Supporting Information

Cyclopeptide Alkaloids from *Ziziphus apetala*

Jing Han,[†,§,‡] Chang-Jiu Ji,[†,§,‡] Wen-Jun He,[†] Yu Shen,[#,§] Ying Leng,[#] Wen-Yan Xu,[†] Jun-Ting Fan,[†] Guang-Zhi Zeng,[†] Ling-Dong Kong,[ℓ] and Ning-Hua Tan[†,*]

[*] To whom correspondence should be addressed. Tel: +86-871-5223800. Fax: +86-871-5223800. E-mail: nhtan@mail.kib.ac.cn.

[†]State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, Yunnan, People's Republic of China

[#]Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, People's Republic of China

[ℓ]Nanjing University, Nanjing 210093, People's Republic of China

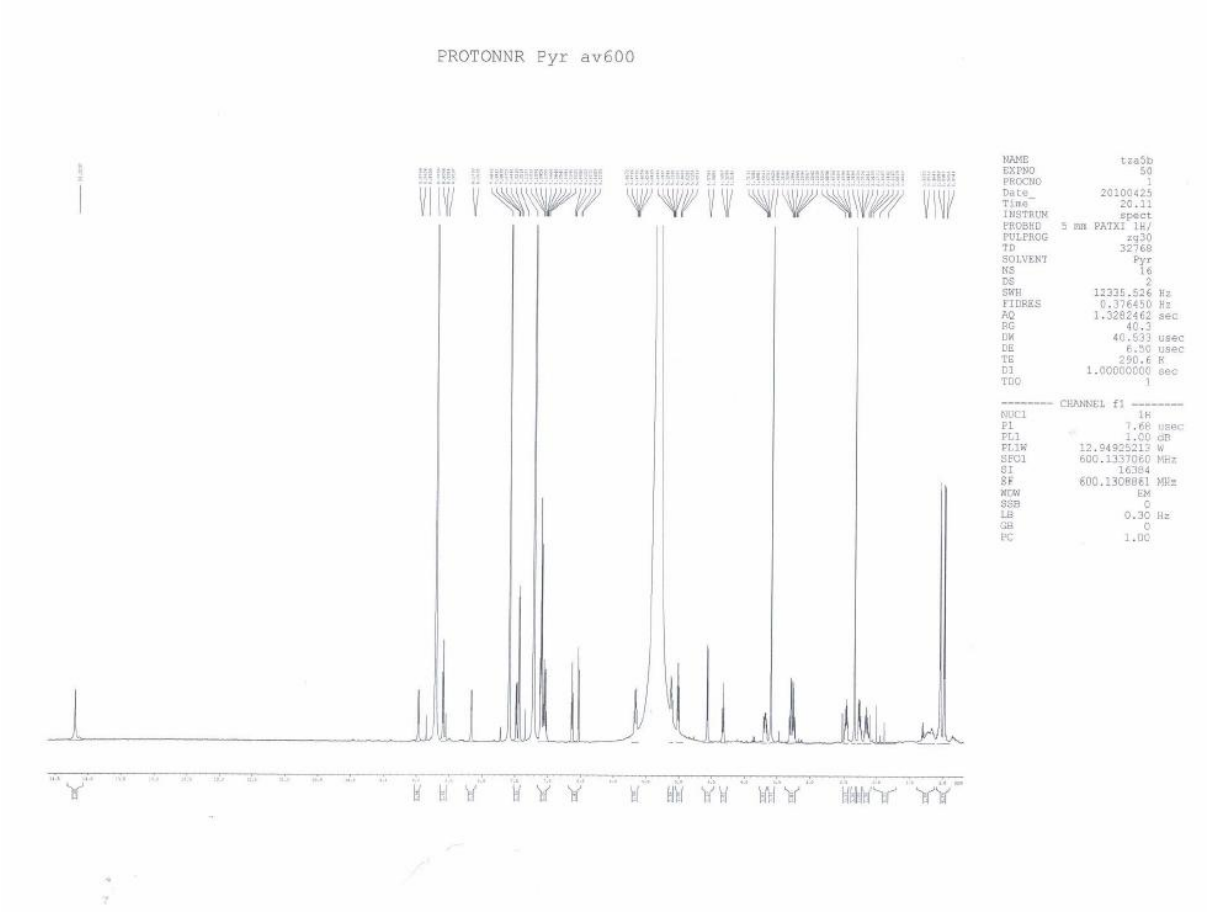
[§]Graduate University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China.

[‡]Contributed equally to this work.

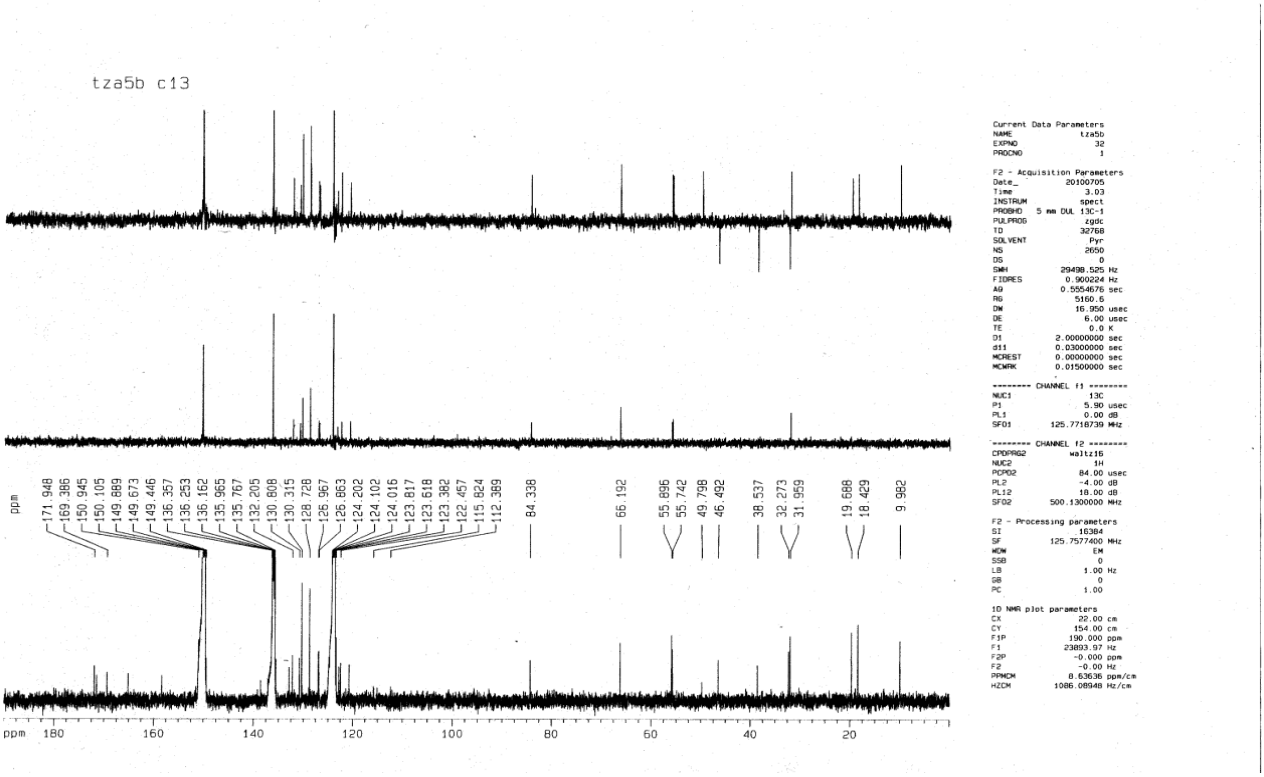
This is the supporting information for "Cyclopeptide Alkaloids from *Ziziphus apetala*", including copies of 1D and 2D NMR, MS, IR, UV, $[\alpha]_D$ and CD spectra of compounds **1**-**8**.

Contents

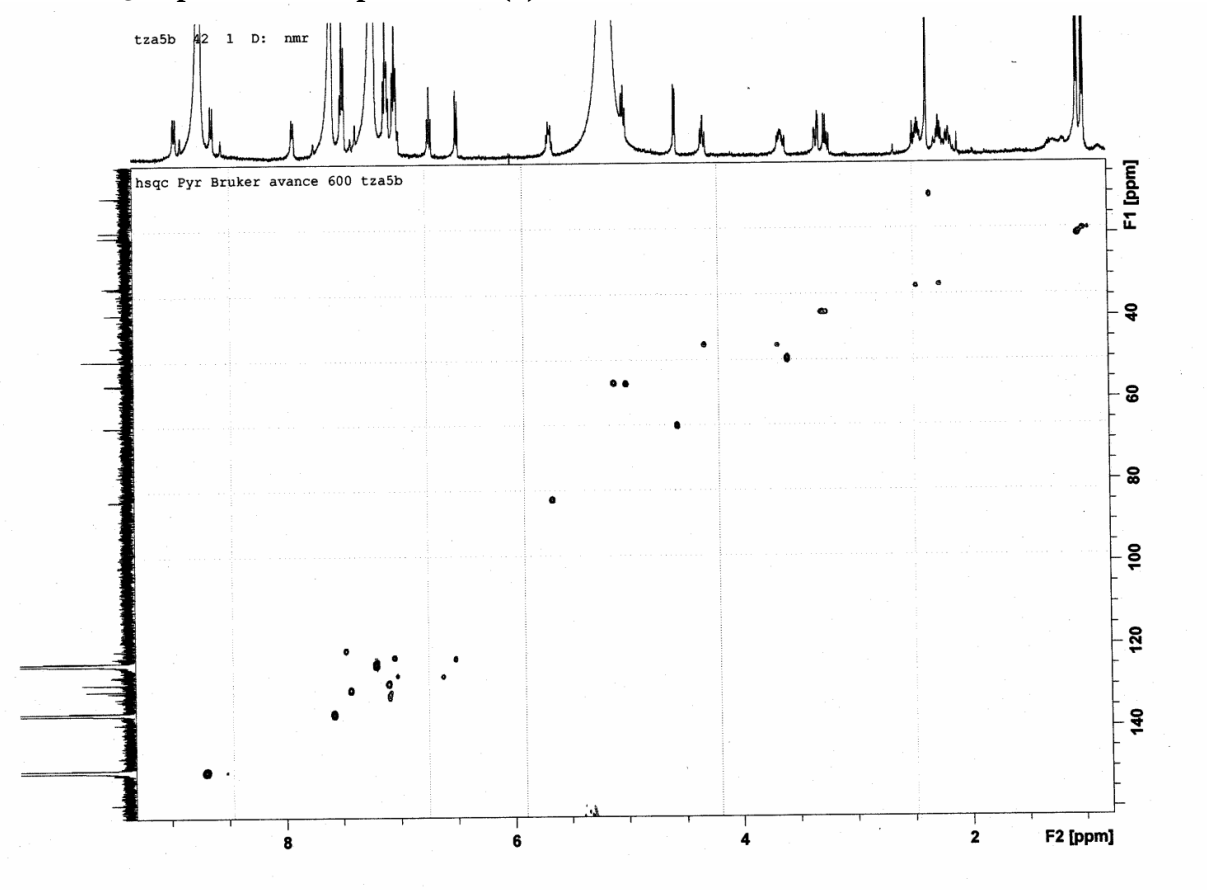
S1 The ^{1}H NMR spectrum of Apetaline A (1) in C_5D_5N



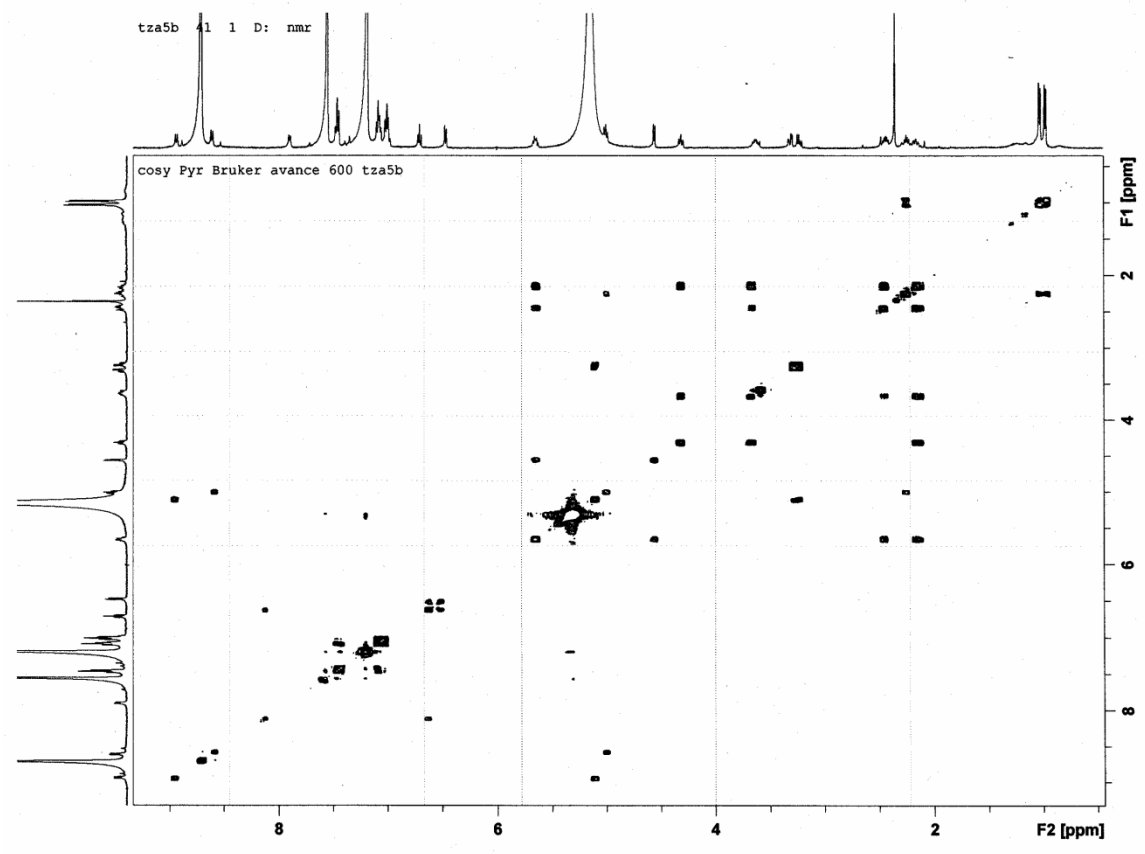
S2 The ^{13}C NMR spectrum of Apetaline A (1) in C_5D_5N



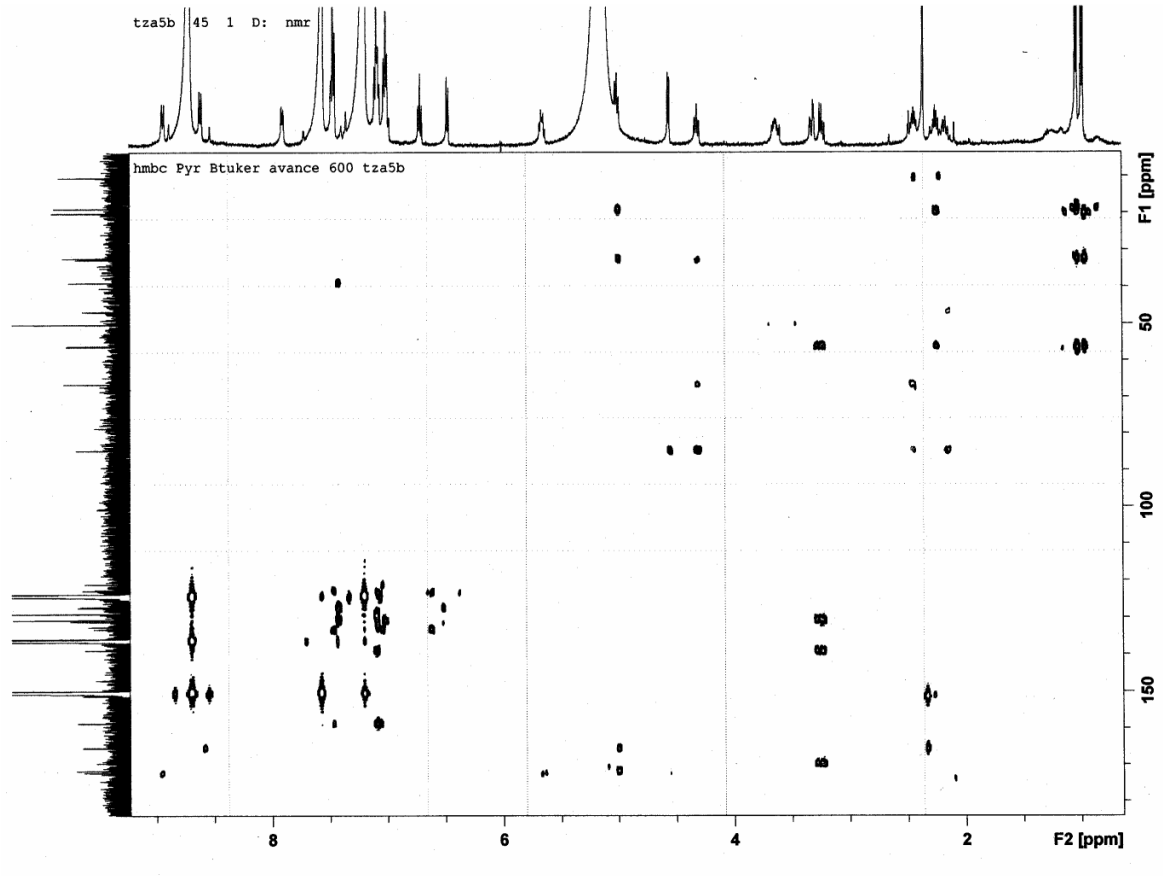
S3 The HSQC spectrum of Apetaline A (1)



