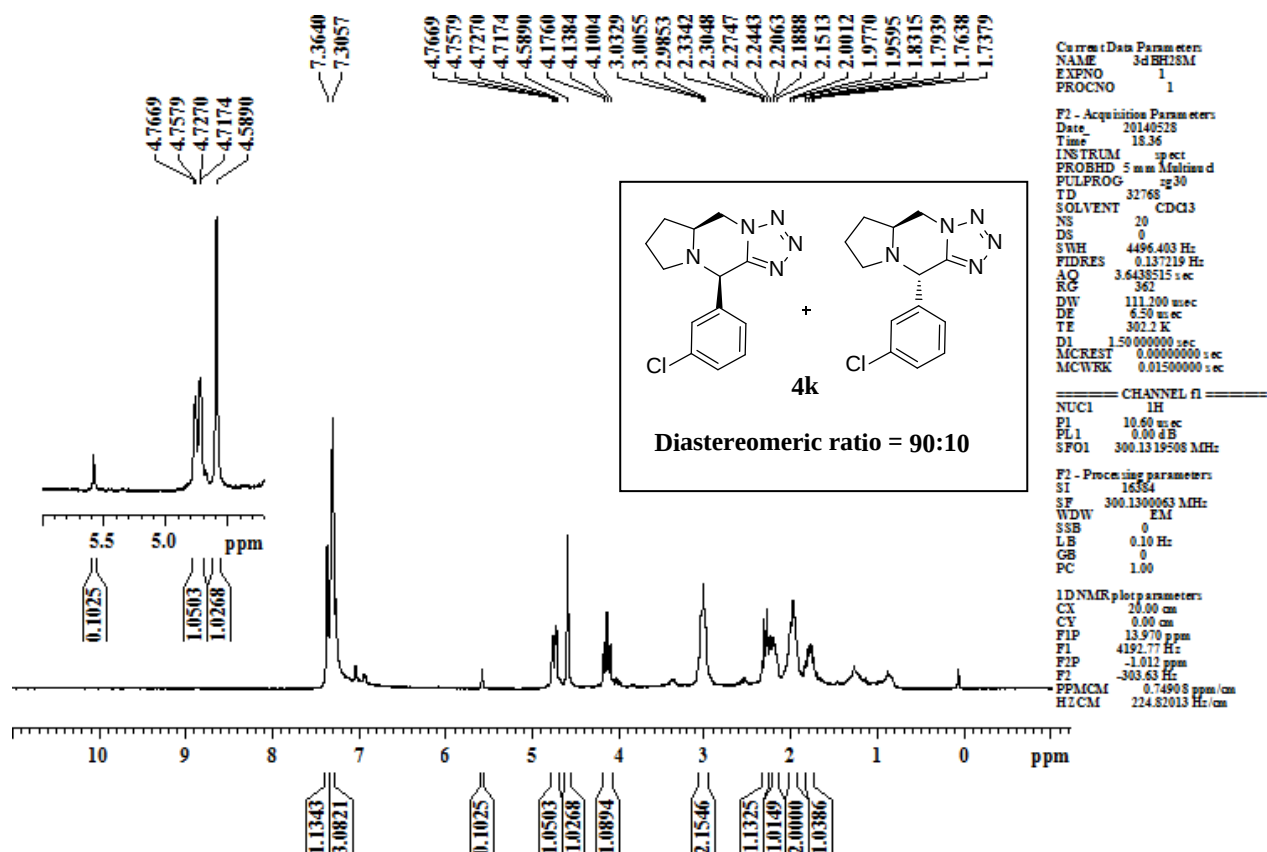


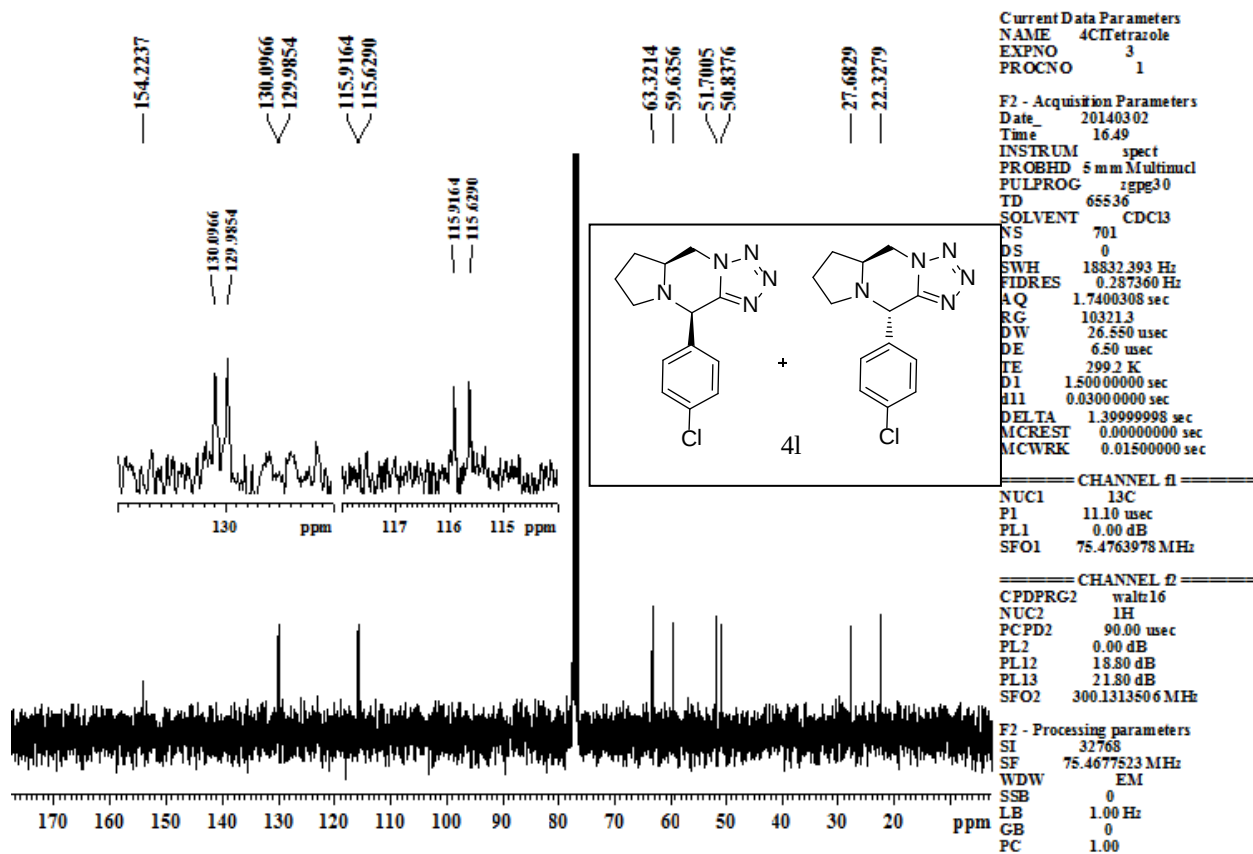
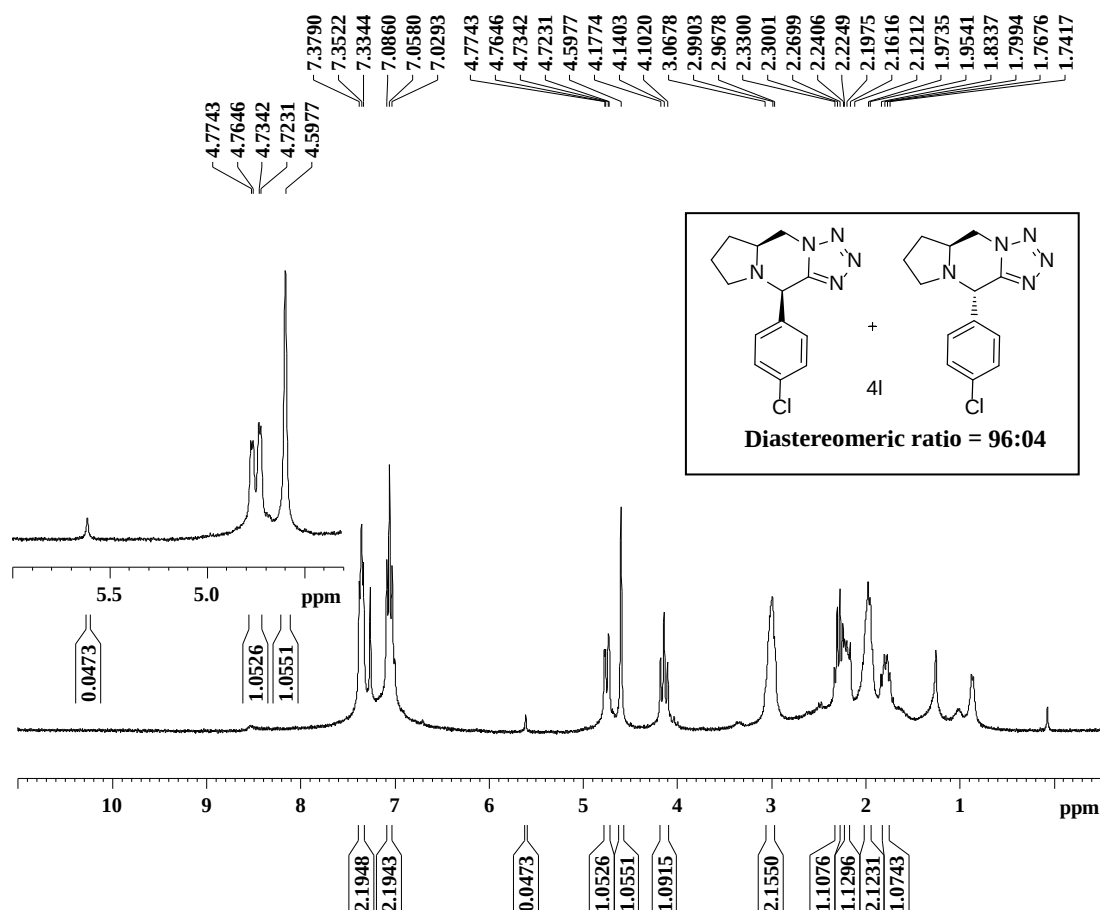