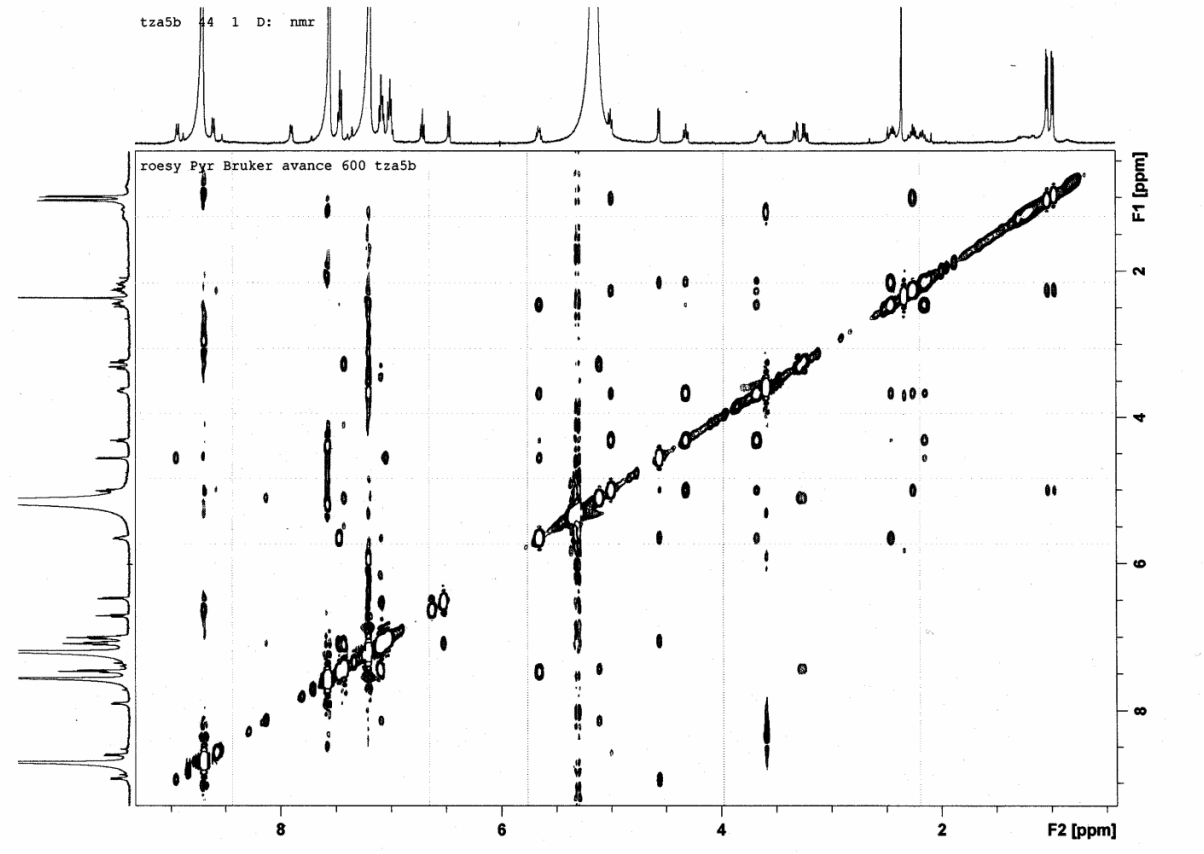
S4 The ^{1}H-^{1}H COSY spectrum of Apetaline A (1)



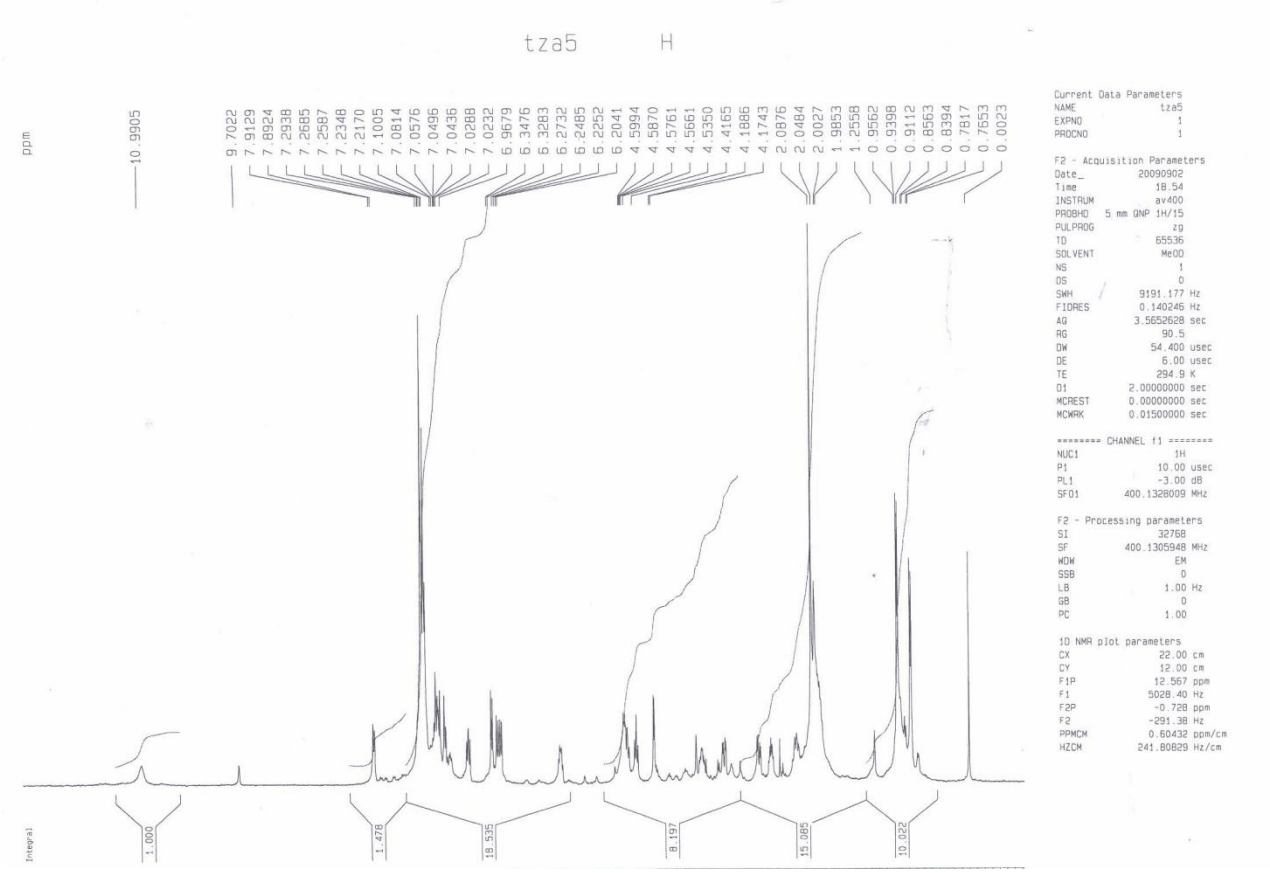
S5 The HMBC spectrum of Apetaline A (1)



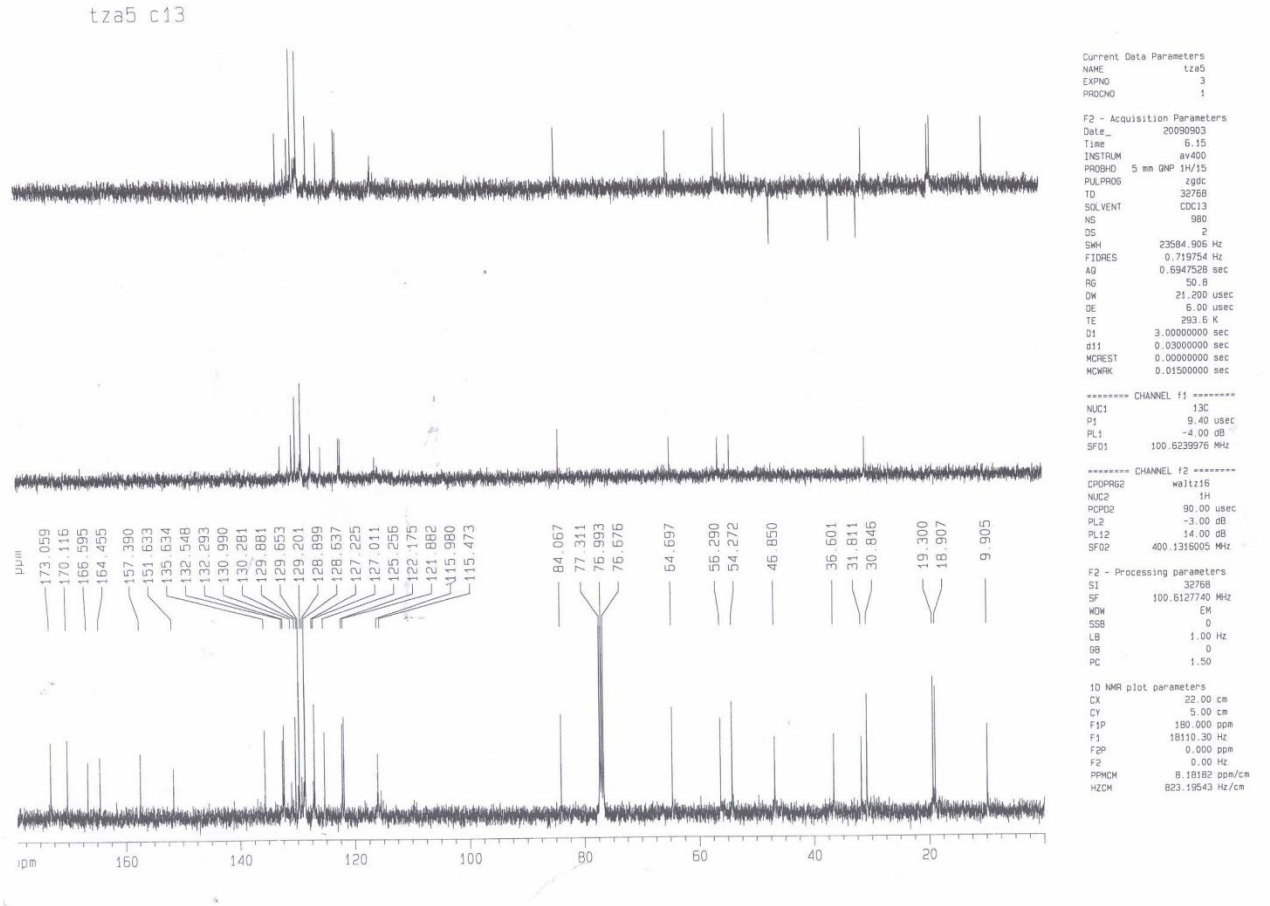
S6 The ROSEY spectrum of Apetaline A (1)



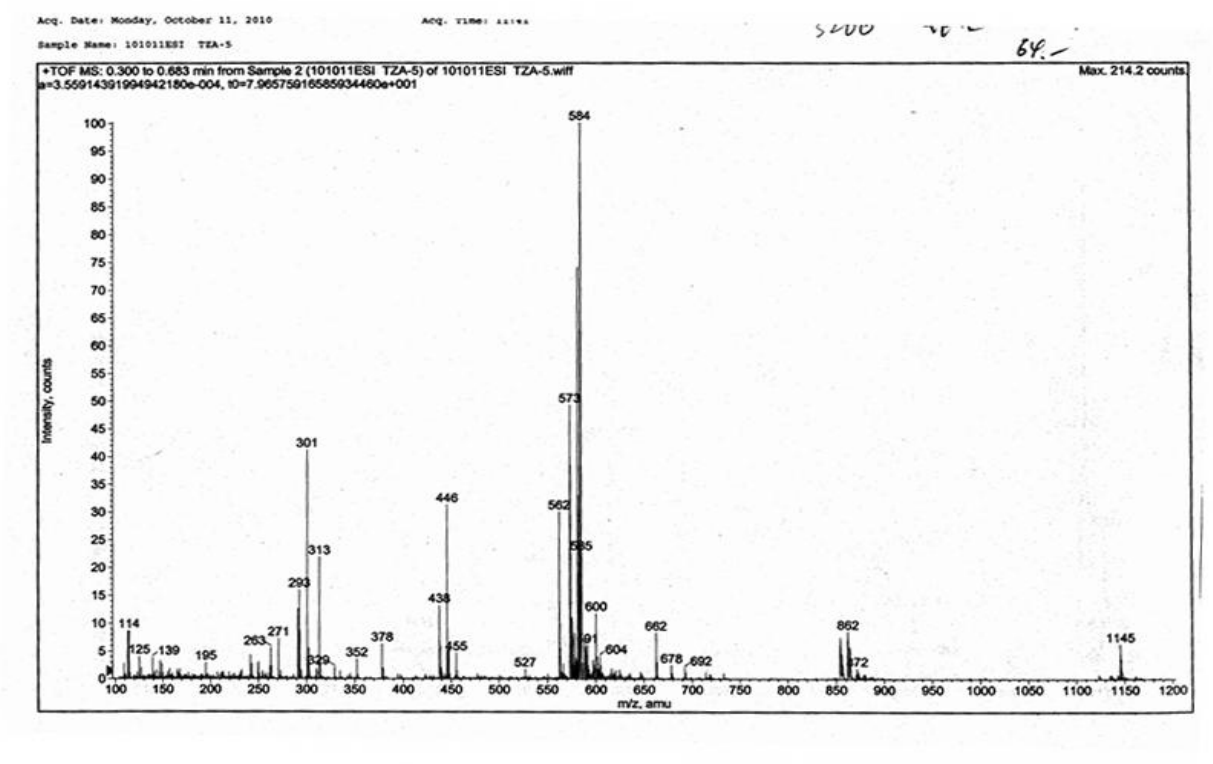
S7 The ^{1}H NMR spectrum of Apetaline A (1) in $CDCl_3$



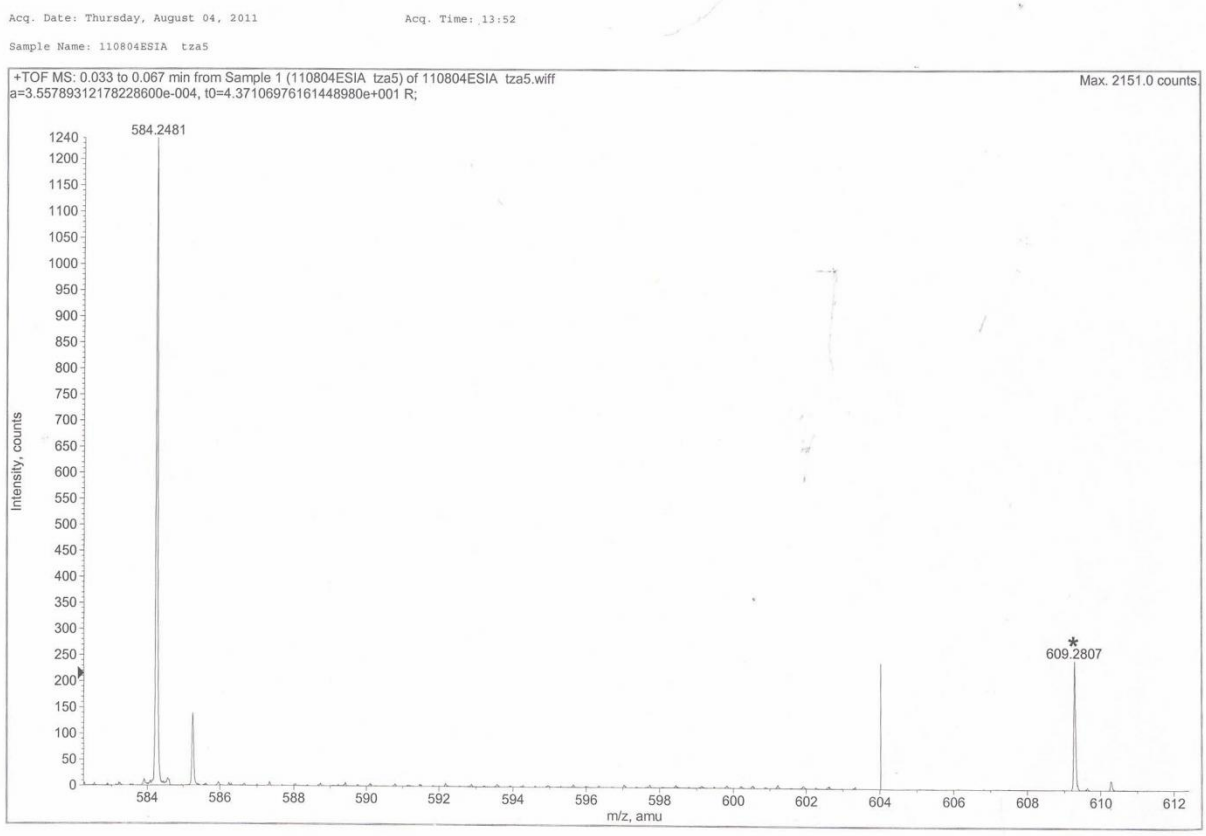
S8 The ^{13}C NMR spectrum of Apetaline A (1) in $CDCl_3$



S9 Positive ESIMS of Apetaline A (1)



S10 Positive HRESIMS of Apetaline A (1)



S10 Positive HRESIMS of Apetaline A (1)

Acq. Date: Thursday, August 04, 2011 Acq. Time: 13:52

Sample Name: 110804ESIA tza5

Elemental composition calculator

Target m/z: +584.2481 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 110804ESIA tza5.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	I	0	0
7	K	0	0
8	N	5	5
9	Na	1	1
10	O	3	6

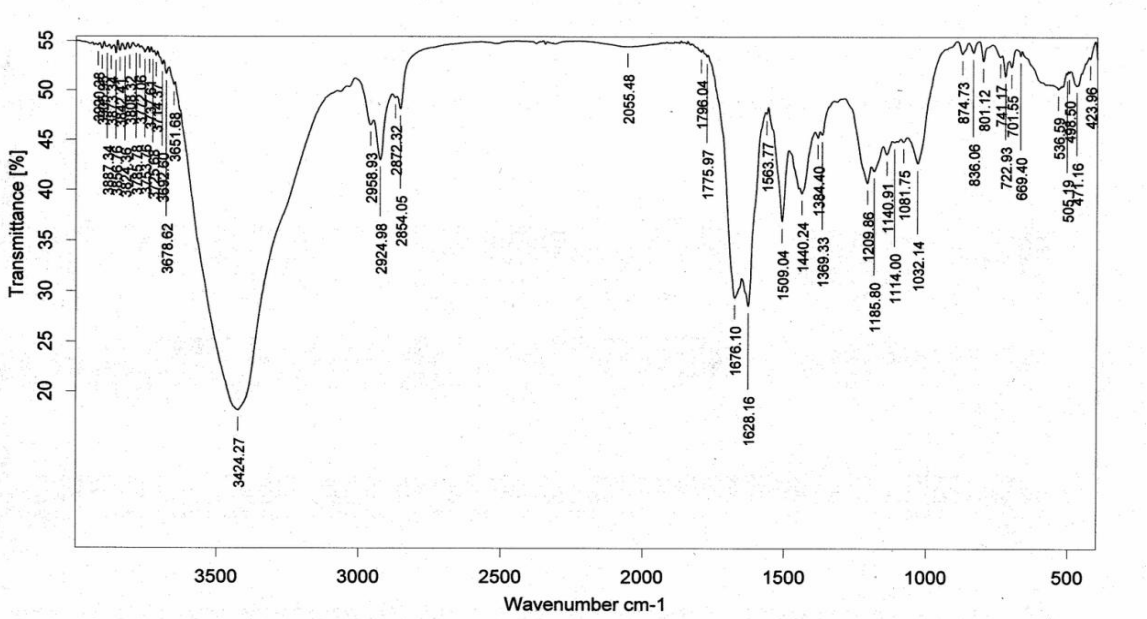
Acq. Date: Thursday, August 04, 2011 Acq. Time: 13:52