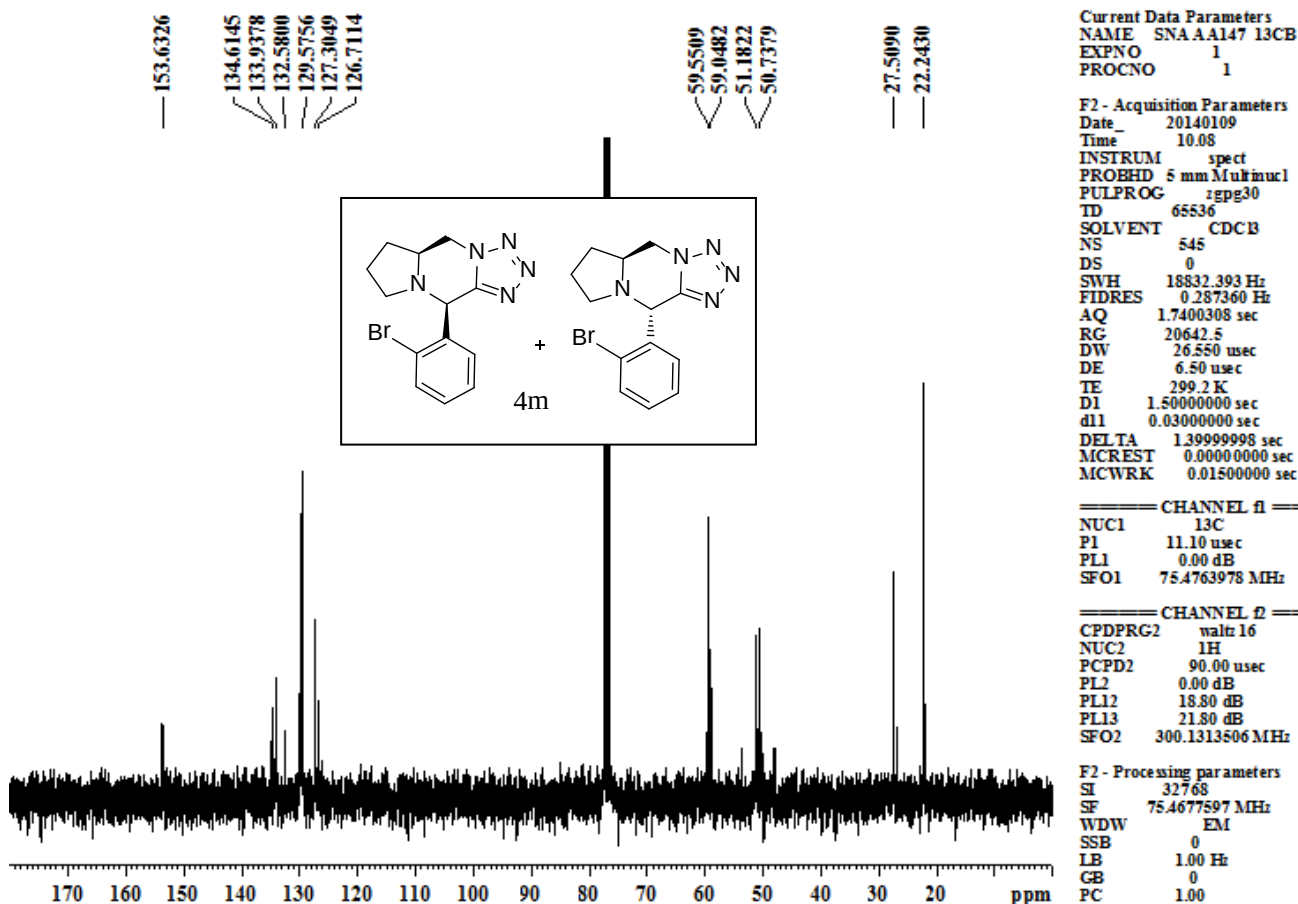
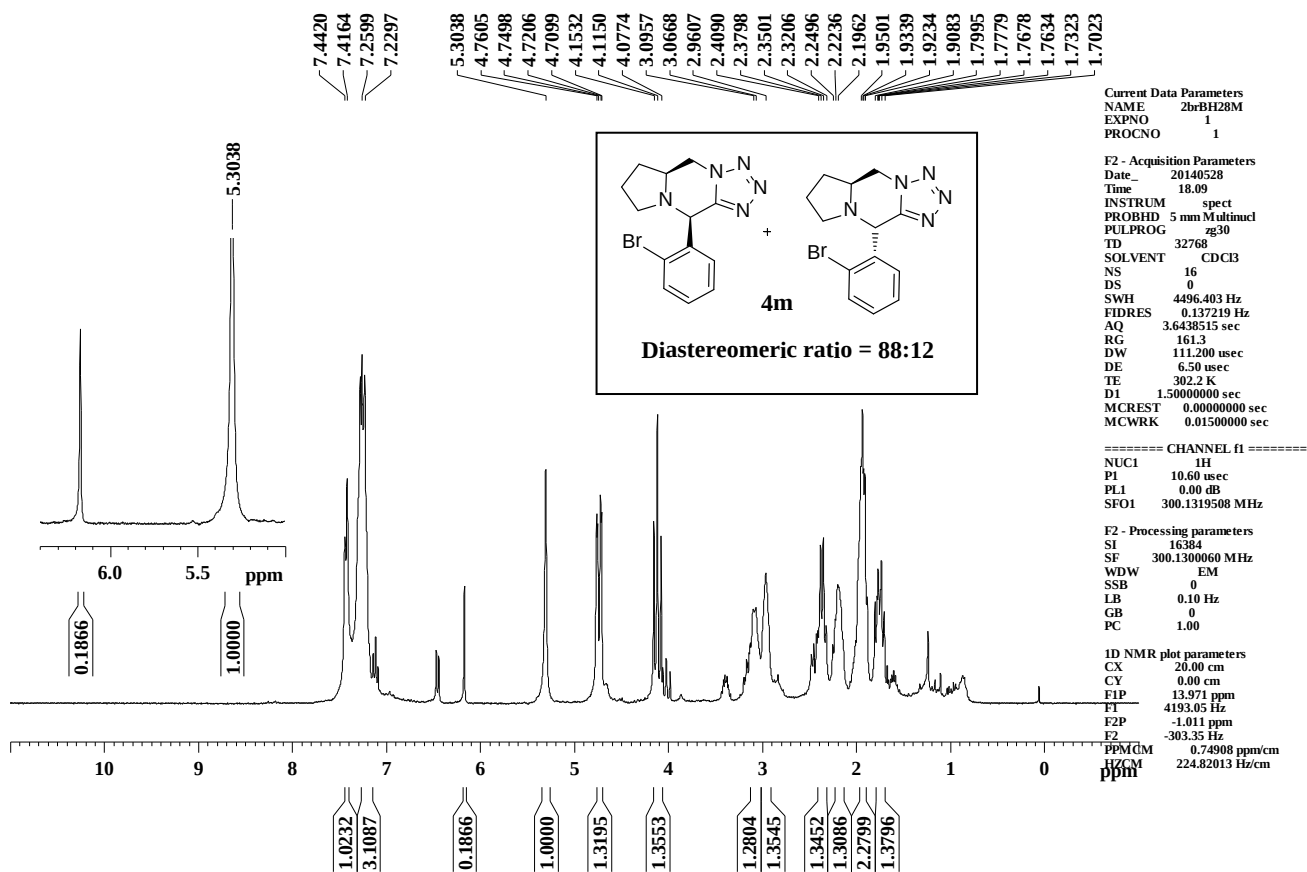


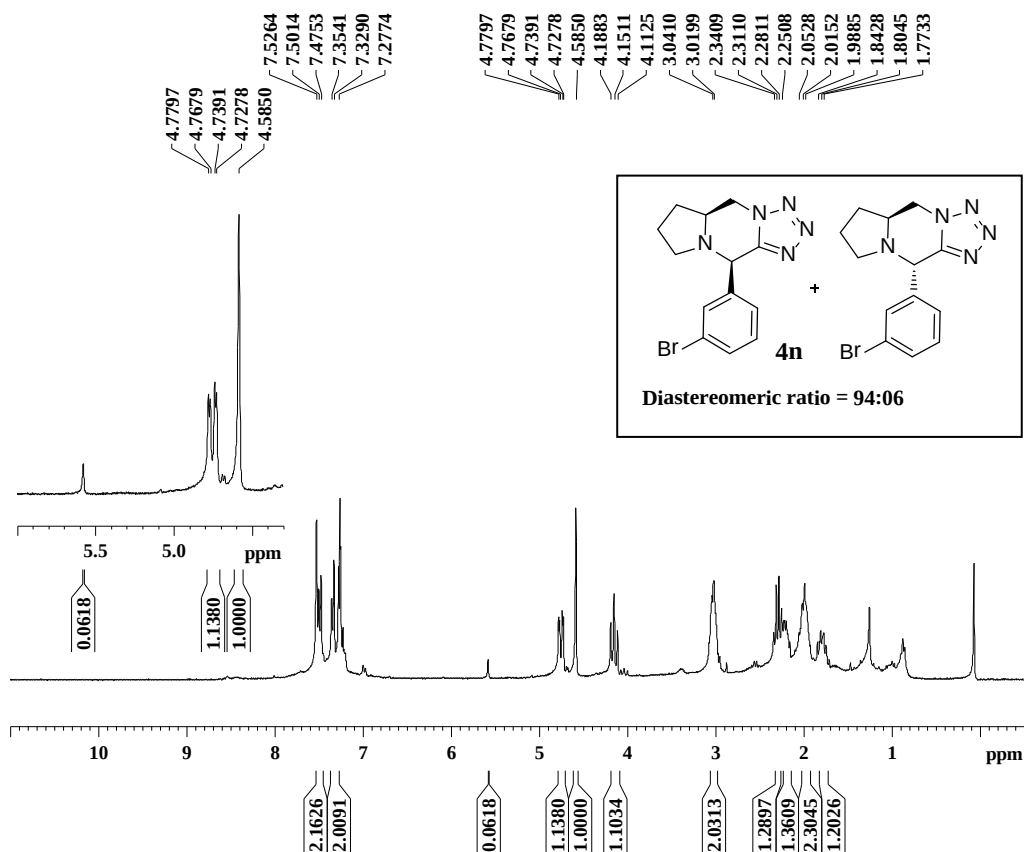












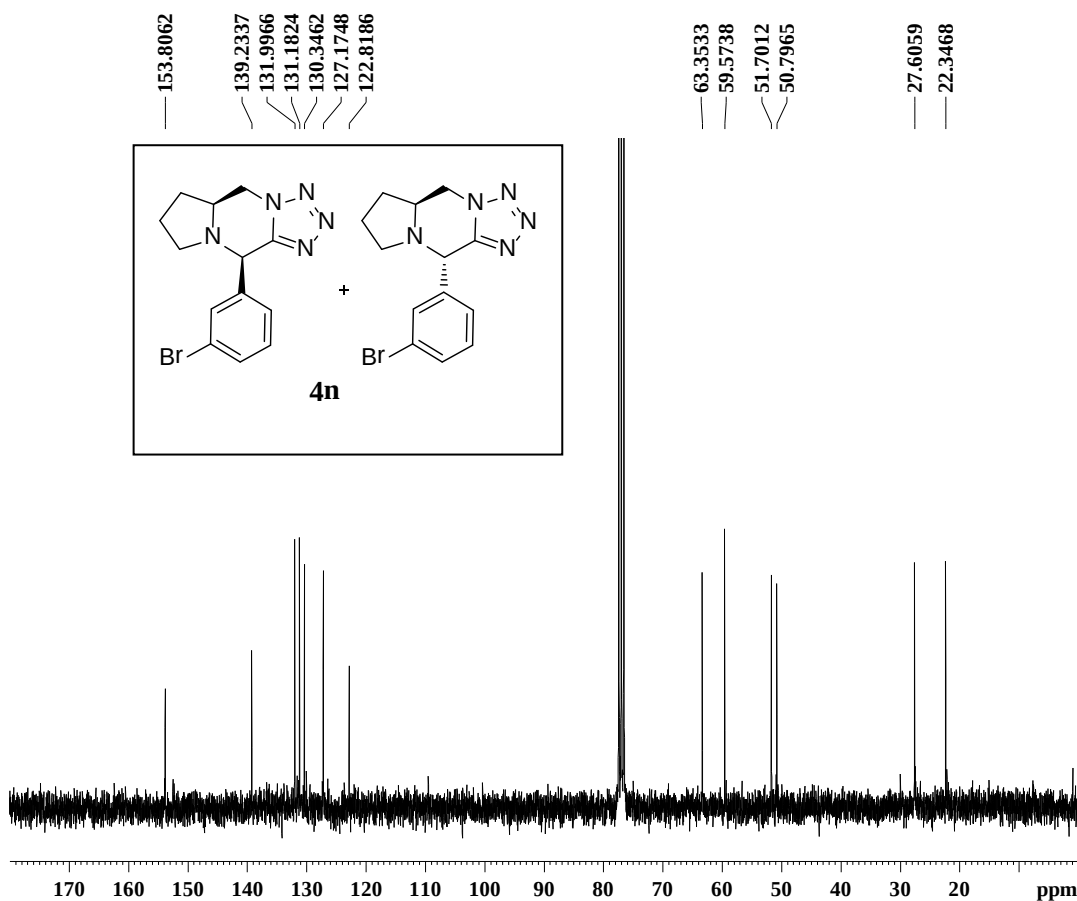
Current Data Parameters
NAME SNA 14BH23M3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140523
Time 14.56
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 36
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 645.1
DW 111.200 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 13.972 ppm
F1 4193.32 Hz
F2P -1.010 ppm
F2 -303.08 Hz
PPMCM 0.74908 ppm/cm
HZCM 224.82013 Hz/cm



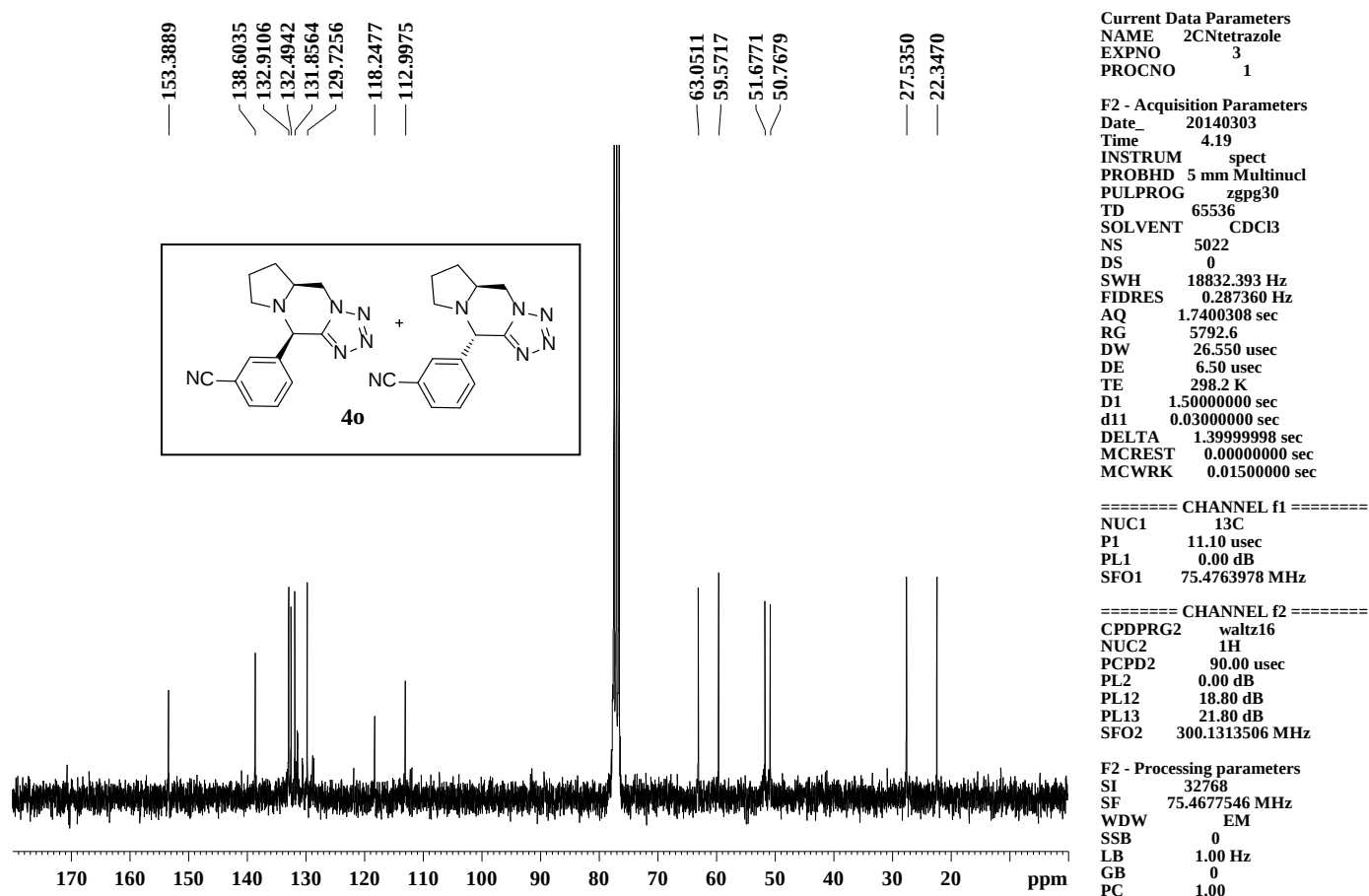
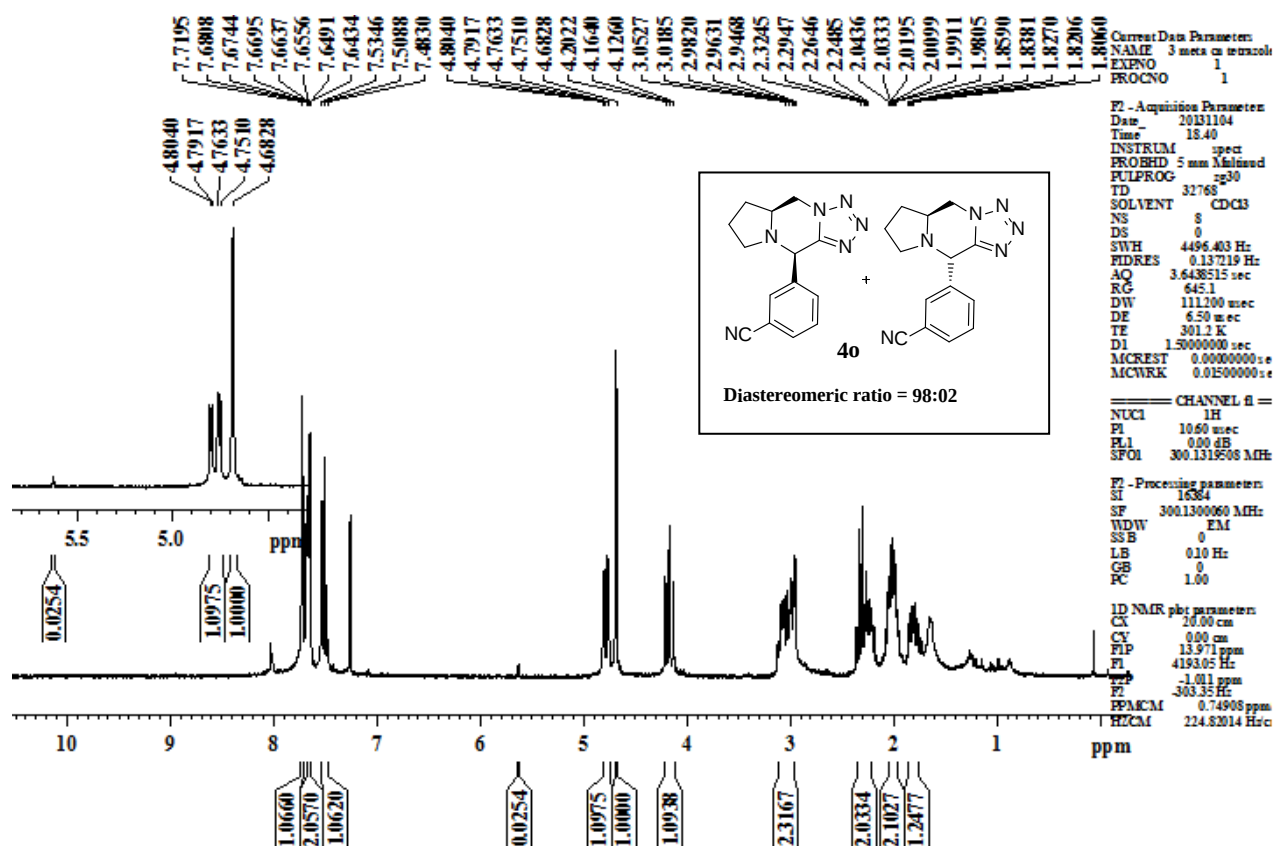
Current Data Parameters
NAME SNA A138 13C B
EXPNO 138
PROCNO 1