Sample Name: 110804ESIA tza5

	Elements	Min Number	Max Number
11	P	0	0
12	Pt	0	0
13	S	0	0
14	Si	0	0

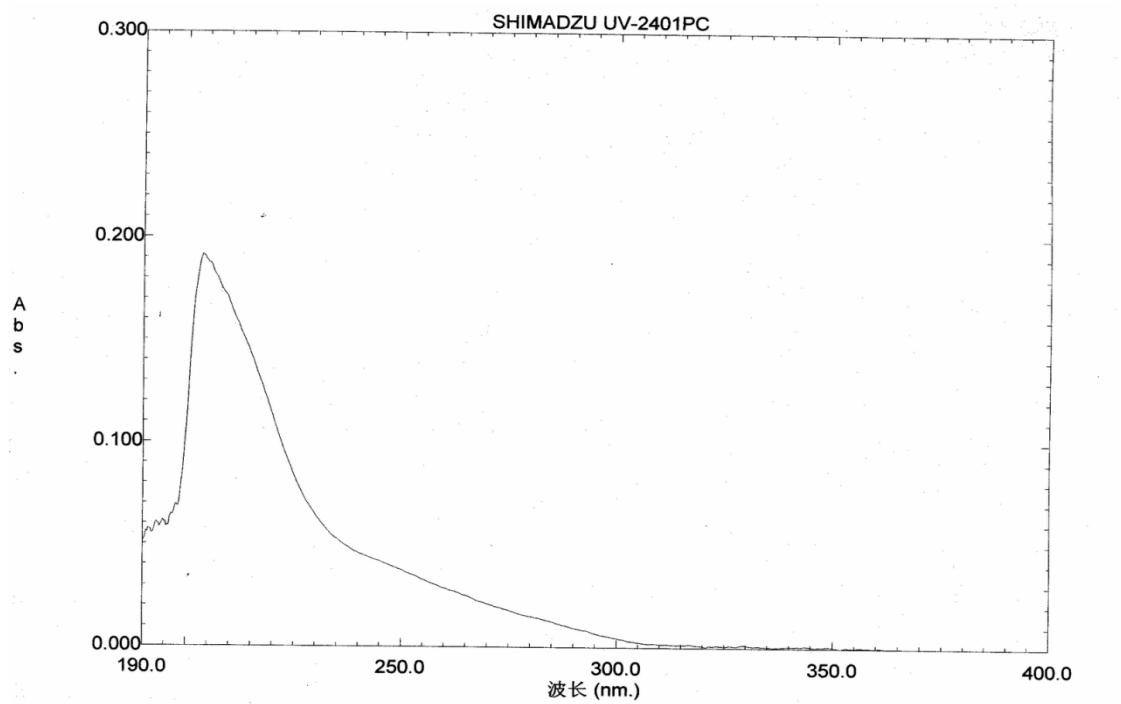
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C30 H35 N5 O6 Na	584.2485	-0.4039	-0.6914	15.5

S11 The IR Spectrum of Apetaline A (1)



Sample : Tza-5	Frequency Range : 399.271 - 3996.57	Measured on : 18/10/2010	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 101018IR2	Zerofilling : 2	Acquisition : Double Sided,For	

S12 The UV Spectrum of Apetaline A (1)



文件名: TZA-5

创建于: 13:48 10-10-12
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 2.0
采样间隔: 0.2

样品浓度：0.0300毫克/毫升
溶剂：甲醇

否.	波长 (nm.)	Abs.
1	203.60	0.1915

S13 The $[\alpha]_D$ of Apetaline A (1)

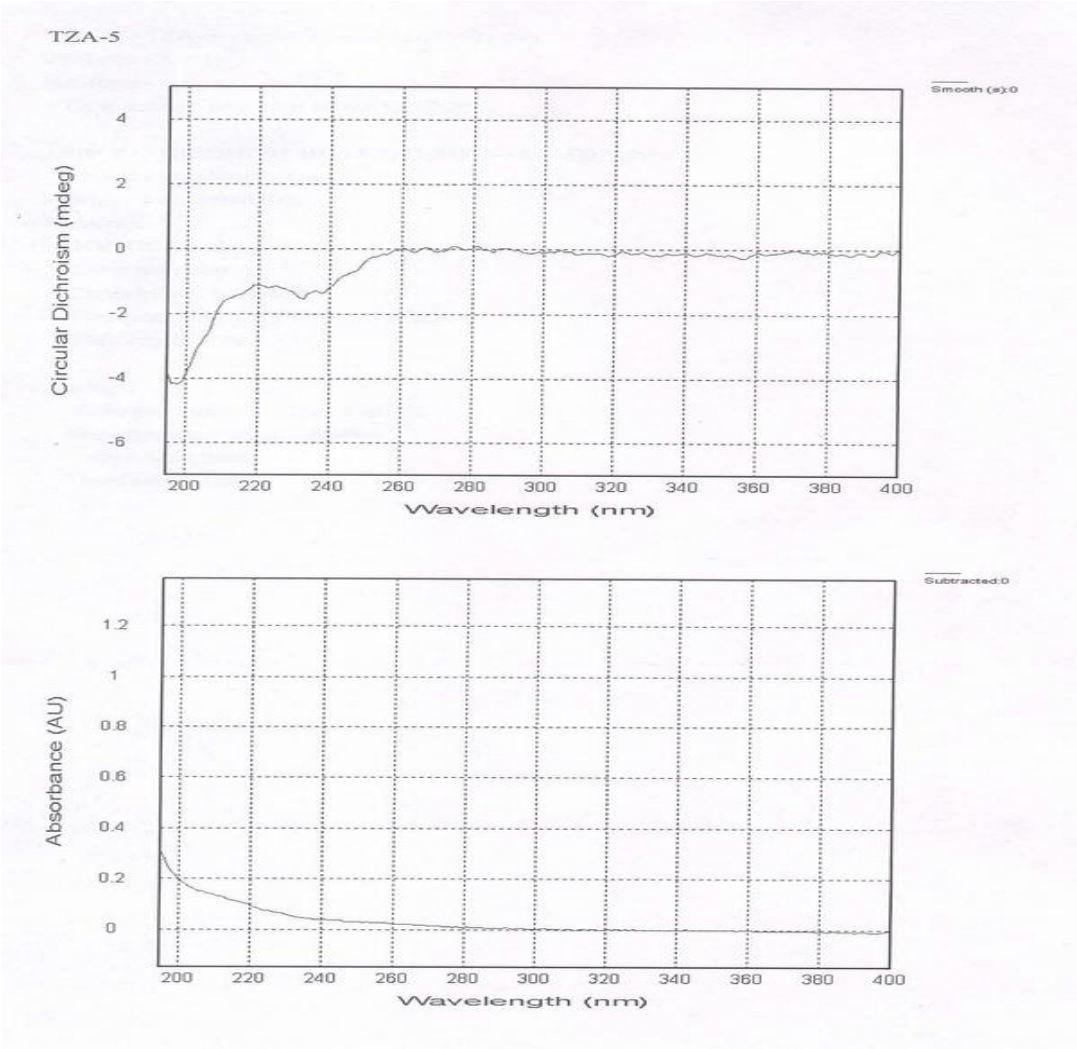
Optical rotation measurement

Model : P-1020 (A060460638)

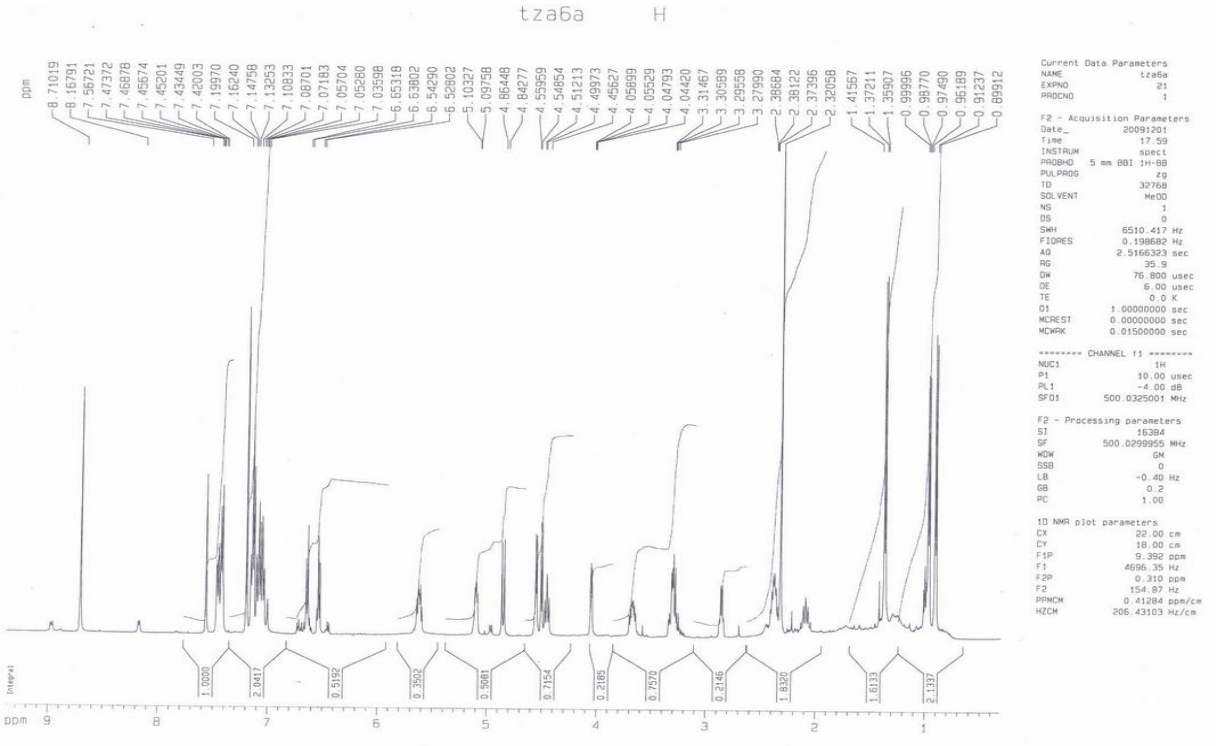
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	1 (1/3)	Sp.Rot	-19.8000	-0.0297 0.0000	22.1 50.00 Cell	Wed Oct 13 11:31:15 2010 0.00300g/mlMeOH TZA-5	Na 589nm	2 sec 10 sec
No.2	1 (2/3)	Sp.Rot	-18.5330	-0.0278 0.0000	22.1 50.00 Cell	Wed Oct 13 11:31:28 2010 0.00300g/mlMeOH TZA-5	Na 589nm	2 sec 10 sec
No.3	1 (3/3)	Sp.Rot	-19.6000	-0.0294 0.0000	22.2 50.00 Cell	Wed Oct 13 11:31:42 2010 0.00300g/mlMeOH TZA-5	Na 589nm	2 sec 10 sec

-19.3111°

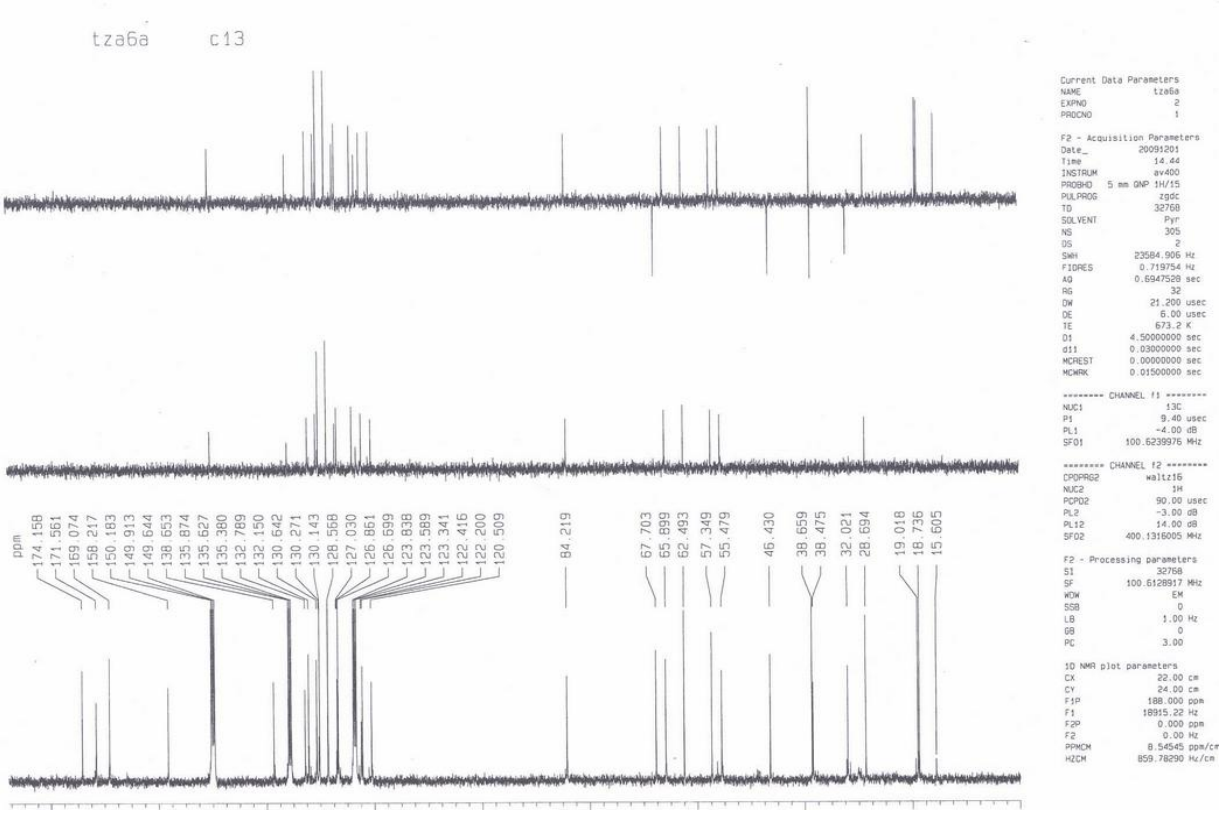
S14 The CD spectrum of Apetaline A (1)



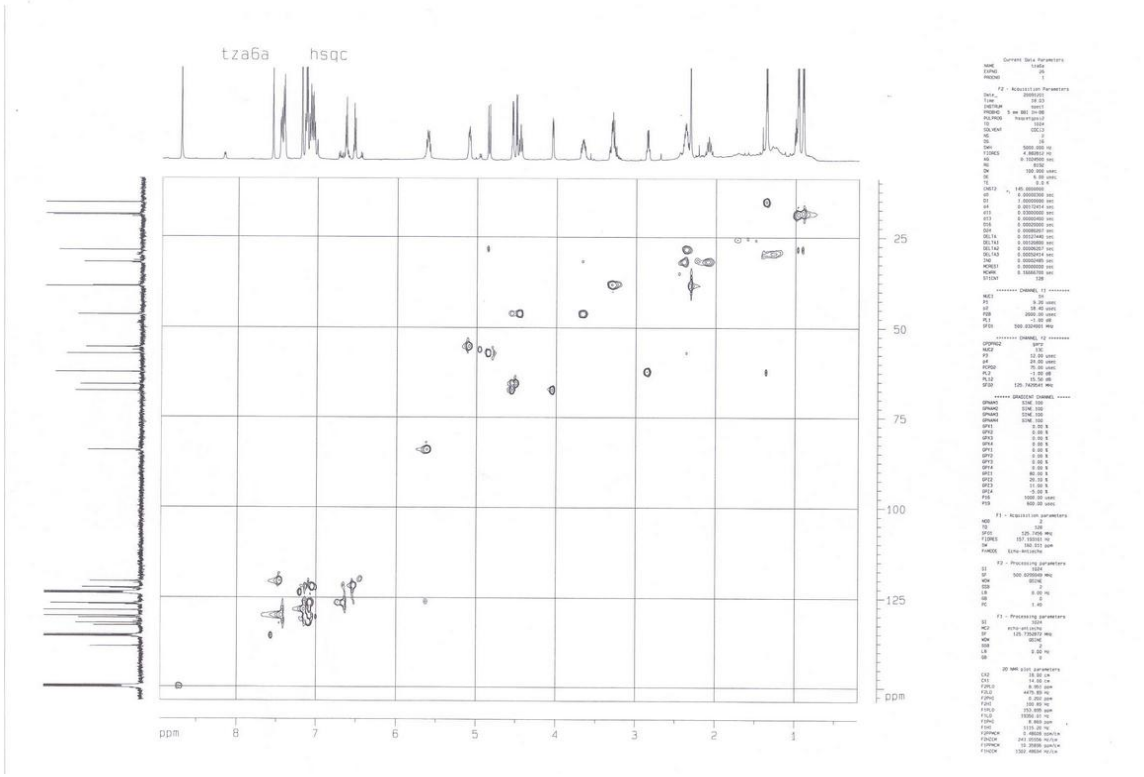
S15 The ^{1}H NMR spectrum of Apetaline B (2) in C_5D_5N