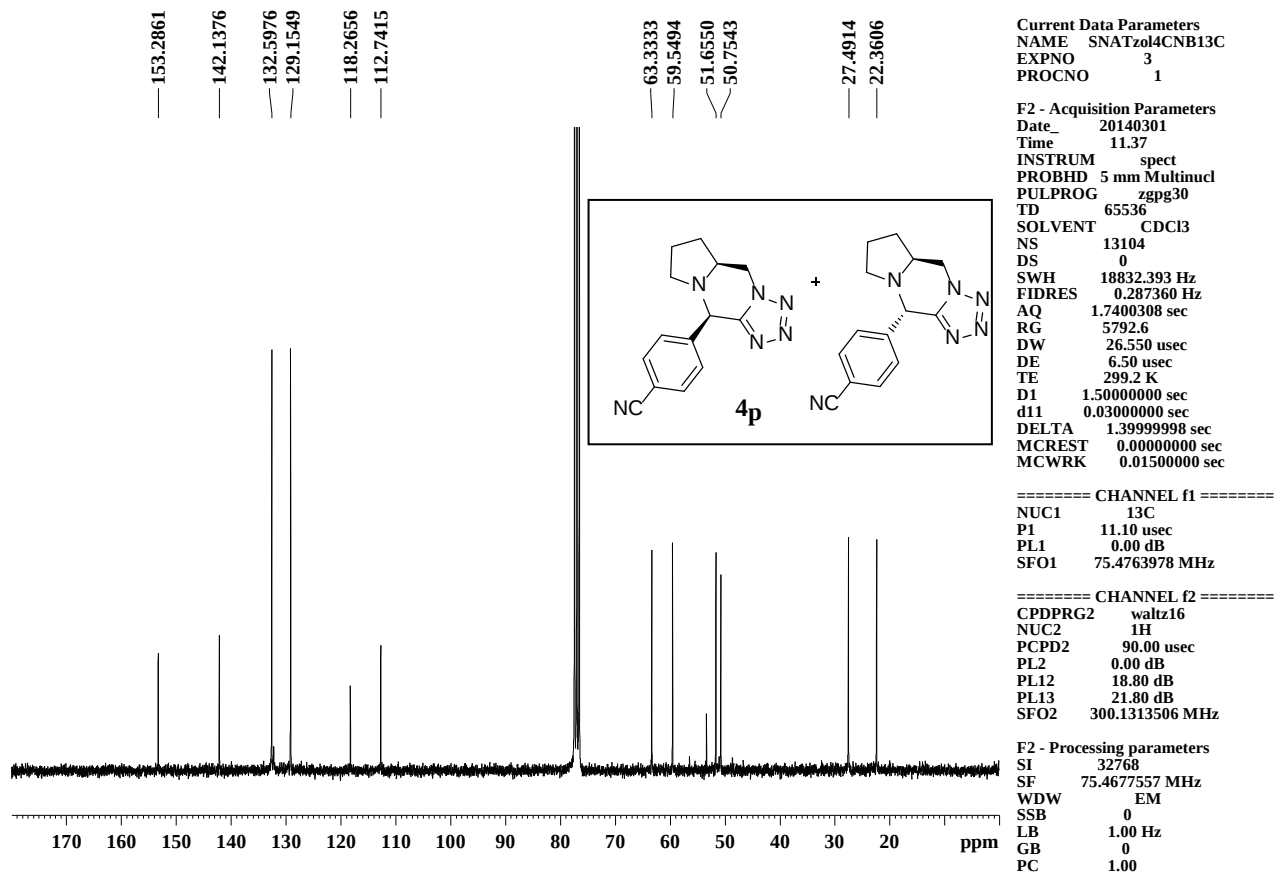
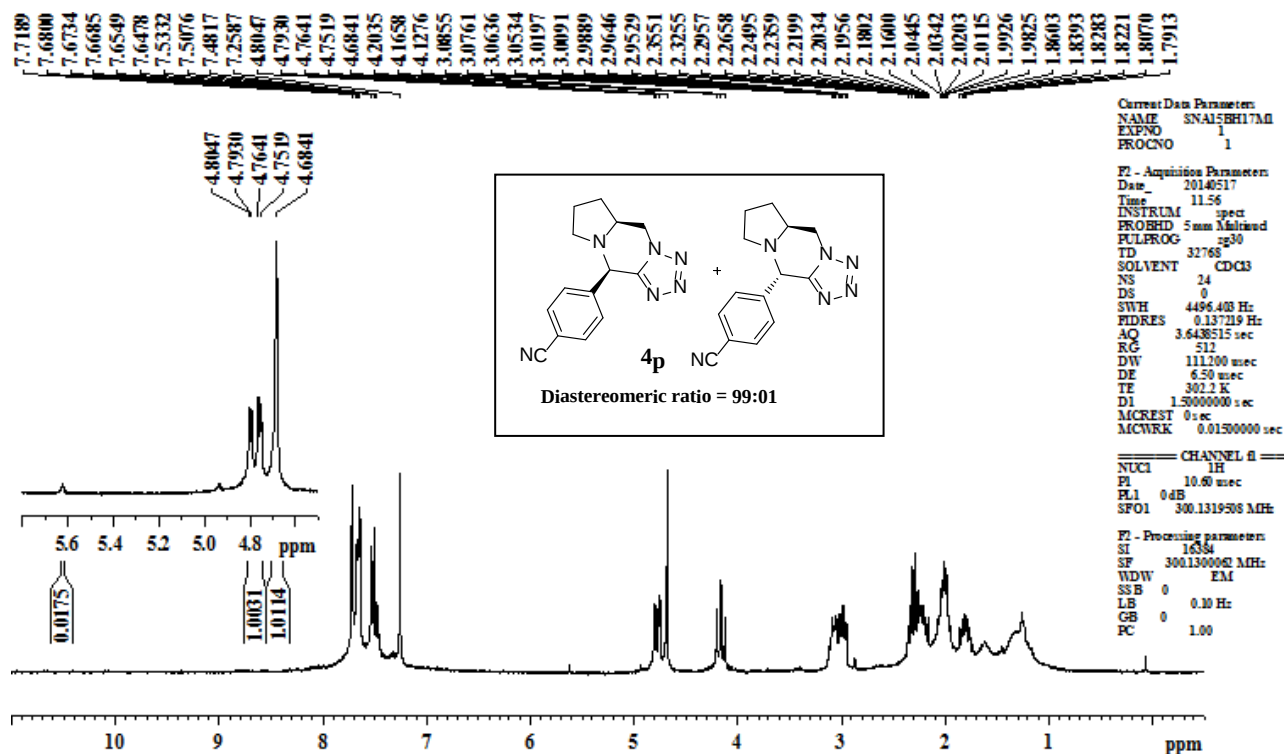
F2 - Acquisition Parameters
Date_ 20140104
Time 18.43
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1440
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