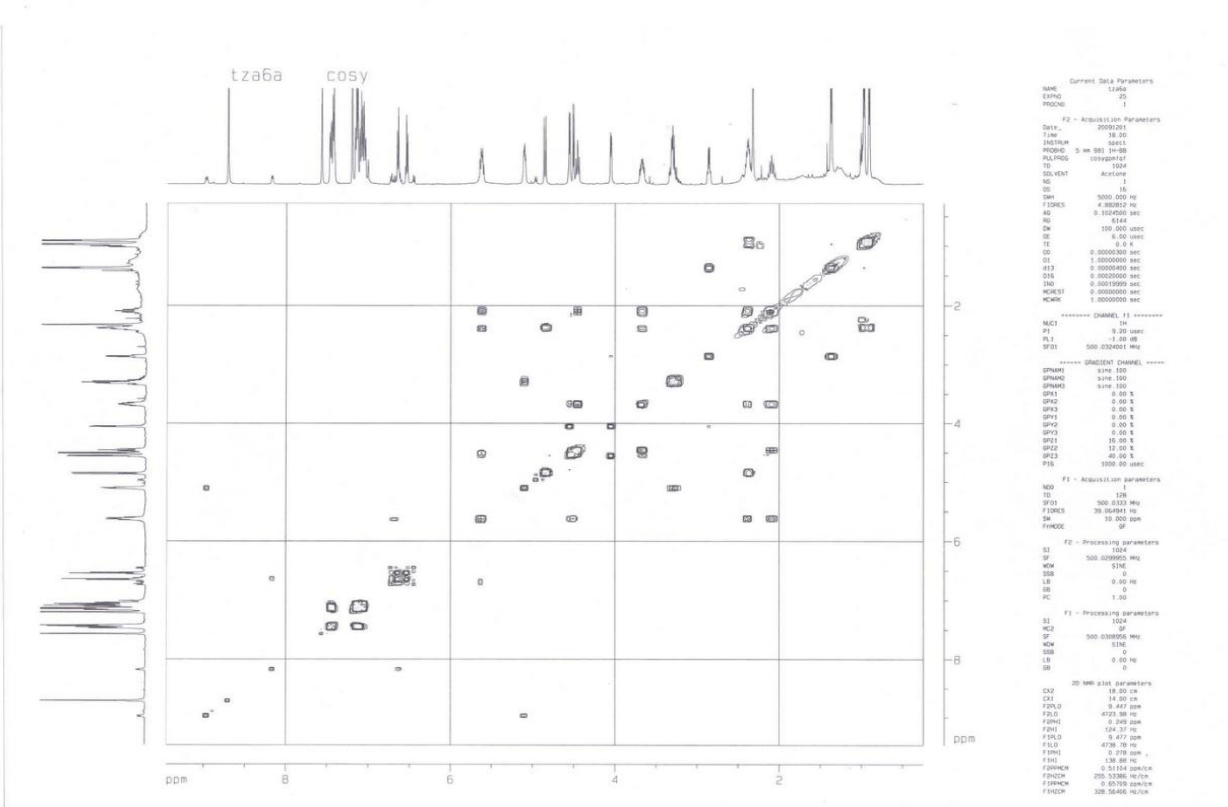
S16 The ^{13}C NMR spectrum of Apetaline B (2) in C_5D_5N



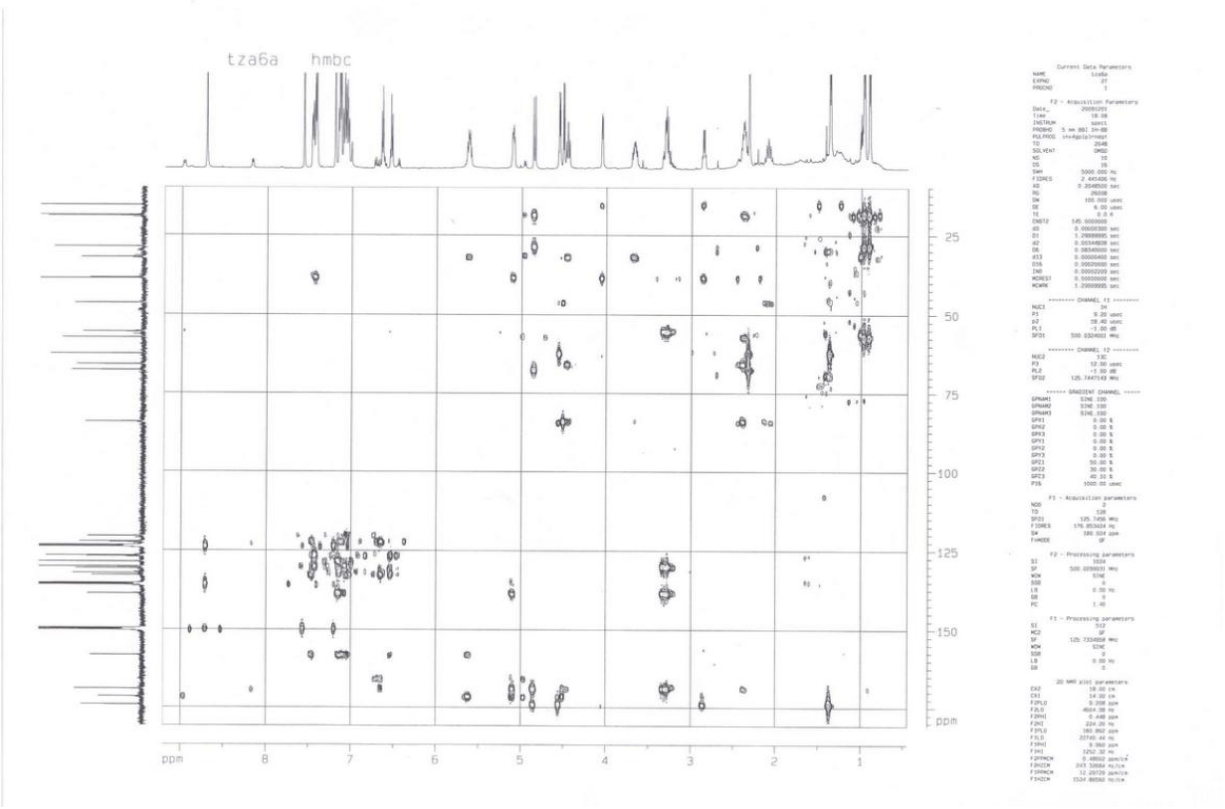
S17 The HSQC spectrum of Apetaline B (2)



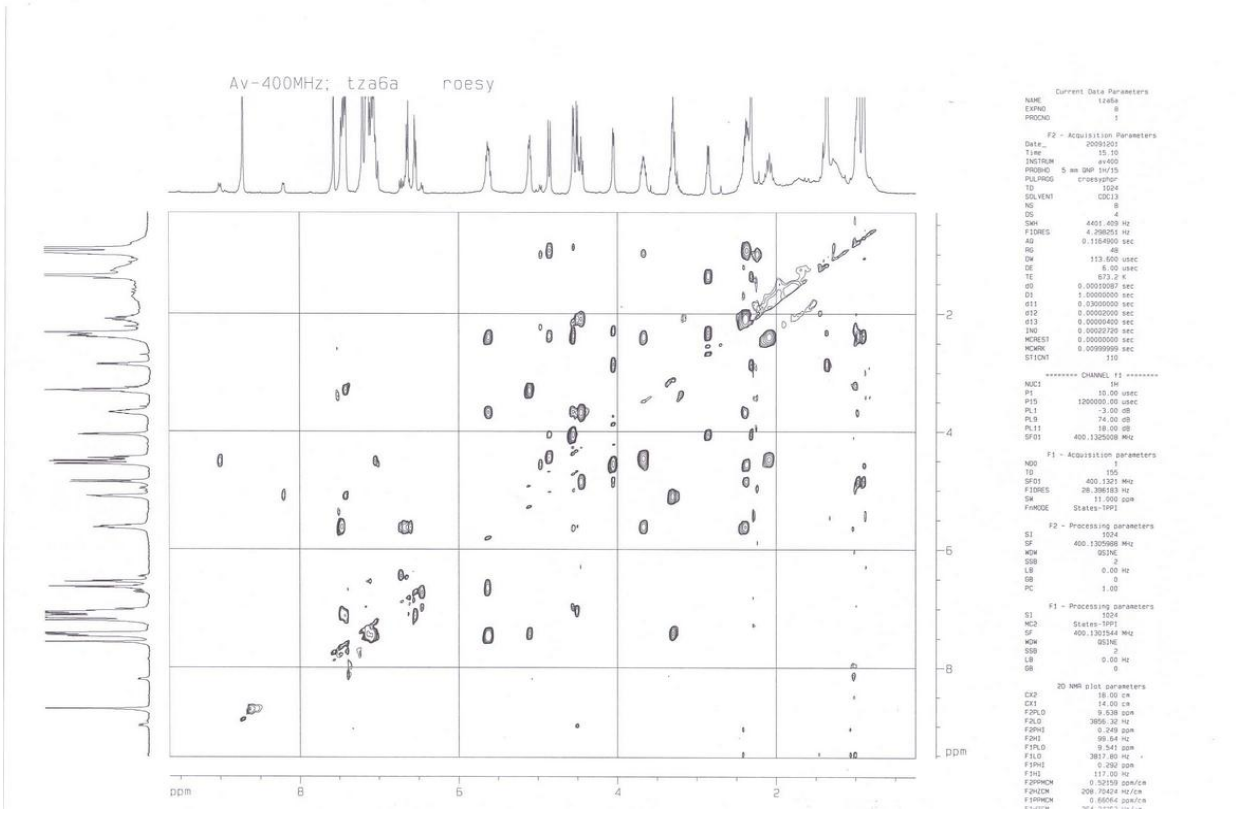
S18 The ^{1}H-^{1}H COSY spectrum of Apetaline B (2)



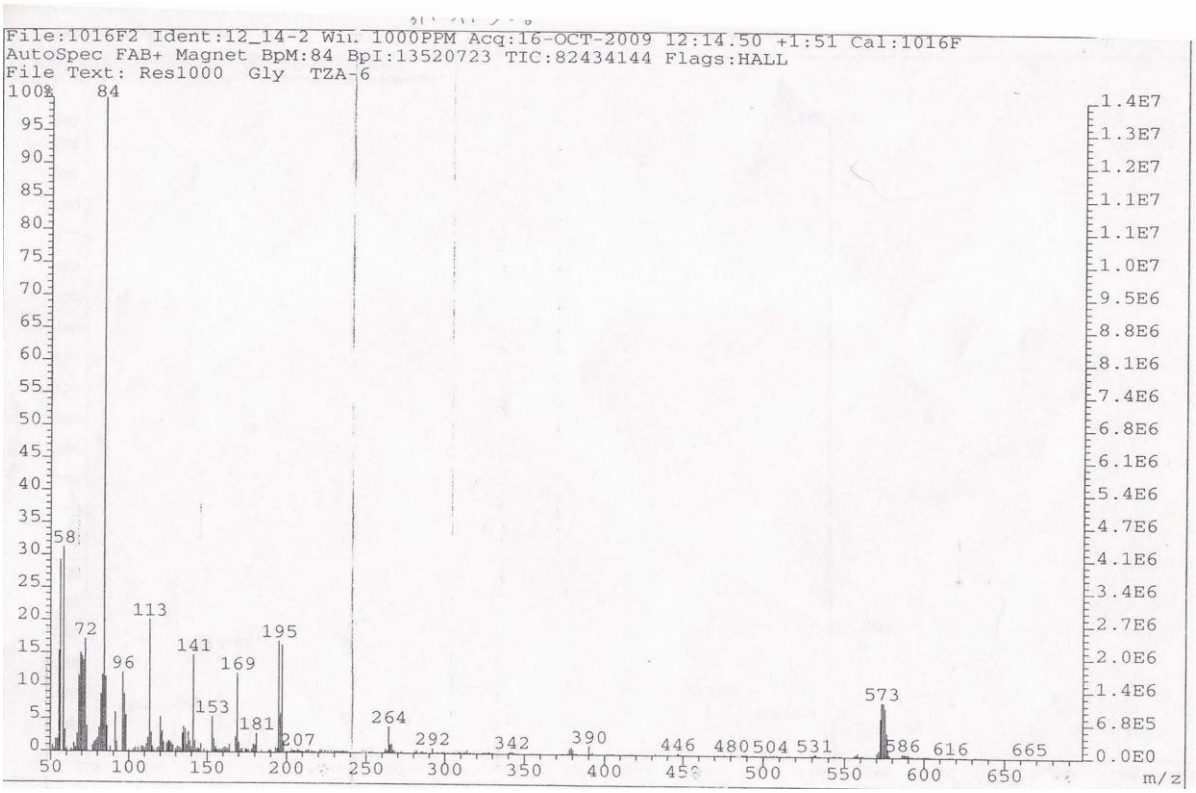
S19 The HMBC spectrum of Apetaline B (2)



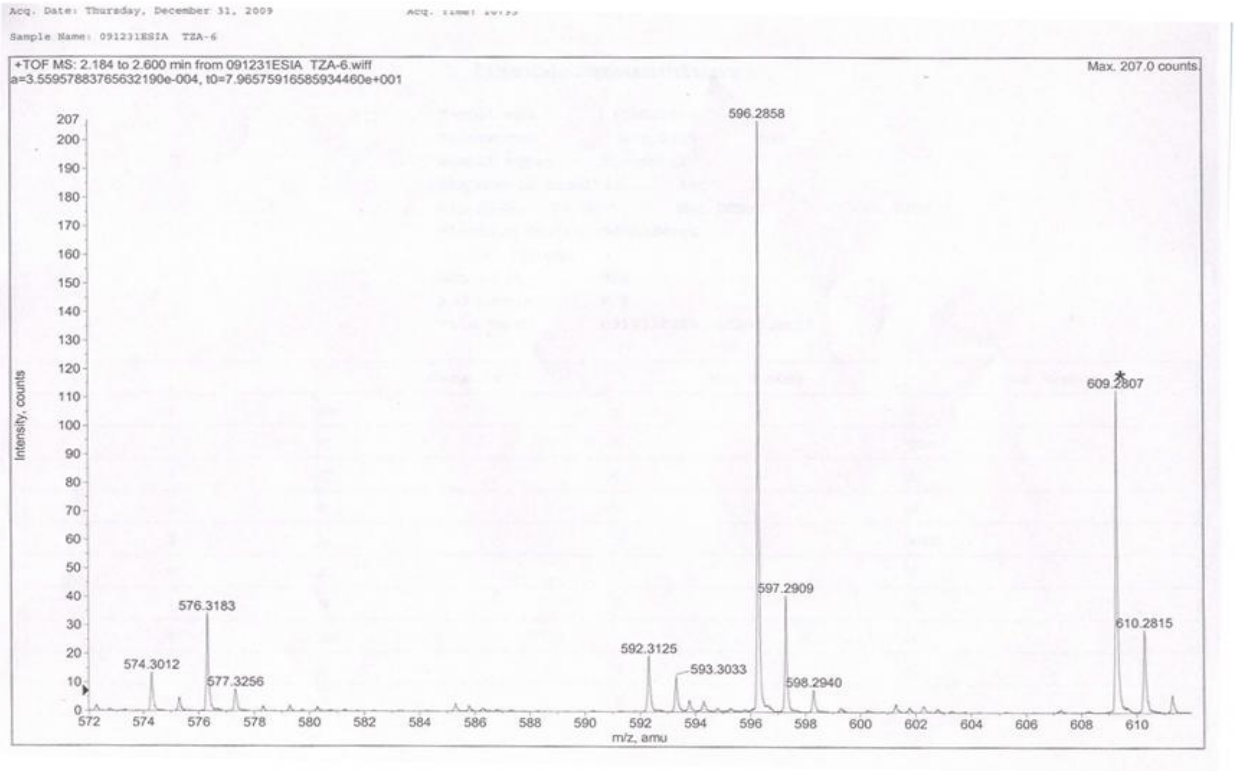
S20 The ROSEY spectrum of Apetaline B (2)



S21 Positive FABMS of Apetaline B (2)



S22 Positive HRESIMS of Apetaline B (2)



S22 Positive HRESIMS of Apetaline B (2)

Acq. Date: Thursday, December 31, 2009 Acq. Time: 10:35

Sample Name: 091231ESIA TZA-6

Elemental composition calculator

Target m/z: +596.2858 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 091231ESIA TZA-6.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	5	5
8	Na	1	1
9	O	4	6
10	S	0	0

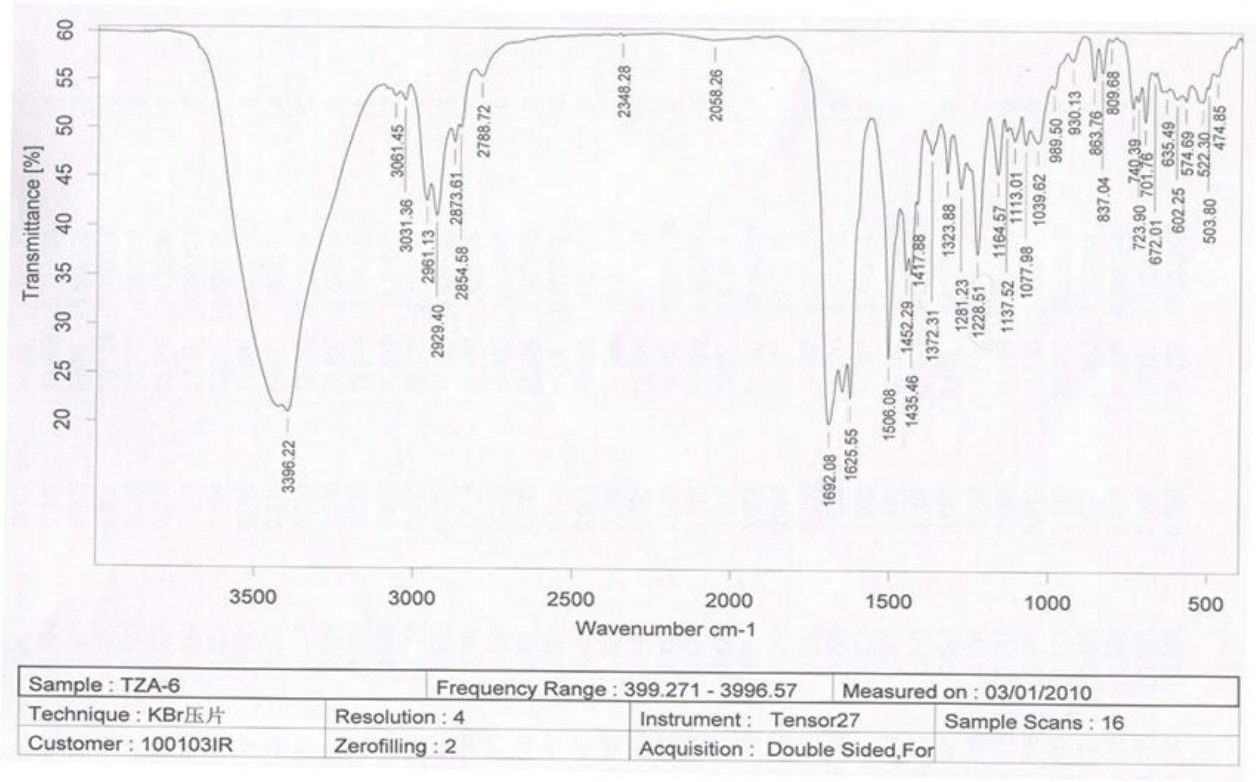
Acq. Date: Thursday, December 31, 2009 Acq. Time: 10:35

Sample Name: 091231ESIA TZA-6

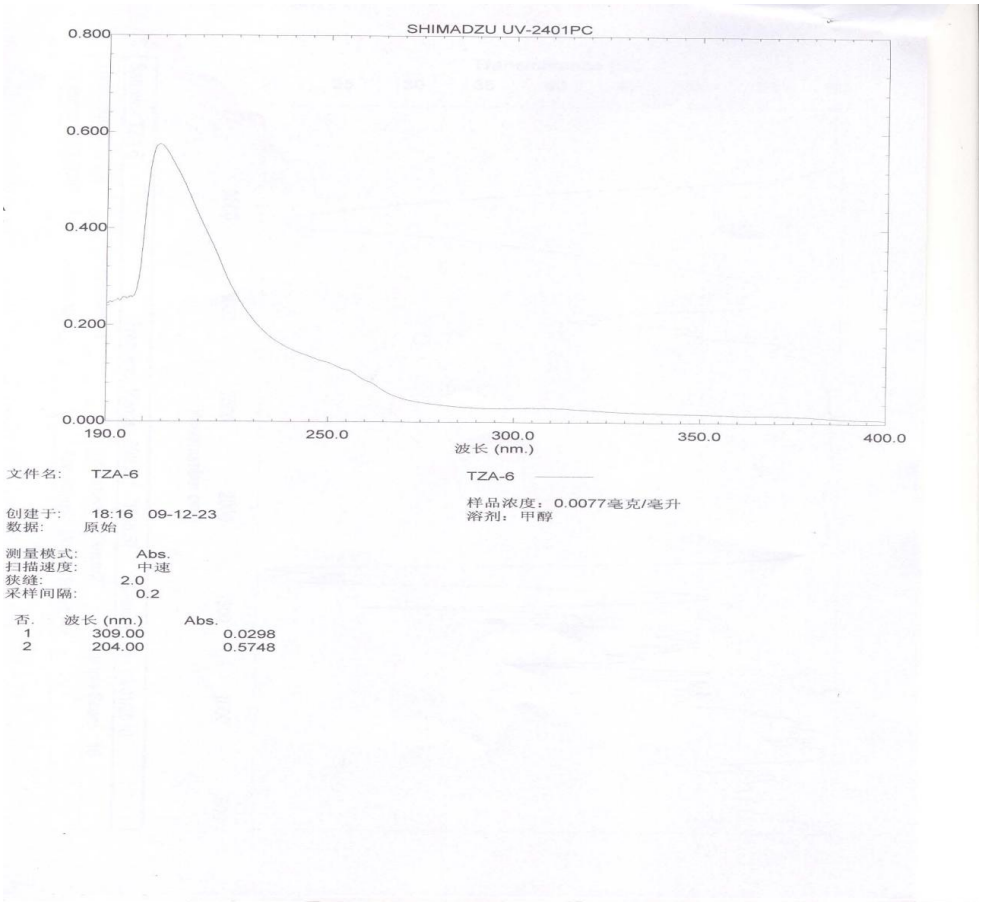
	Elements	Min Number	Max Number
11	Si	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C32 H39 N5 O5 Na	596.2848	0.9105	1.5269	15.5

S23 The IR spectrum of Apetaline B (2)



S24 The UV spectrum of Apetaline B (2)



S25 The $[\alpha]_D$ of Apetaline B (2)

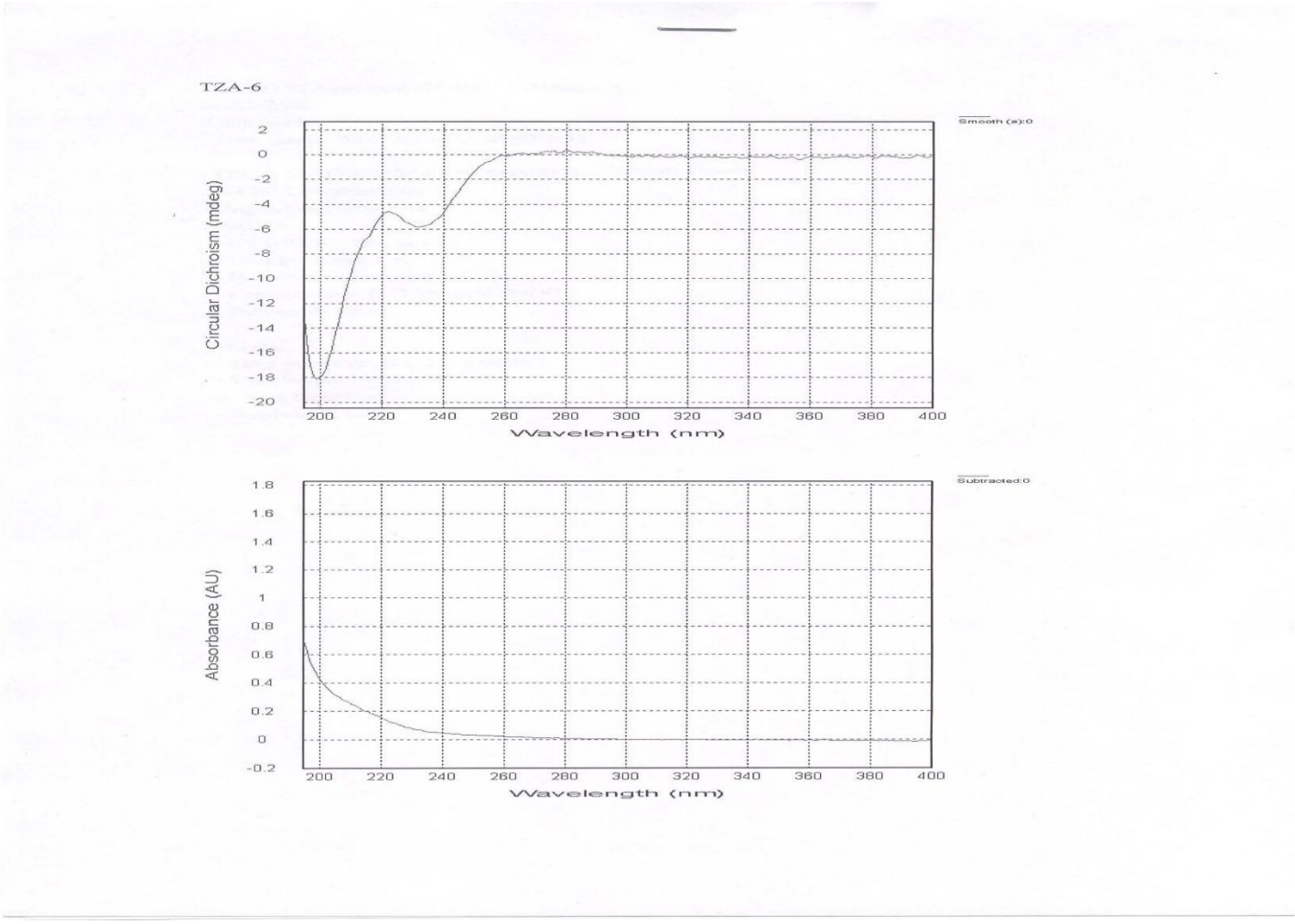
Optical rotation measurement

Model : P-1020 (A060460638)

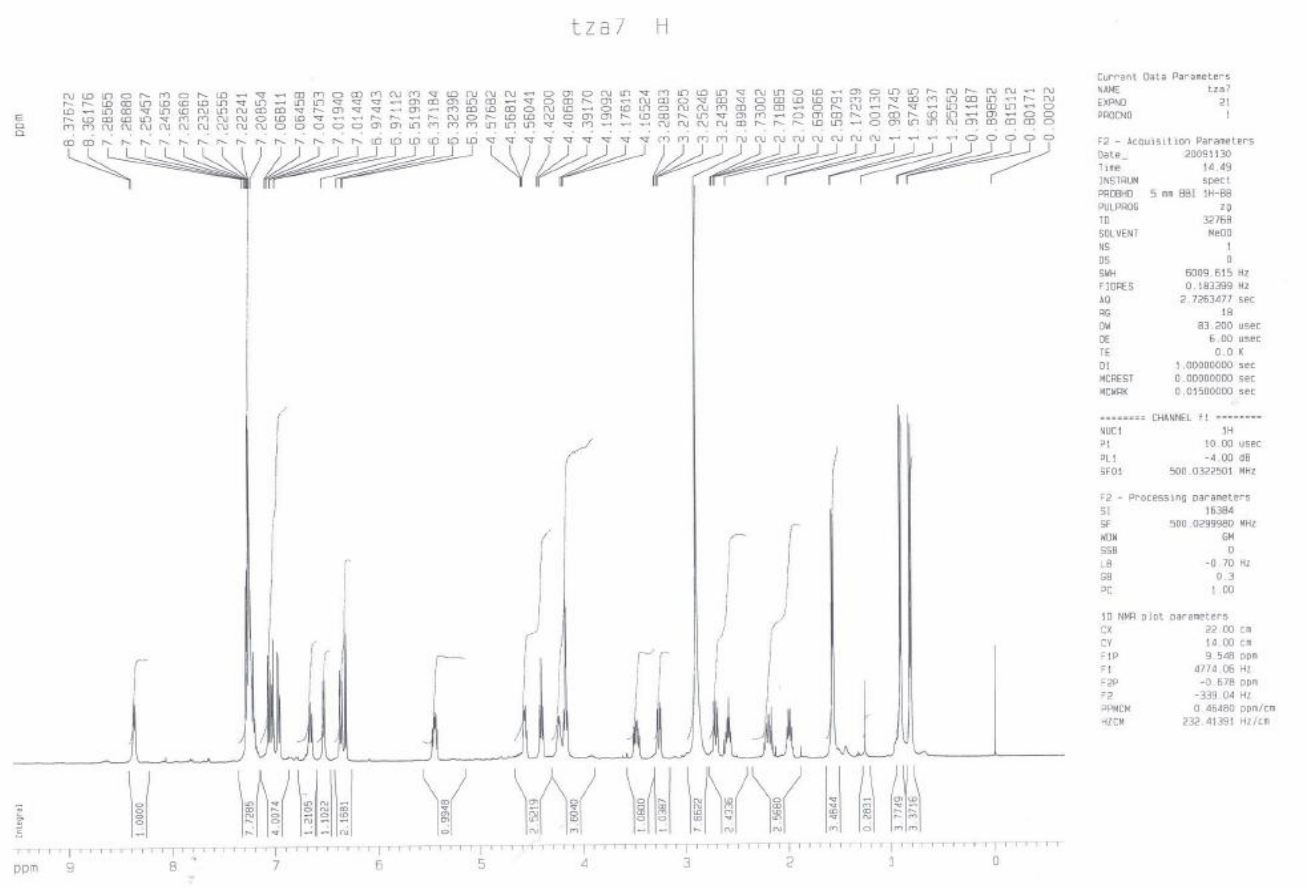
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	4 (1/3)	Sp.Rot	-259.0000	-0.6475 0.0000	16.4 50.00 Cell	Thu Dec 24 16:04:27 2009 0.00500g/mlMeOH TZA-6	Na 589nm	2 sec 10 sec
No.2	4 (2/3)	Sp.Rot	-259.3200	-0.6483 0.0000	16.5 50.00 Cell	Thu Dec 24 16:04:40 2009 0.00500g/mlMeOH TZA-6	Na 589nm	2 sec 10 sec
No.3	4 (3/3)	Sp.Rot	-259.0400	-0.6476 0.0000	16.4 50.00 Cell	Thu Dec 24 16:04:53 2009 0.00500g/mlMeOH TZA-6	Na 589nm	2 sec 10 sec

-259.1200°

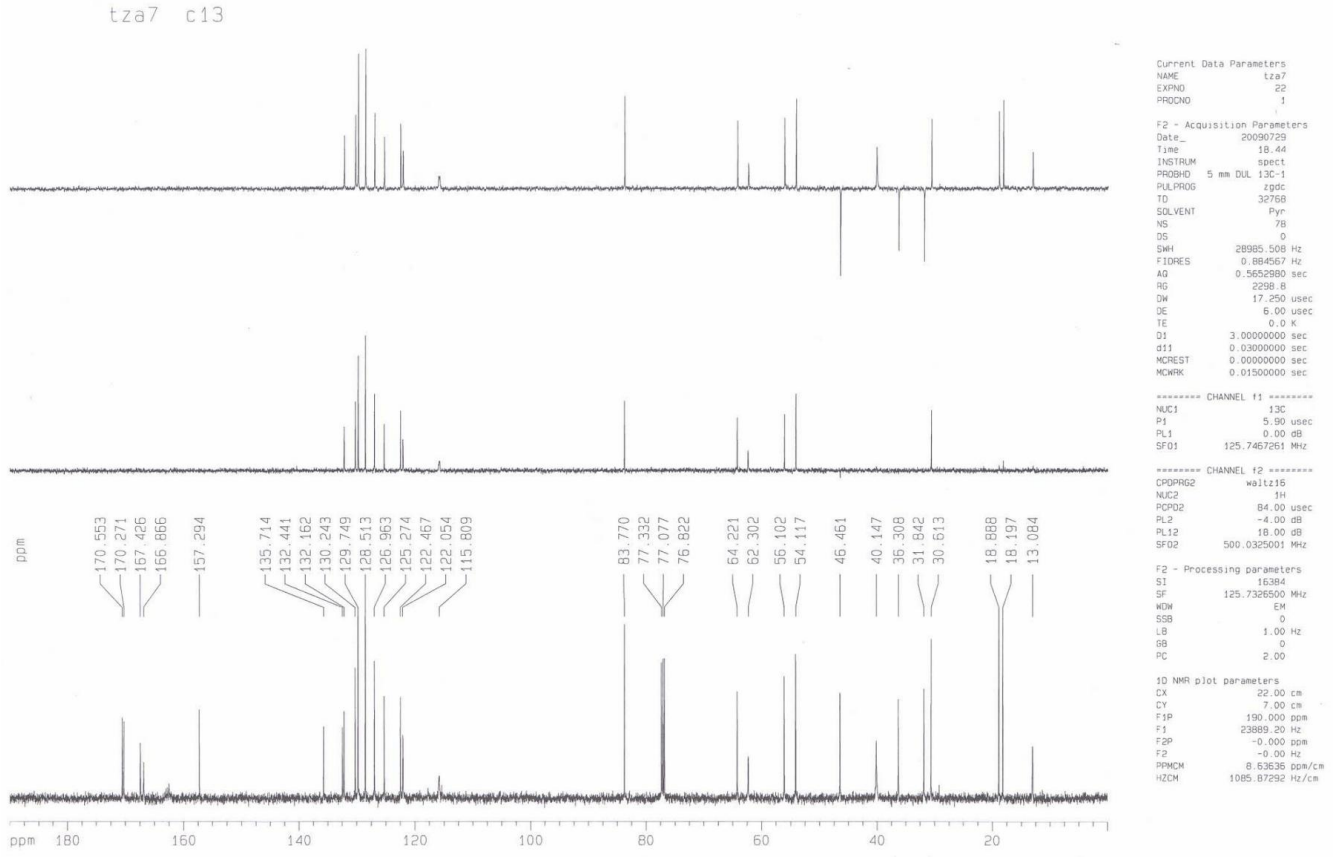
S26 The CD spectrum of Apetaline B (2)



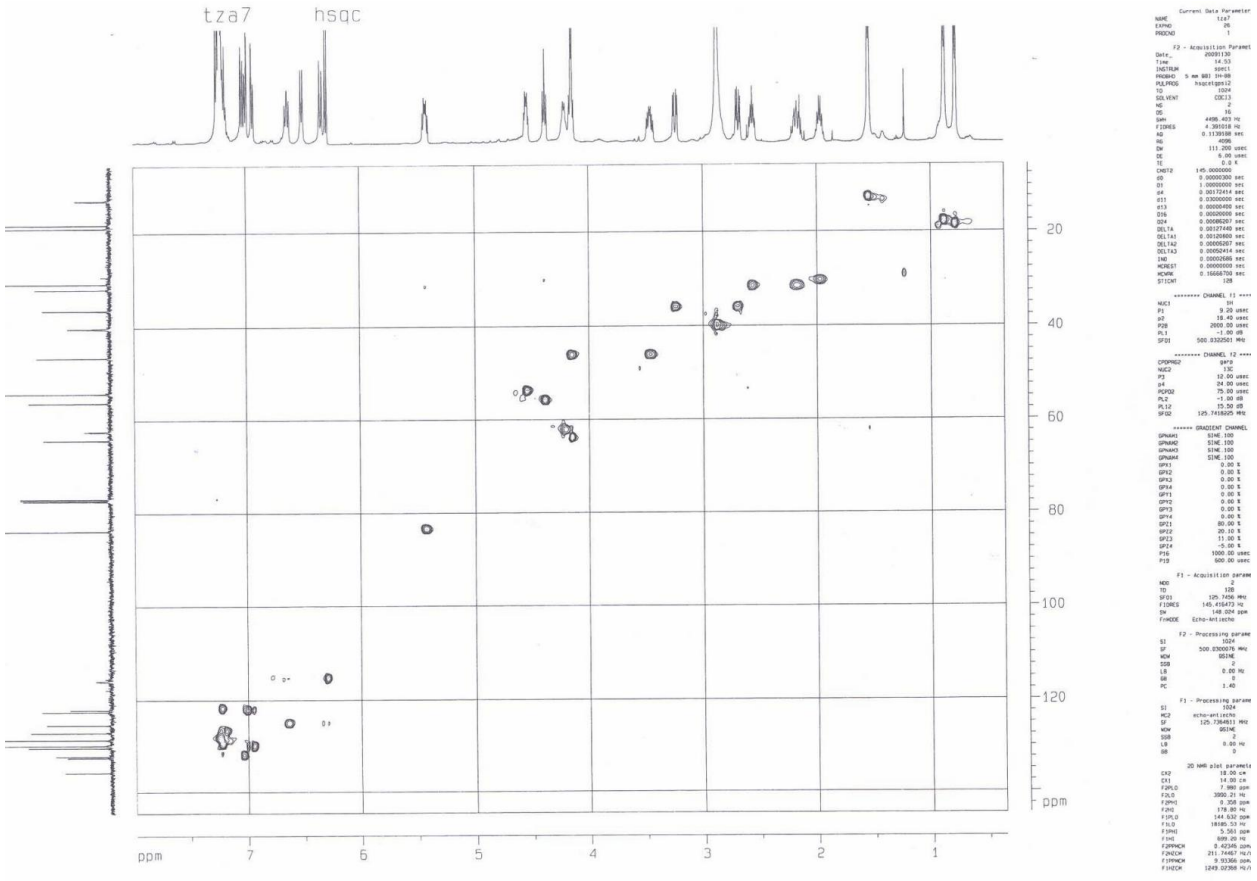
S27 The ^{1}H NMR spectrum of *epi*-Mauritine A (3) in $CDCl_3$