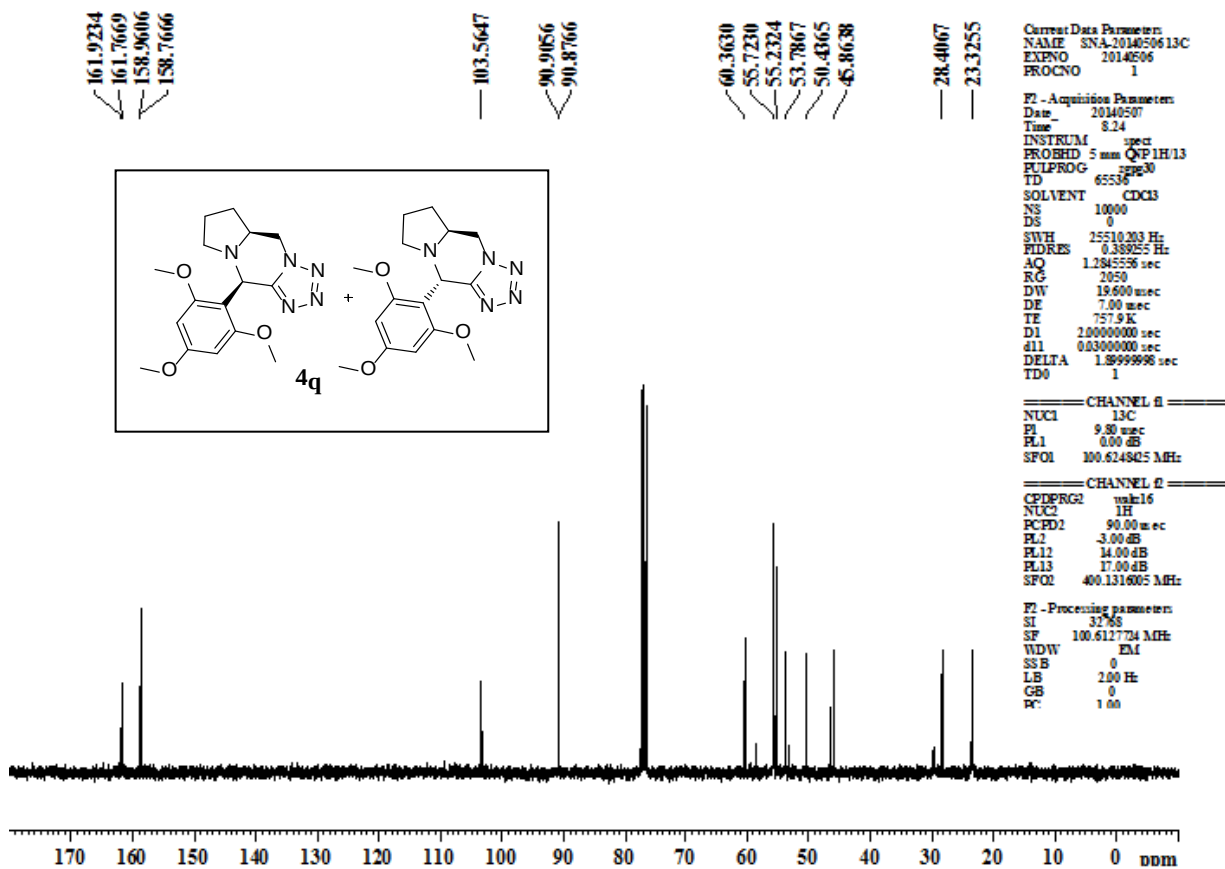
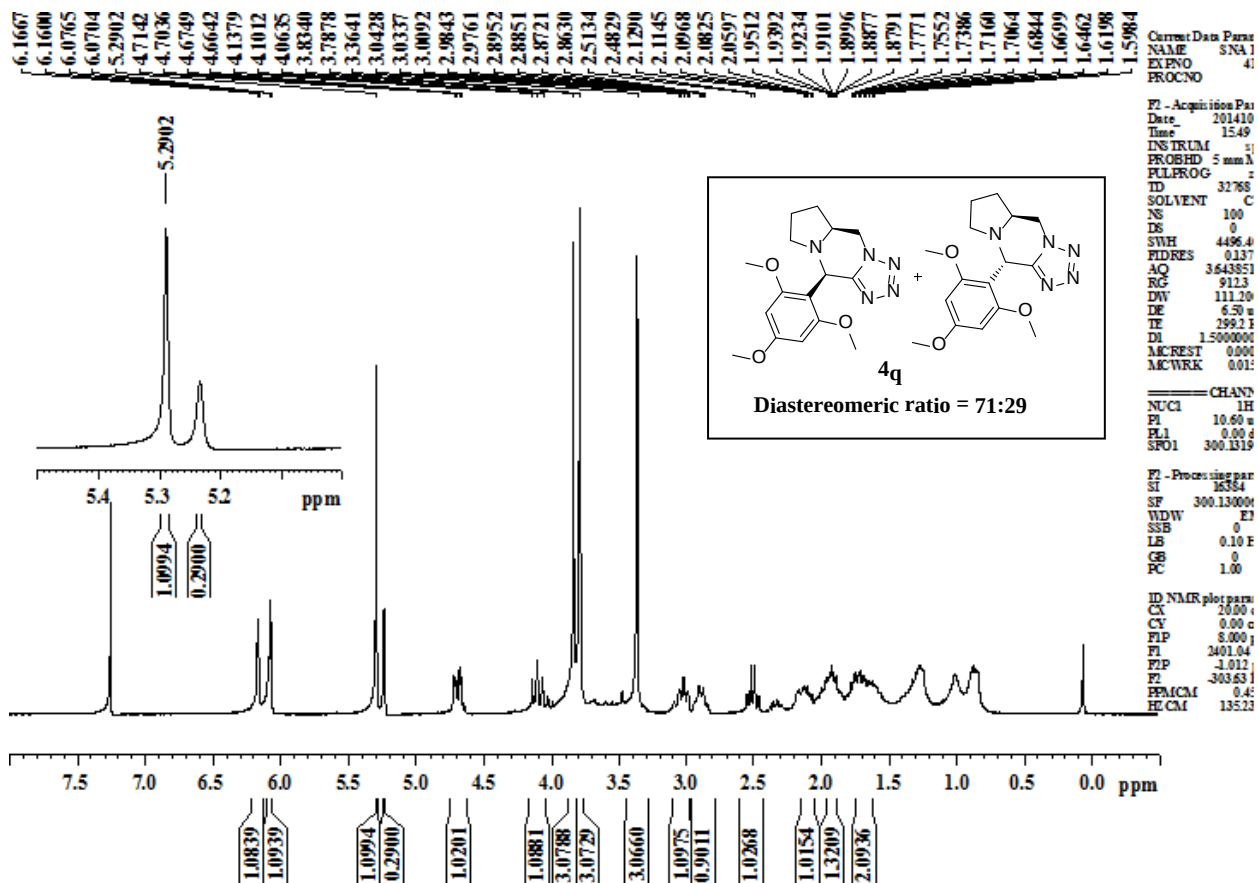
===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

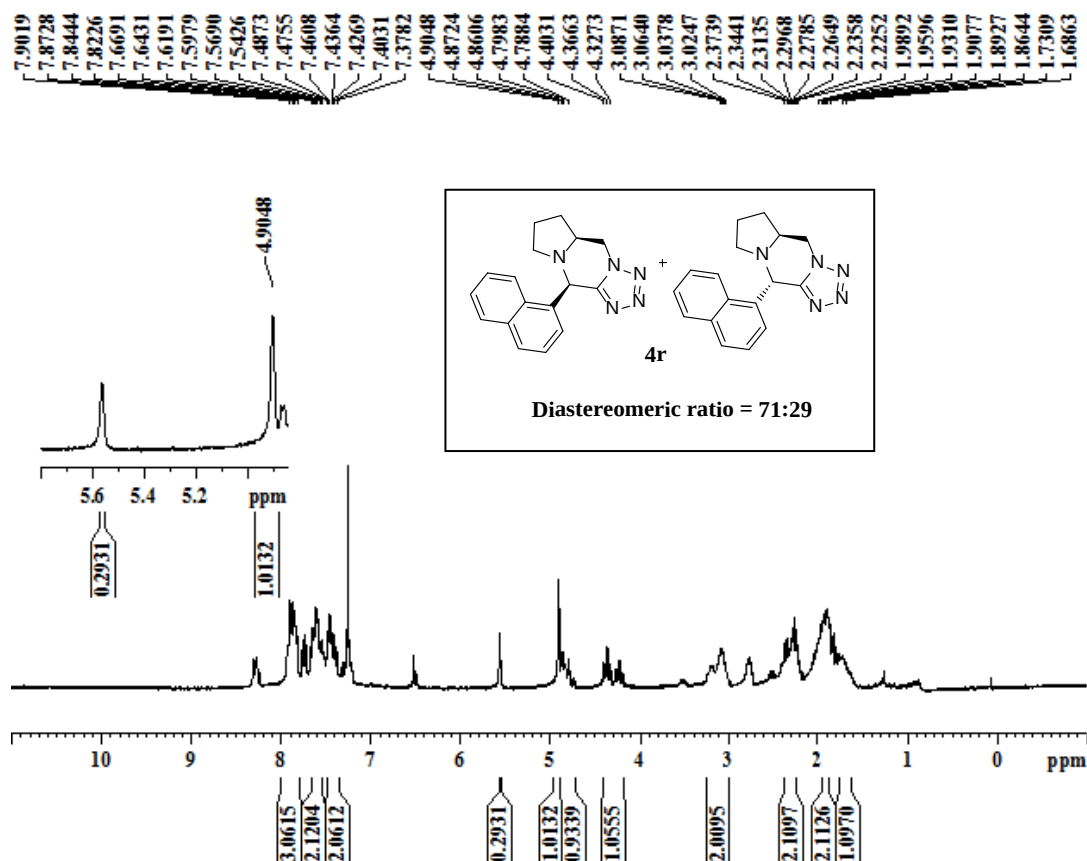
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00