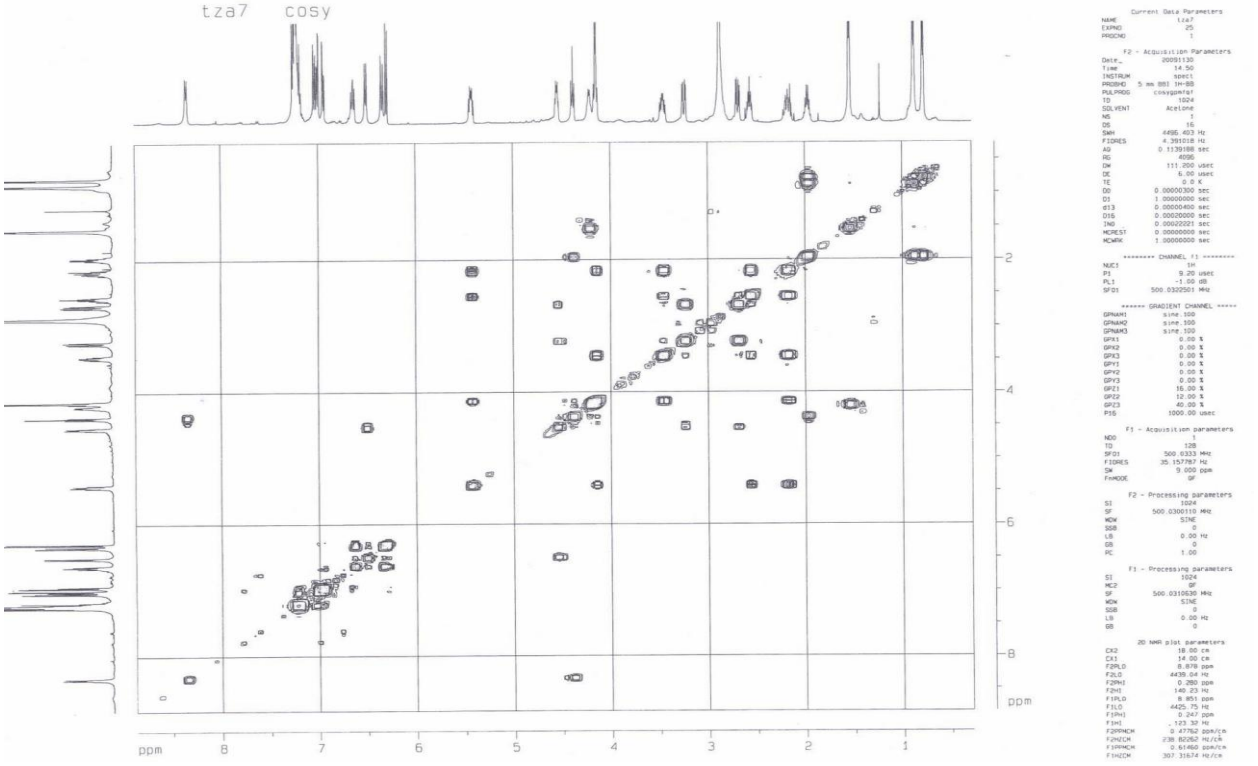
S28 The ^{13}C NMR spectrum of *epi*-Mauritine A (3) in $CDCl_3$



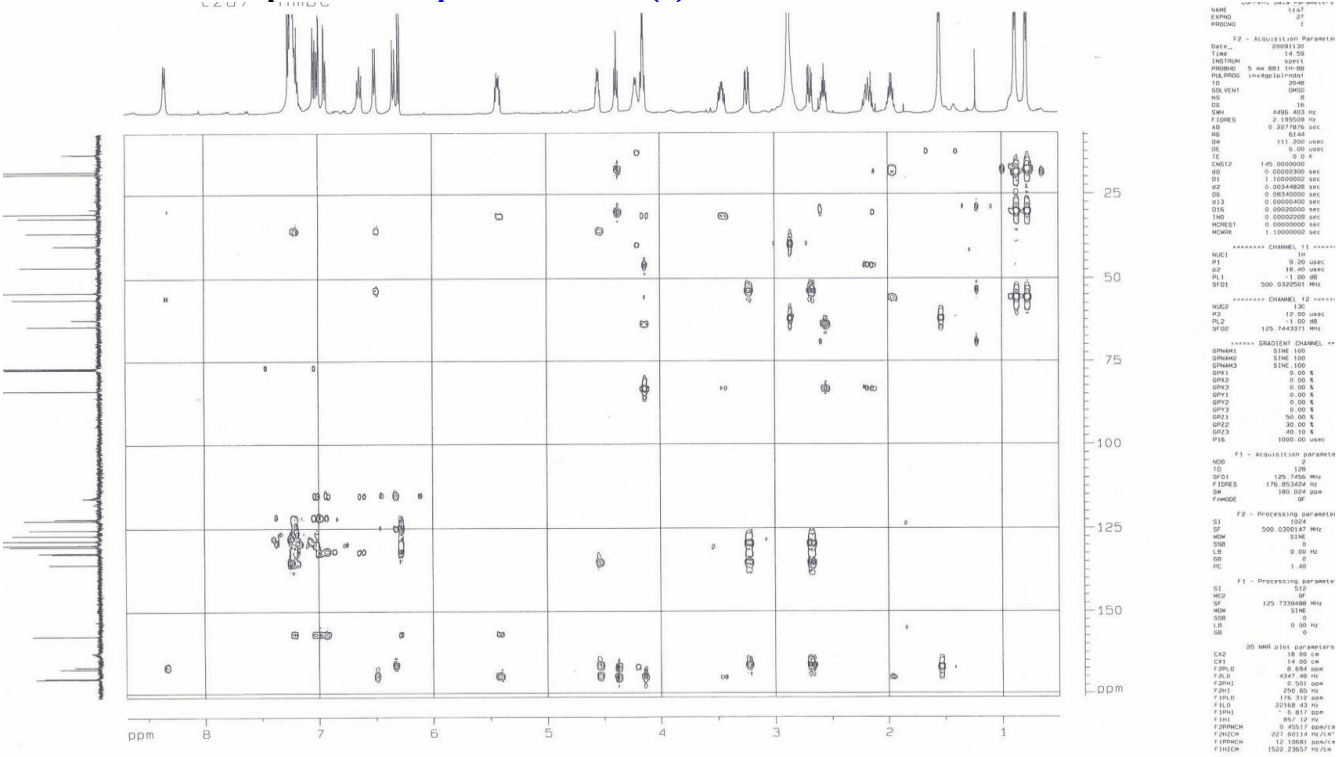
S29 The HSQC spectrum of *epi*-Mauritine A (3)



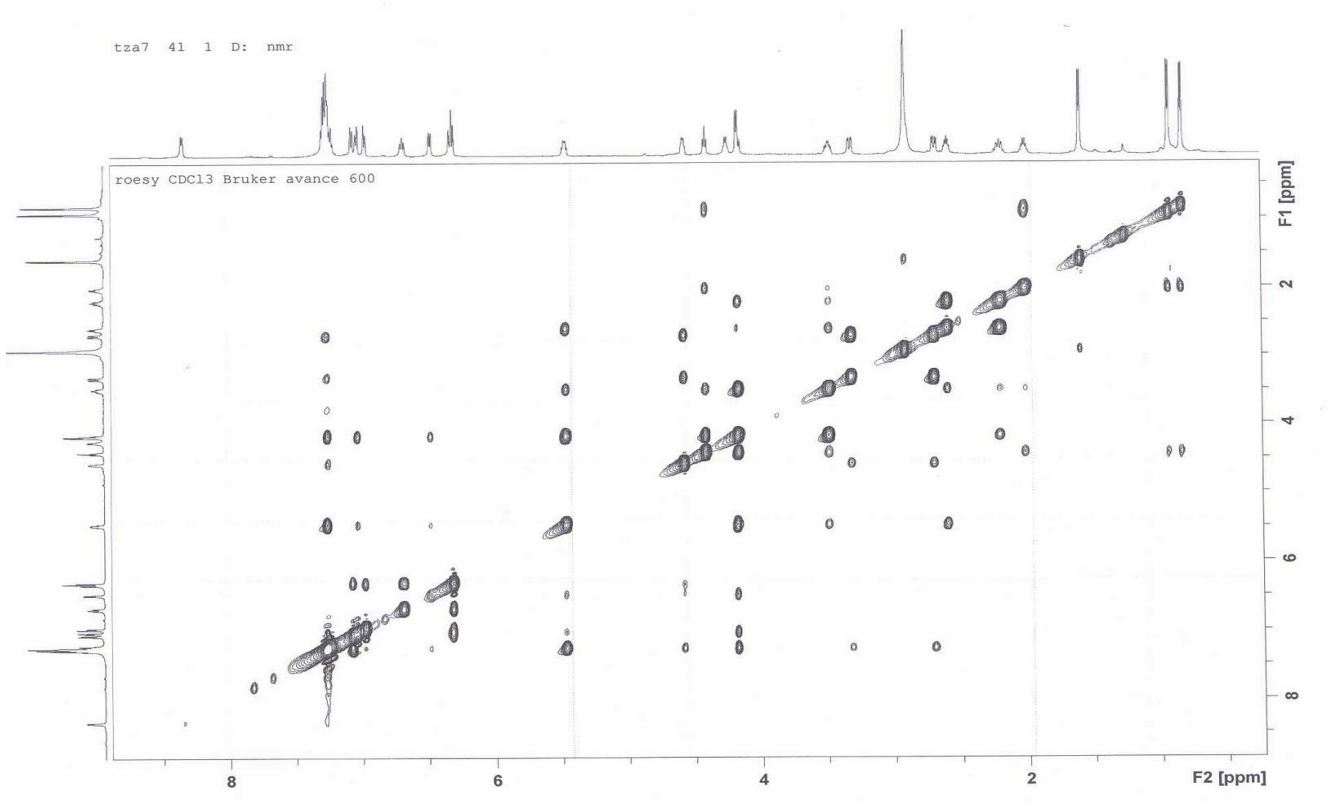
S30 The H-H COSY spectrum of *epi*-Mauritine A (3)



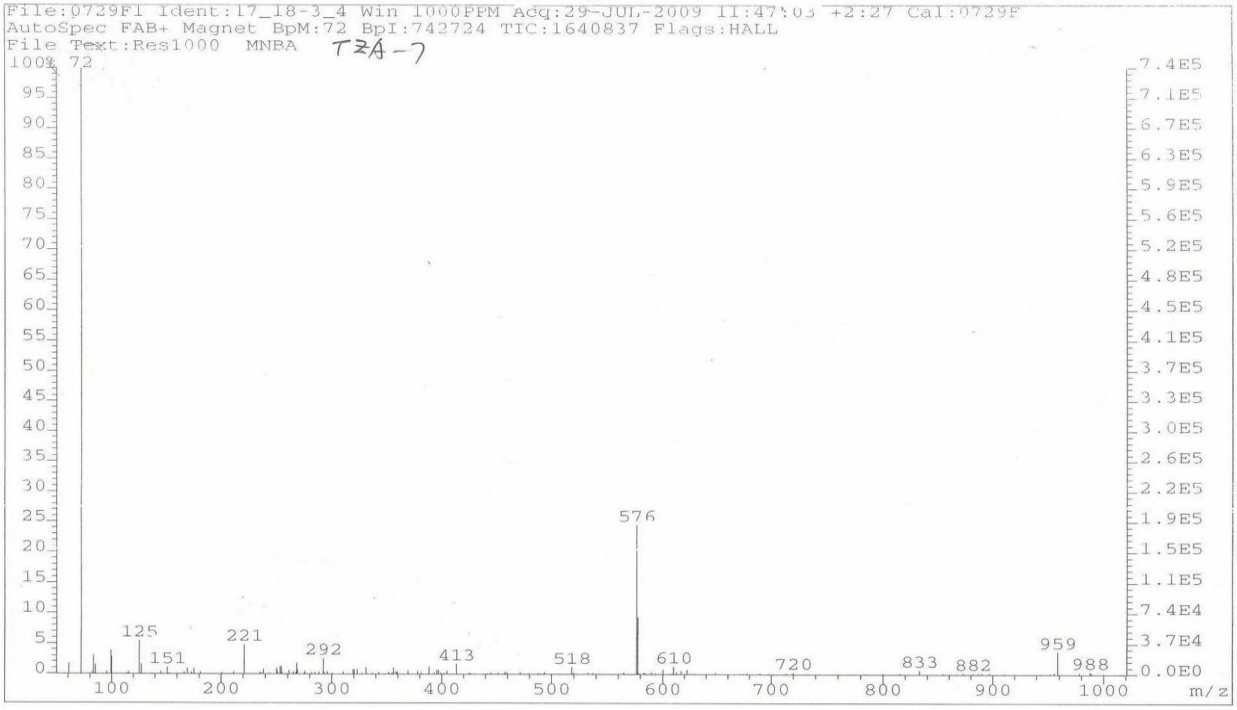
S31 The HMBC spectrum of *epi*-Mauritine A (3)



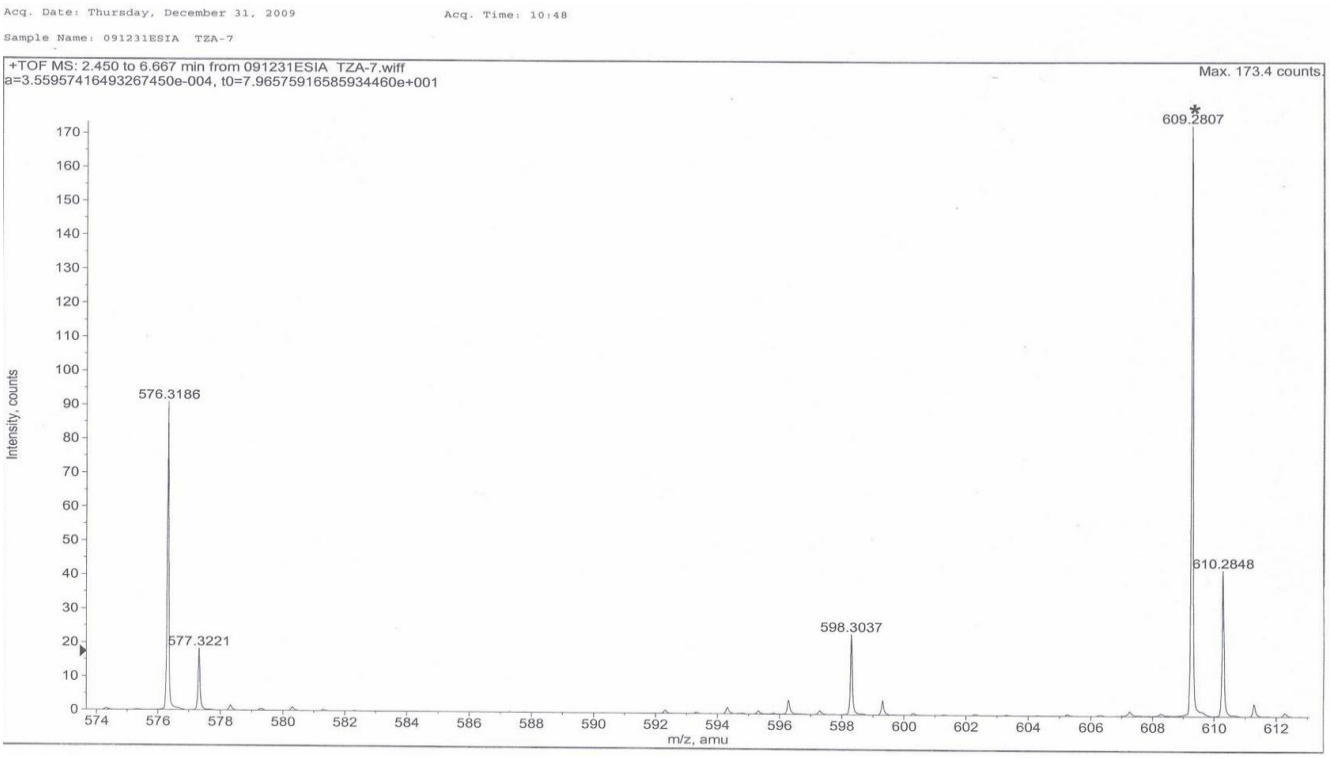
S32 The ROESY spectrum of *epi*-Mauritine A (3)



S33 The Positive FABMS of *epi*-Mauritine A (3)



S34 The Positive HRESIMS of *epi*-Mauritine A (3)



S34 The Positive HRESIMS of *epi*-Mauritine A (3)

Acq. Date: Thursday, December 31, 2009 Acq. Time: 10:48

Sample Name: 091231ESIA TZA-7

Elemental composition calculator

Target m/z: +576.3186 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 091231ESIA TZA-7.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	5	5
8	Na	0	0
9	O	4	6
10	S	0	0