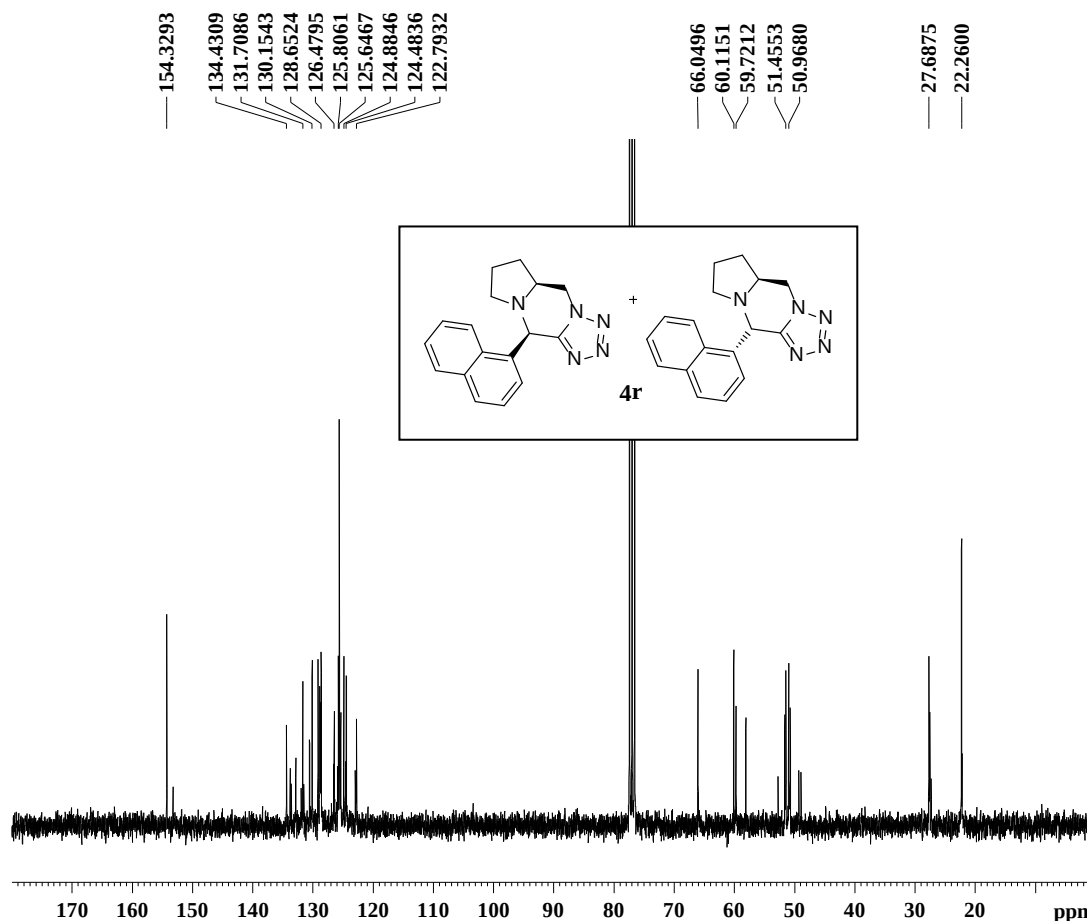


Current Data Parameters
NAME SNA15BH17M
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140517
Time 12.18
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 48
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 724.1
DVI 111.200 usec
DE 6.50 usec
TE 302.2 K
D1 1.50000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 10.60 usec
PL1 0 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



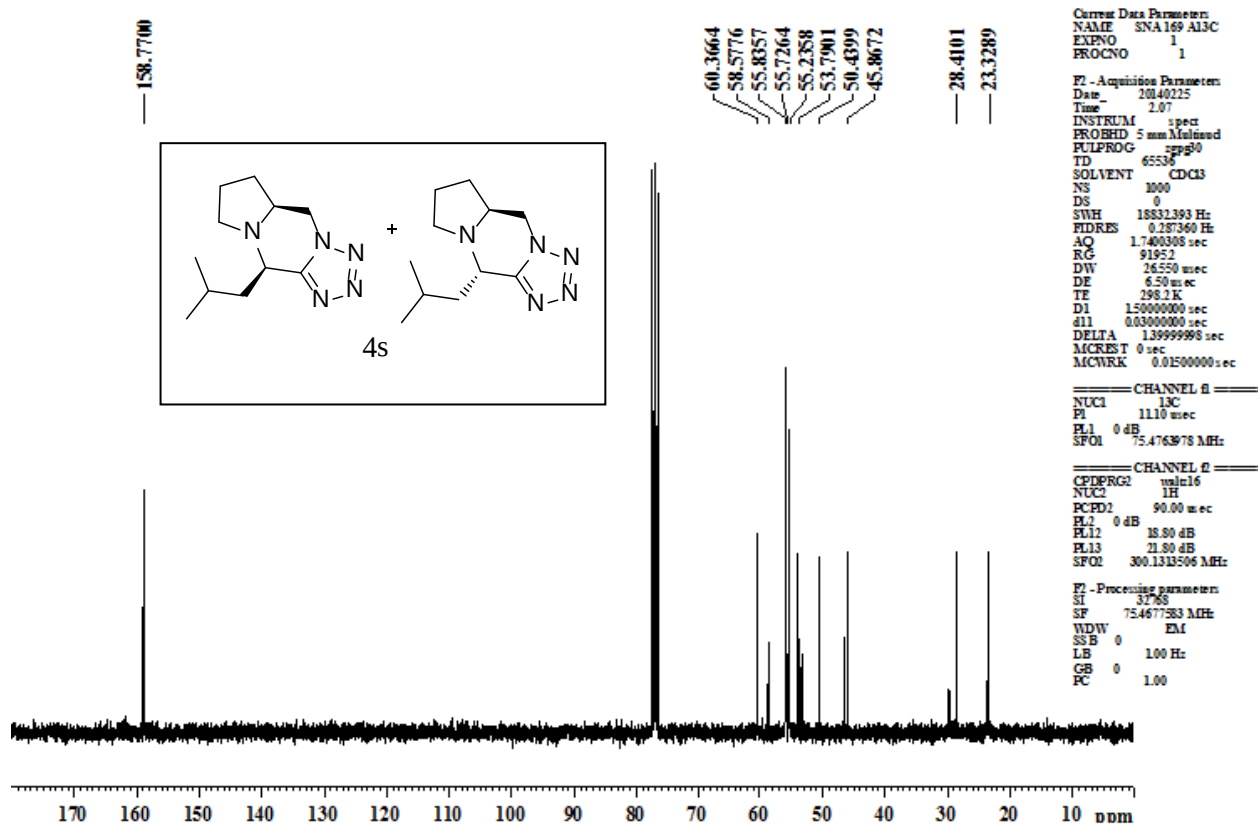
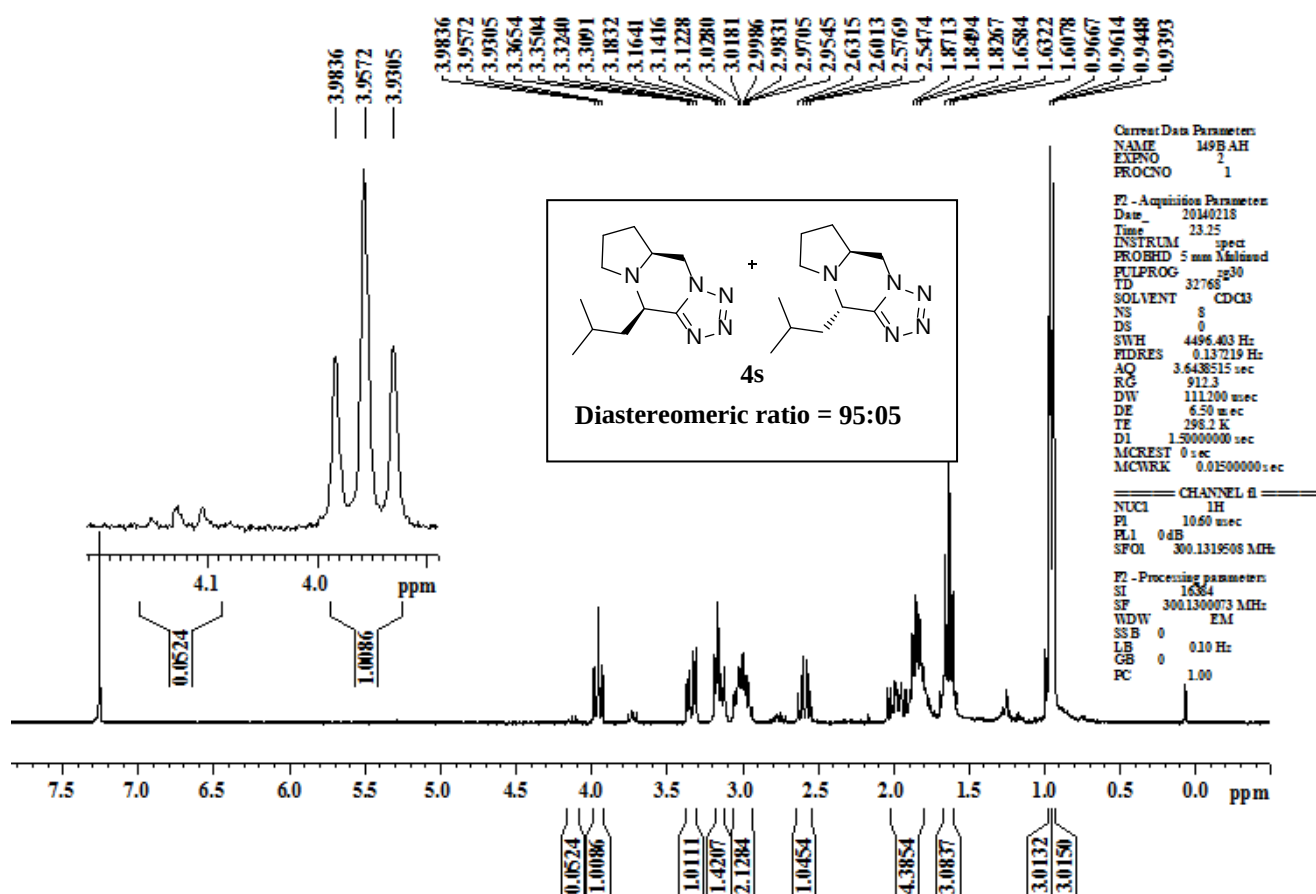
Current Data Parameters
NAME SNA A132A 13CB
EXPNO 132
PROCNO 1