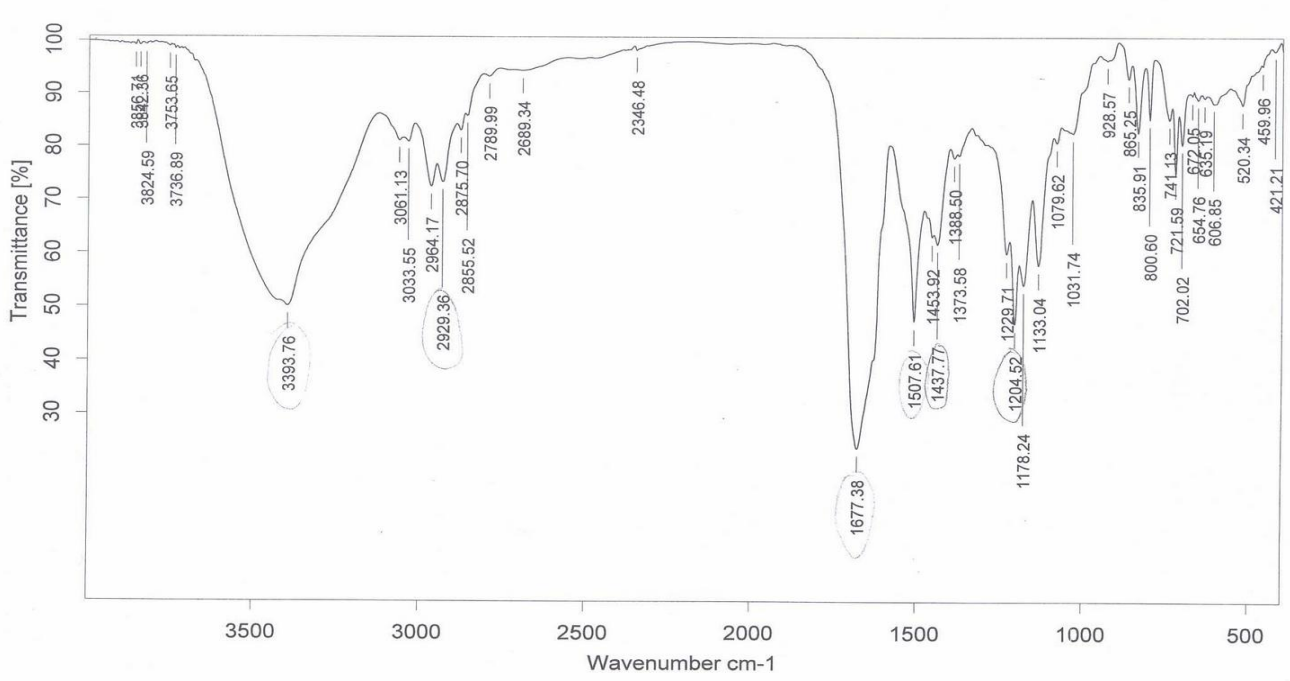
Acq. Date: Thursday, December 31, 2009 Acq. Time: 10:48

Sample Name: 091231ESIA TZA-7

	Elements	Min Number	Max Number
11	Si	0	0

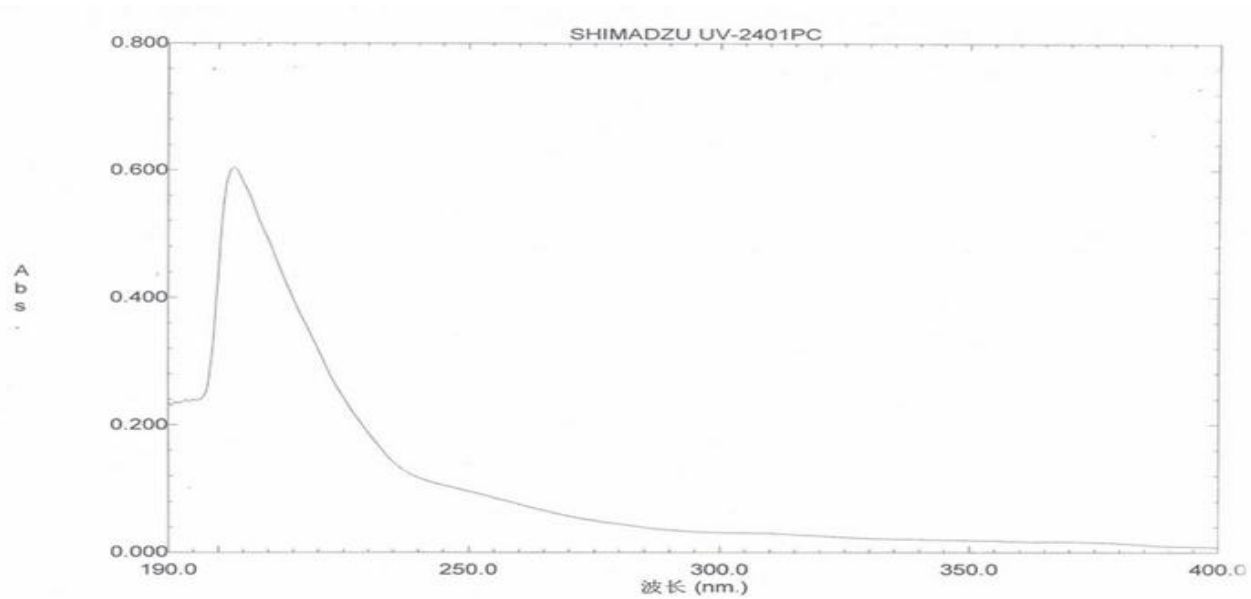
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C32 H42 N5 O5	576.3185	0.0050	0.0088	14.5

S35 The IR spectrum of *epi*-Mauritine A (3)



Sample : TZA-7	Frequency Range : 399.271 - 3996.57	Measured on : 03/01/2010	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 100103IR1	Zerofilling : 2	Acquisition : Double Sided,For	

S36 The UV spectrum of *epi*-Mauritine A (3)



文件名: TZA-7

TZA-7

样品浓度: 0.0077毫克/毫升
溶剂: 甲醇

创建于: 17:25 09-12-23
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 2.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	203.00	0.6040
2	193.40	0.2393

S37 The $[\alpha]_D$ of *epi*-Mauritine A (3)

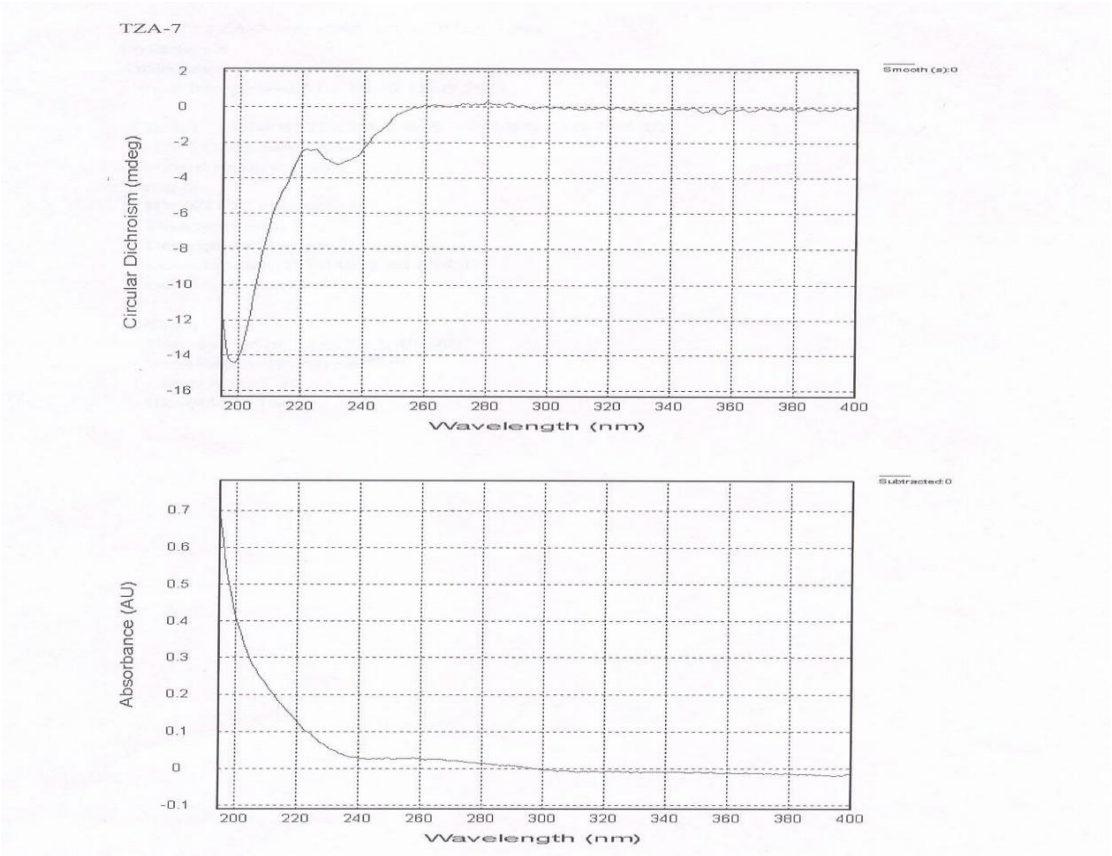
Optical rotation measurement

Model : P-1020 (A060460638)

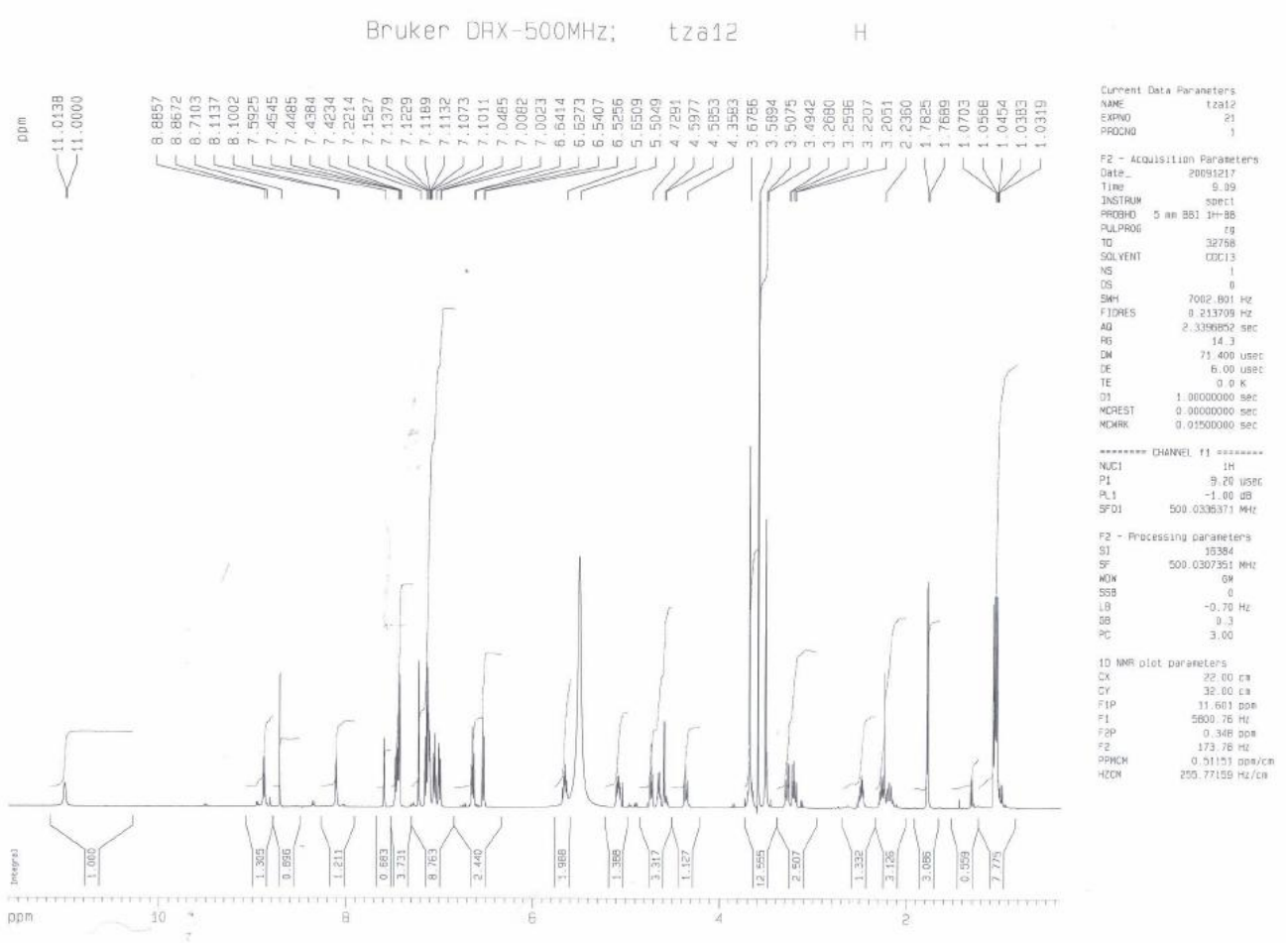
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	1 (1/3)	Sp.Rot	-231.2800	-0.5782 0.0000	15.2 50.00 Cell	Thu Dec 24 14:53:01 2009 0.00500g/mlMeOH TZA-7	Na 589nm	2 sec 10 sec
No.2	1 (2/3)	Sp.Rot	-231.0000	-0.5775 0.0000	15.3 50.00 Cell	Thu Dec 24 14:53:14 2009 0.00500g/mlMeOH TZA-7	Na 589nm	2 sec 10 sec
No.3	1 (3/3)	Sp.Rot	-231.2000	-0.5780 0.0000	15.3 50.00 Cell	Thu Dec 24 14:53:27 2009 0.00500g/mlMeOH TZA-7	Na 589nm	2 sec 10 sec

-231.1600°

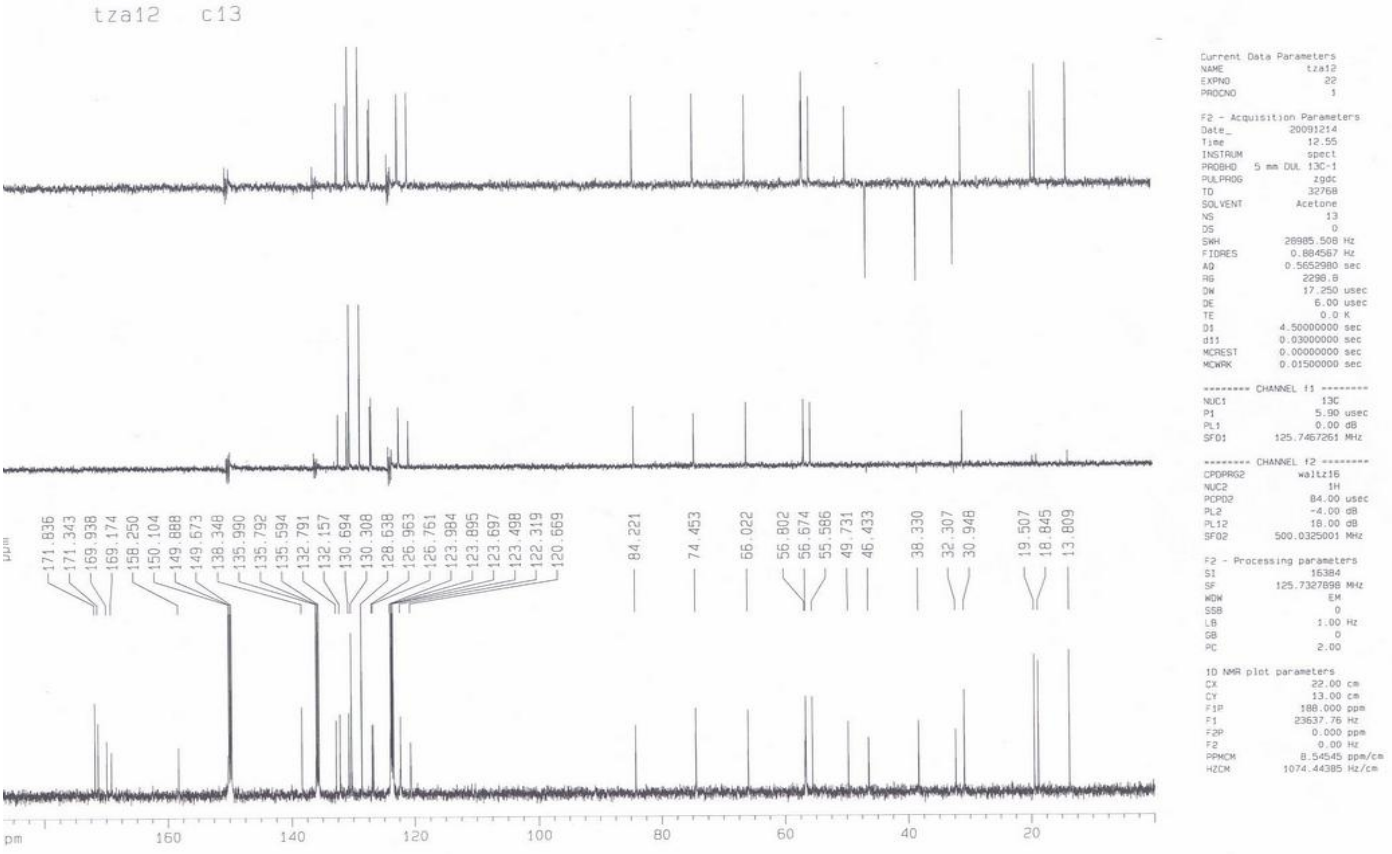
S38 The CD spectrum of *epi*-Mauritine A (3)