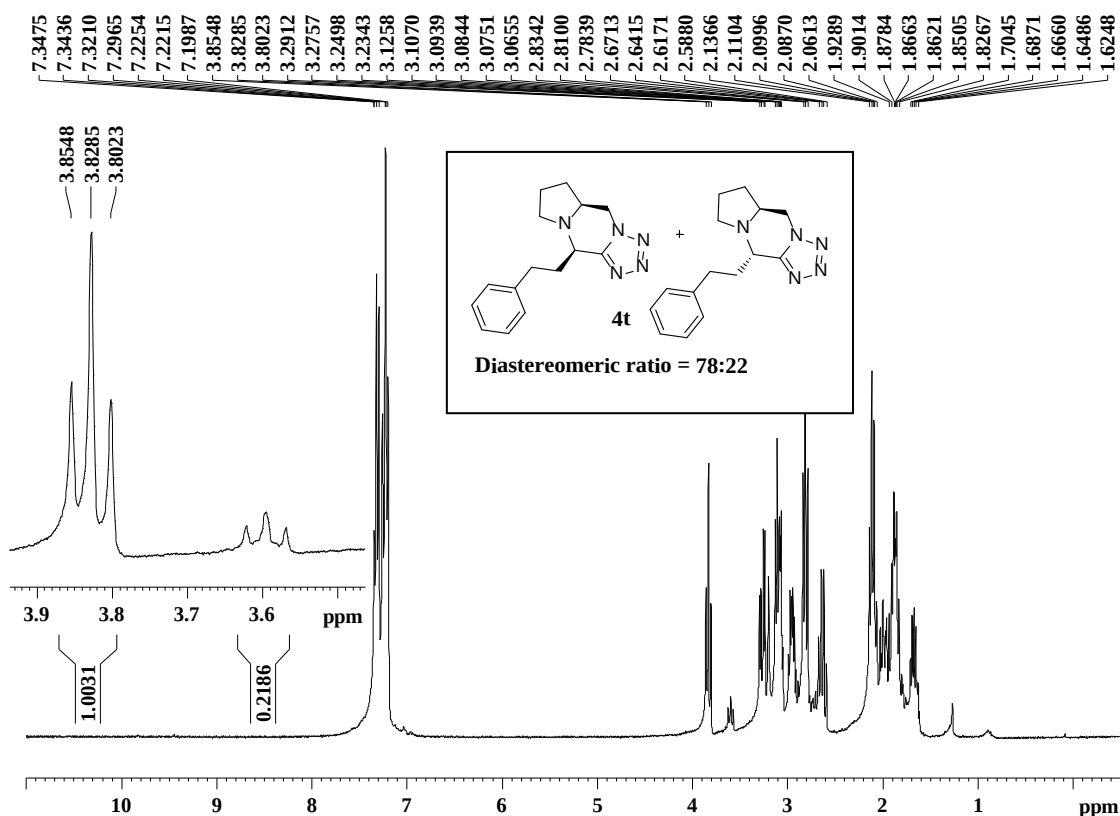
F2 - Acquisition Parameters
Date_ 20140104
Time 14.14
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1194
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677626 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00





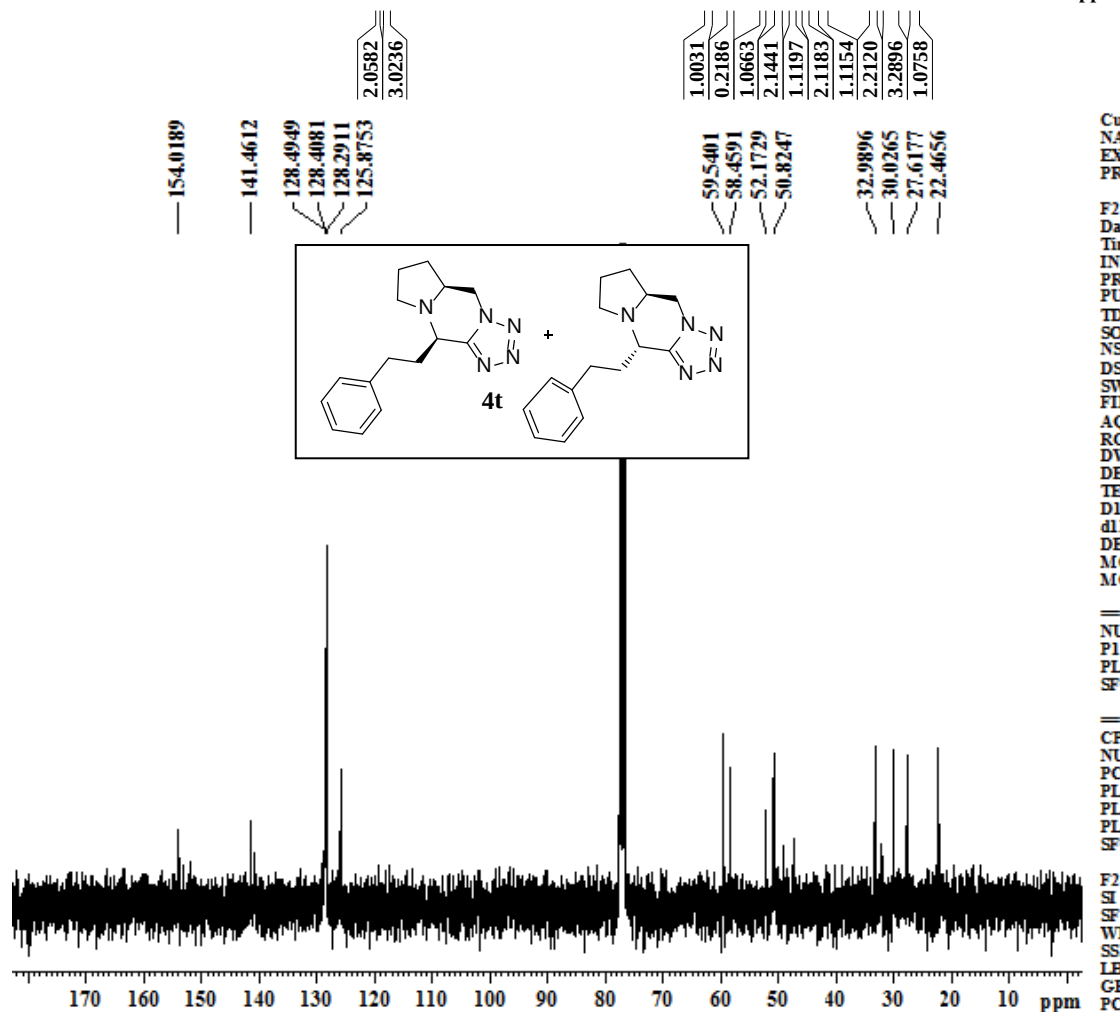
Current Data Parameters
NAME SNA 20AD
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141028
Time 10.04
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 287.4
DW 111.200 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 8.000 ppm
F1 2401.04 Hz
F2P -1.010 ppm
F2 -303.08 Hz
PPMCM 0.45049 ppm/cm
HZCM 135.20598 Hz/cm



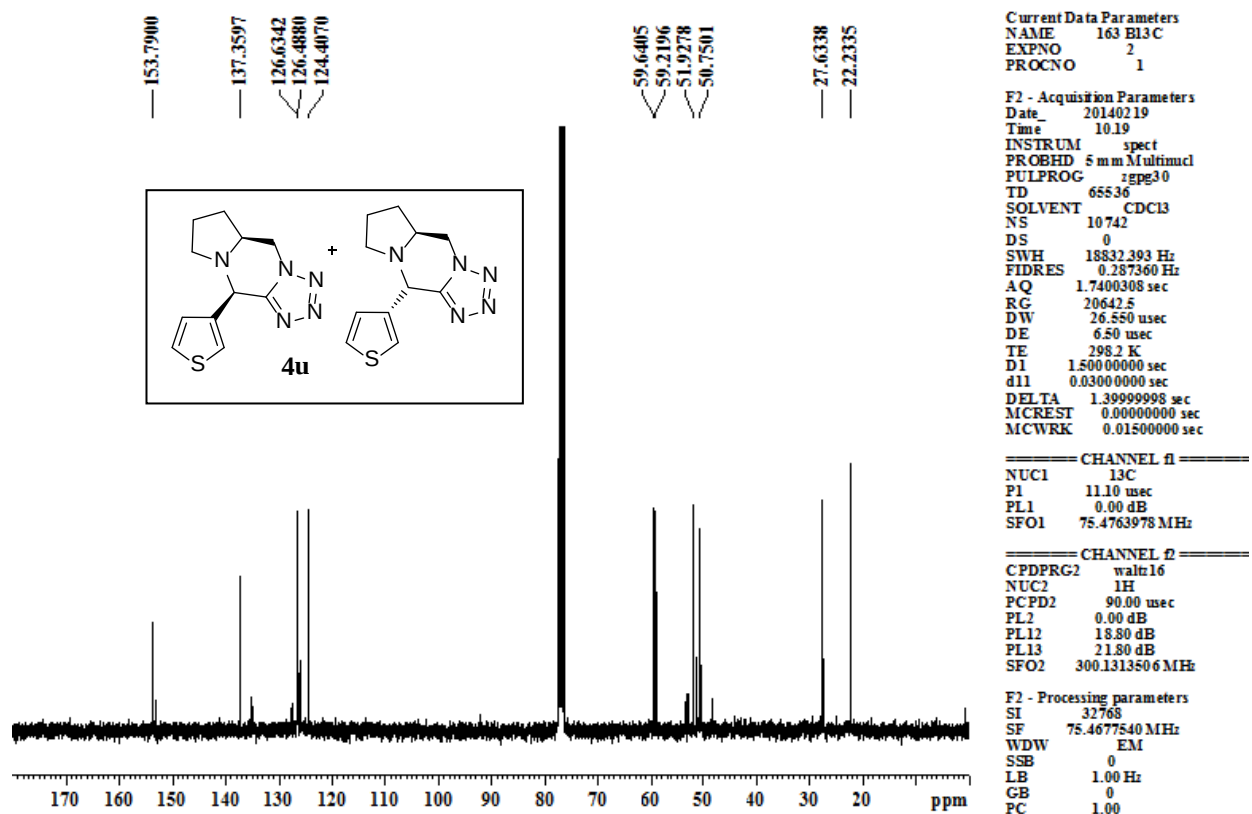
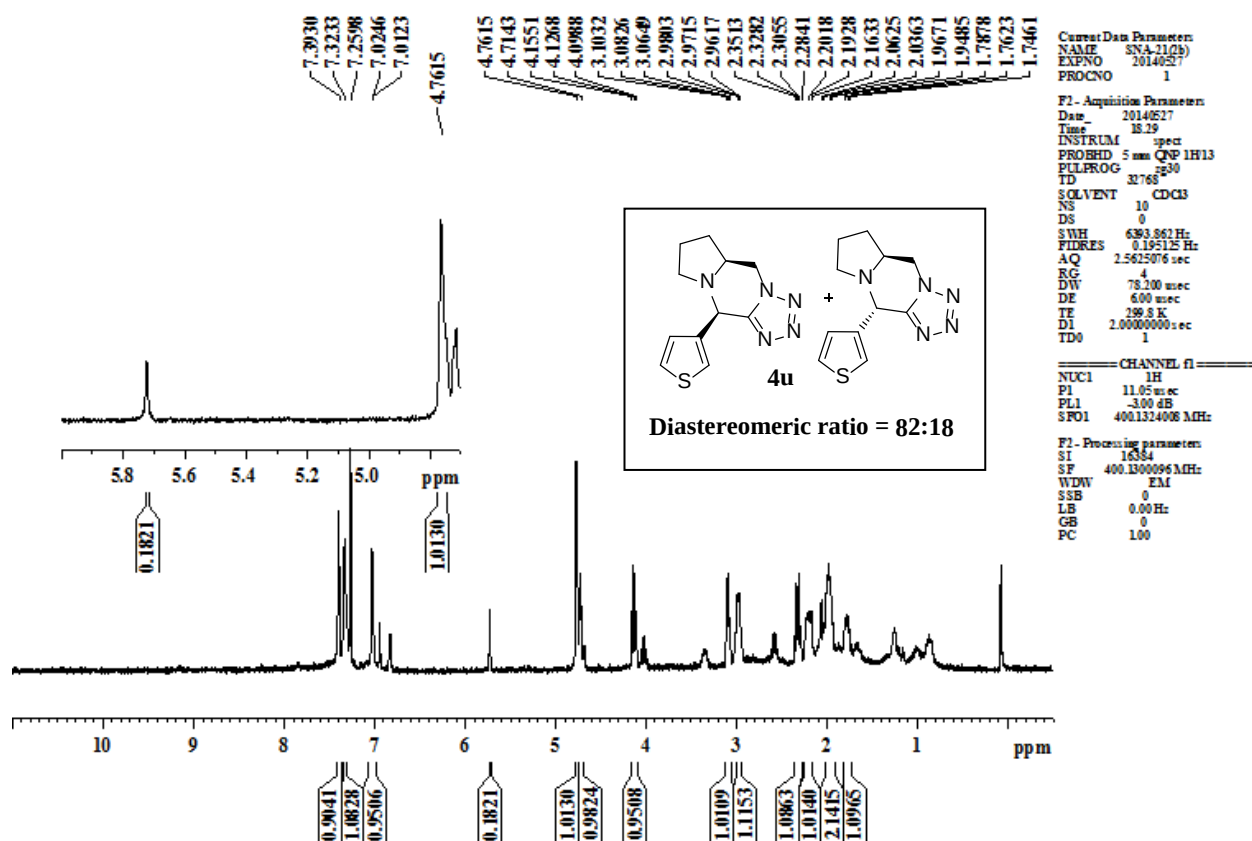
Current Data Parameters
NAME SNA 172 dnm B13C
EXPNO 1
PROCNO 1

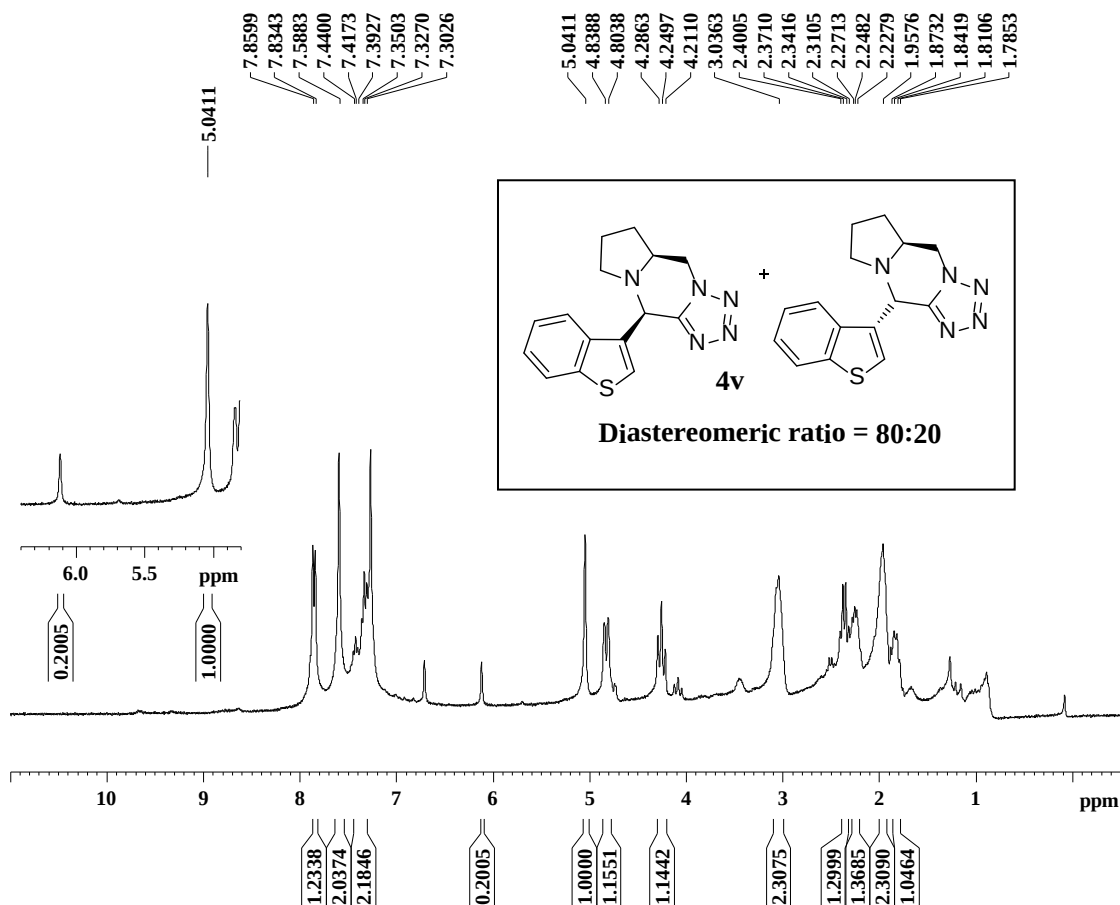
F2 - Acquisition Parameters
Date_ 20140225
Time 6.47
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG :gpg30
TD 65536
SOLVENT CDCl3
NS 1170
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00





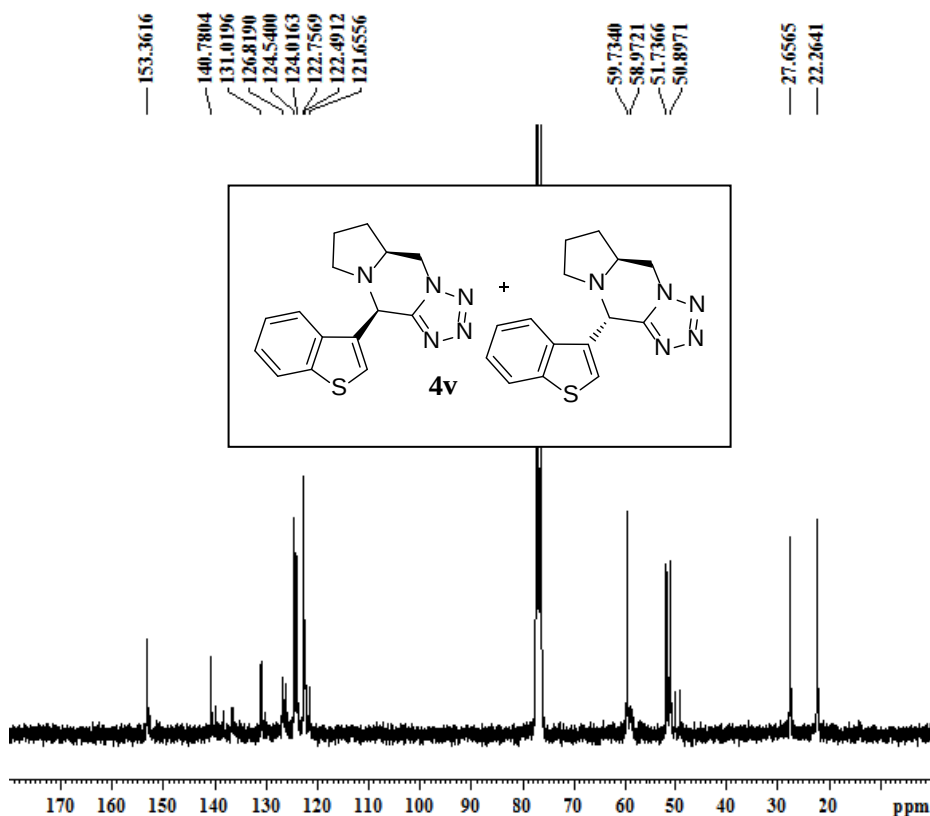
Current Data Parameters
NAME SNA22BH23M2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140523
Time 16.53
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 47
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 645.1
DW 111.200 usec
DE 6.50 usec
TE 301.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.60 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 16384
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
FIP 13.972 ppm
F1 4193.32 Hz
F2P -1.010 ppm
F2 -303.08 Hz
PPMCM 0.74908 ppm/c
HZCM 224.82013 Hz/cm



Current Data Parameters
NAME SNA B thianapT
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140212
Time 9.54
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11465
DS 0
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 5792.6
DW 26.550 usec
DE 6.50 usec
TE 296.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.10 usec
PL1 0.00 dB
SFO1 75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 18.80 dB
PL13 21.80 dB
SFO2 300.1313506 MHz

F2 - Processing parameters
SI 32768
SF 75.4677597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00