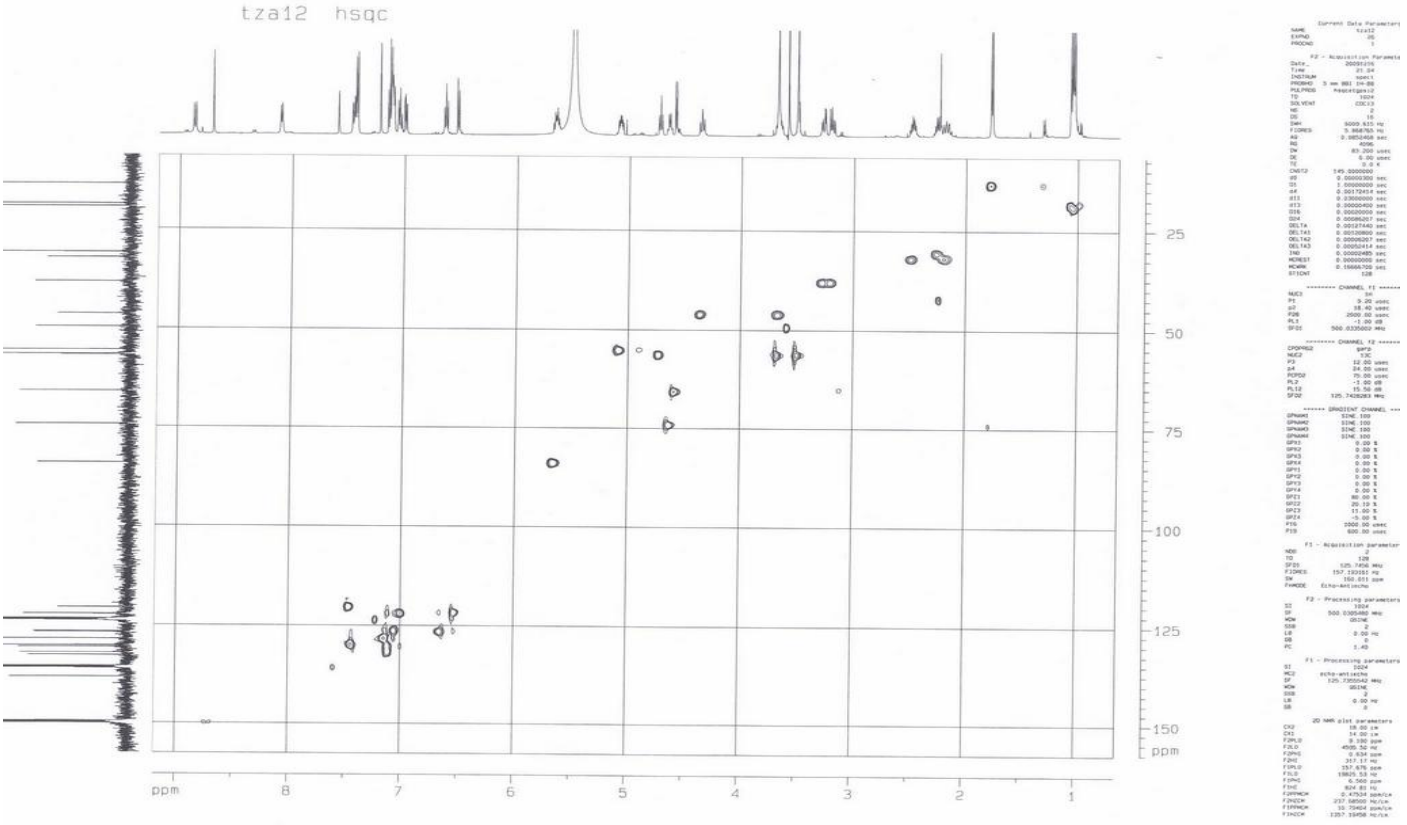
S39 The ^{1}H NMR spectrum of *epi*-Mauritine A *N*-oxide (4) in C_5D_5N



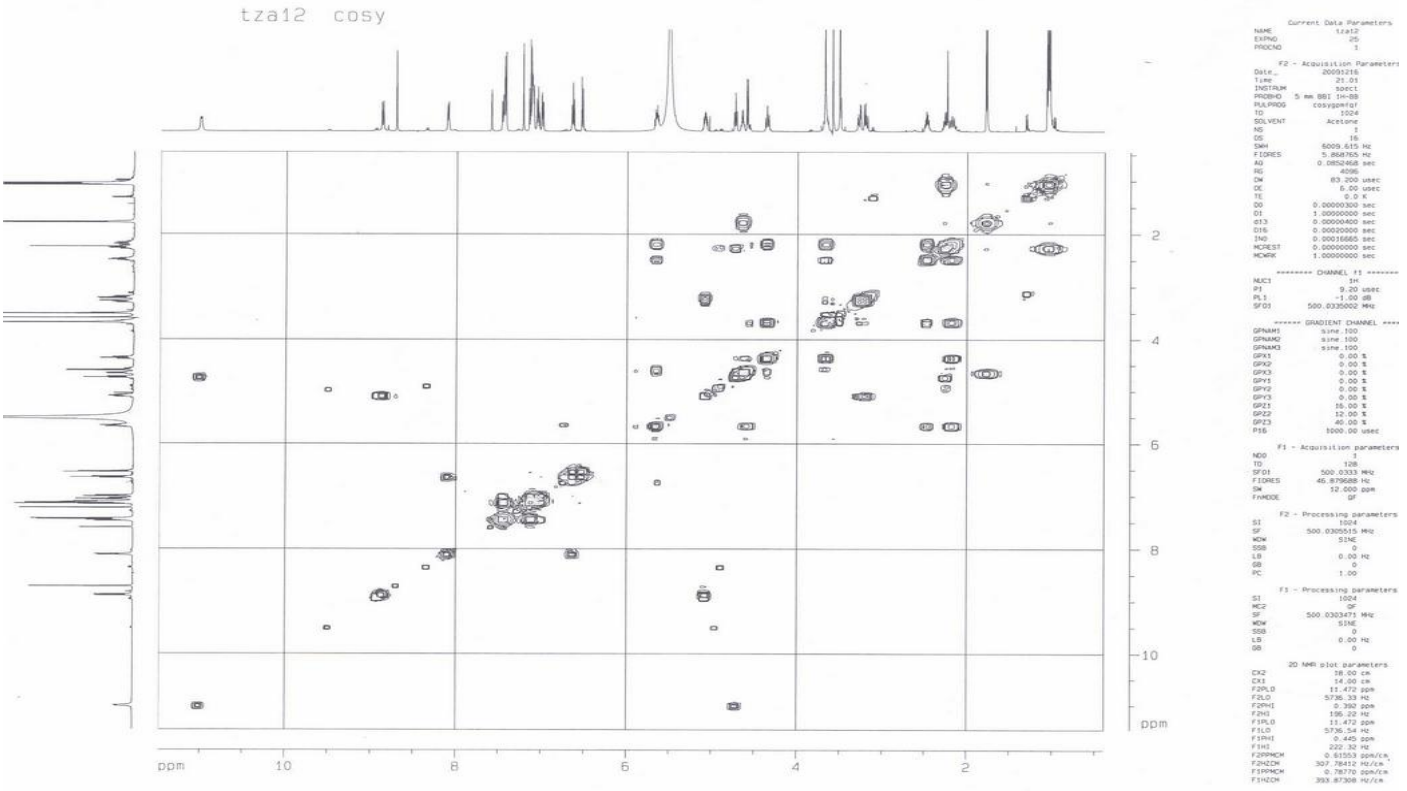
S40 The ^{13}C NMR spectrum of *epi*-Mauritine A *N*-oxide (4) in C_5D_5N



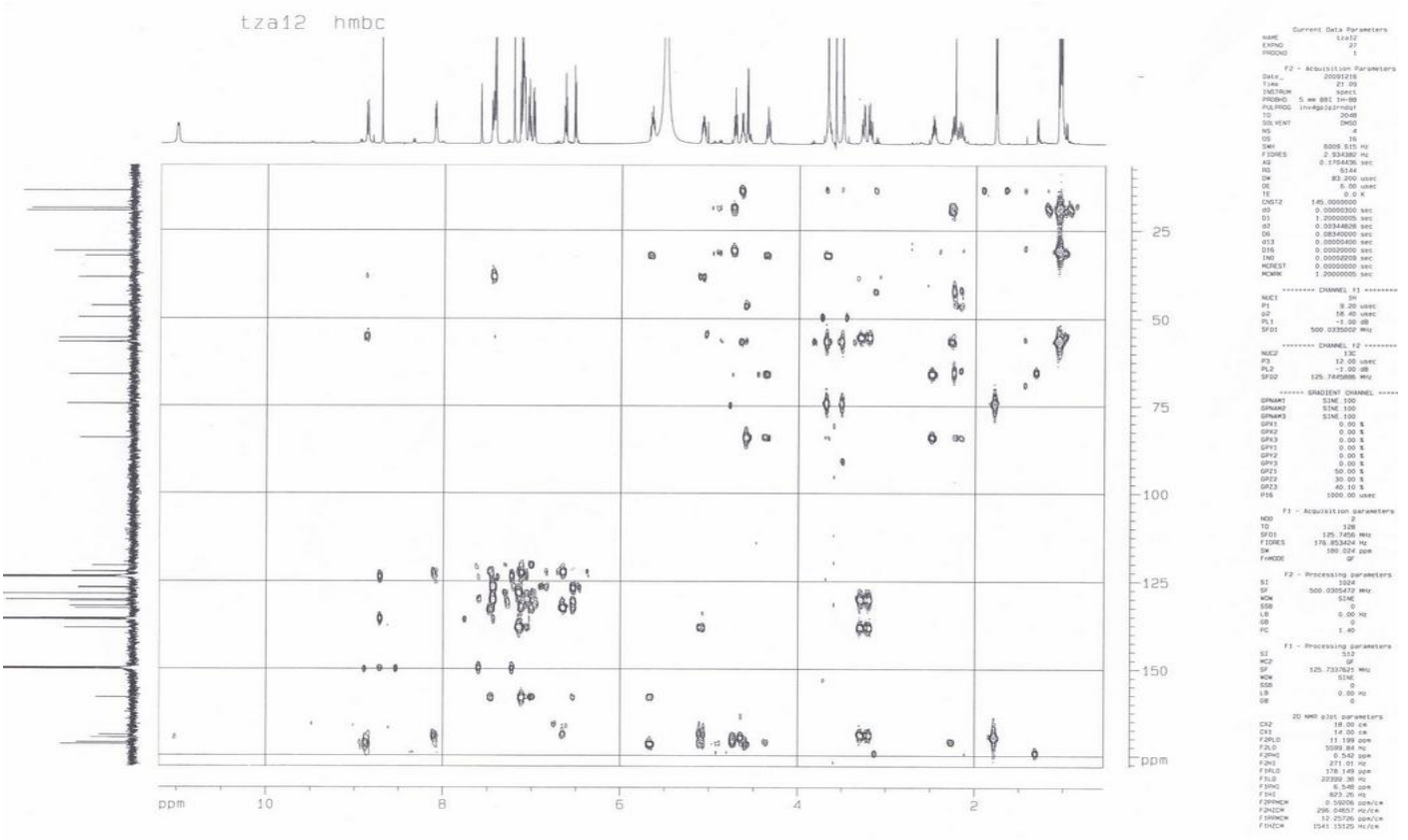
S41 The HSQC spectrum of *epi*-Mauritine A *N*-oxide (4)



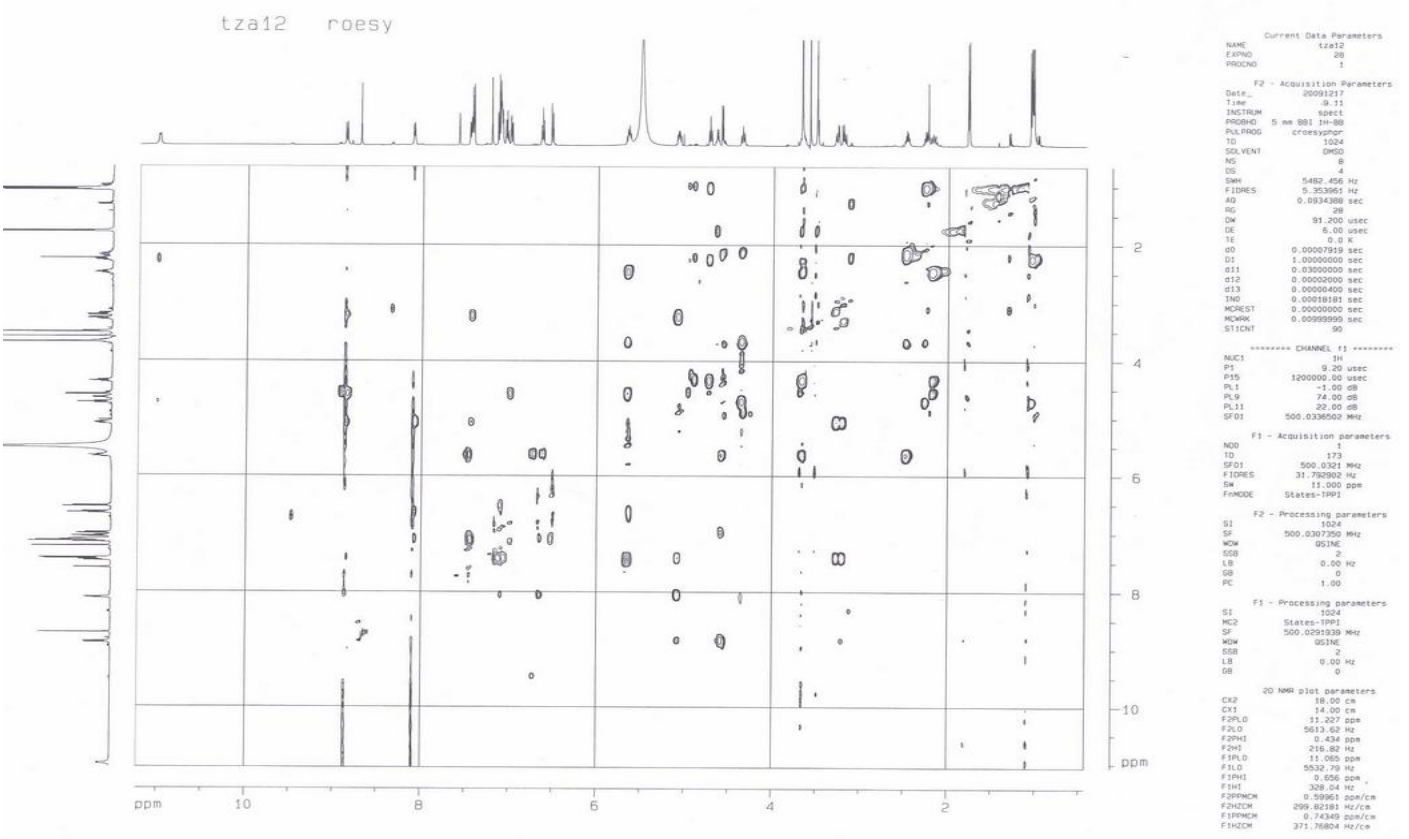
S42 The ^{1}H-^{1}H COSY spectrum of *epi*-Mauritine A *N*-oxide (4)



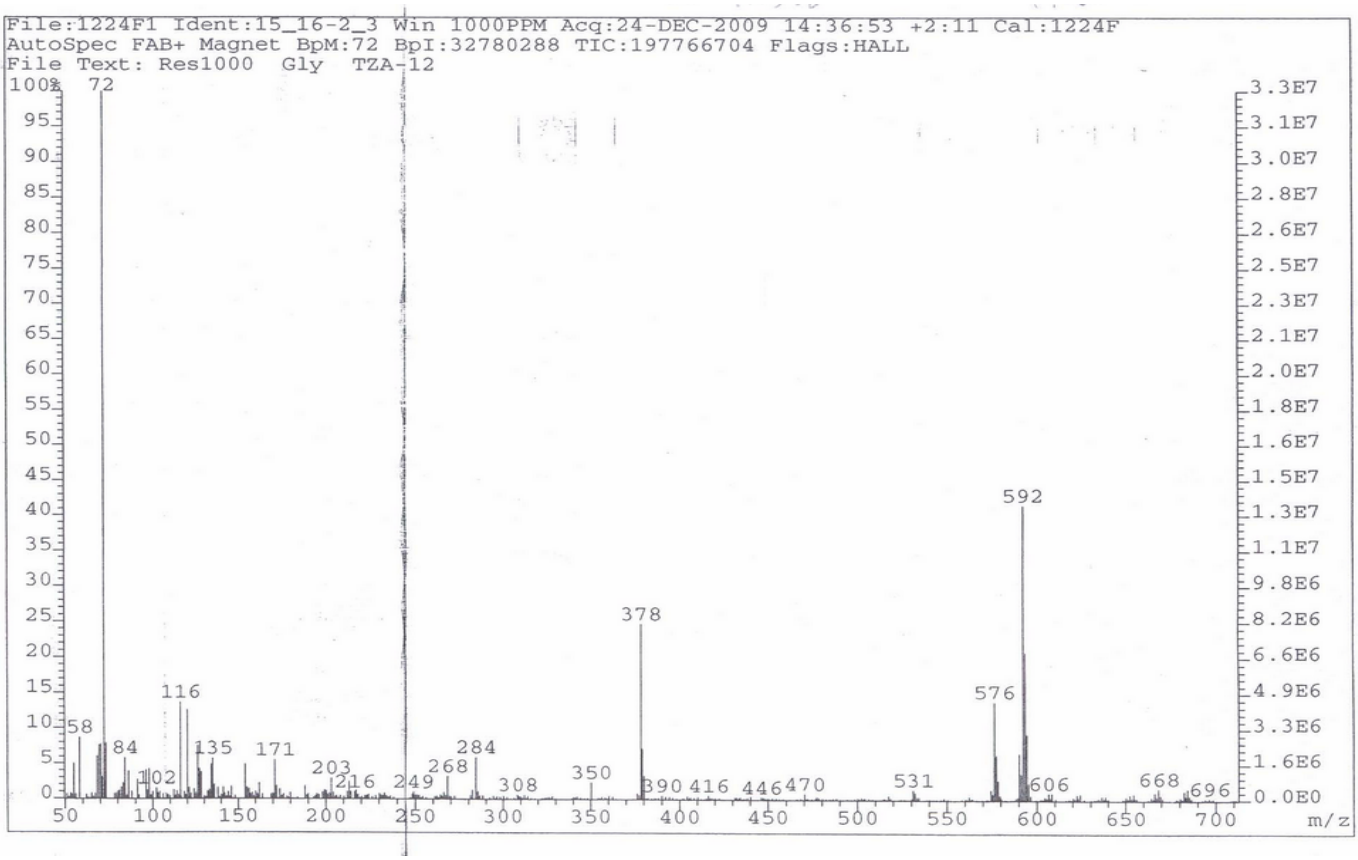
S43 The HMBC spectrum of *epi*-Mauritine A *N*-oxide (4)



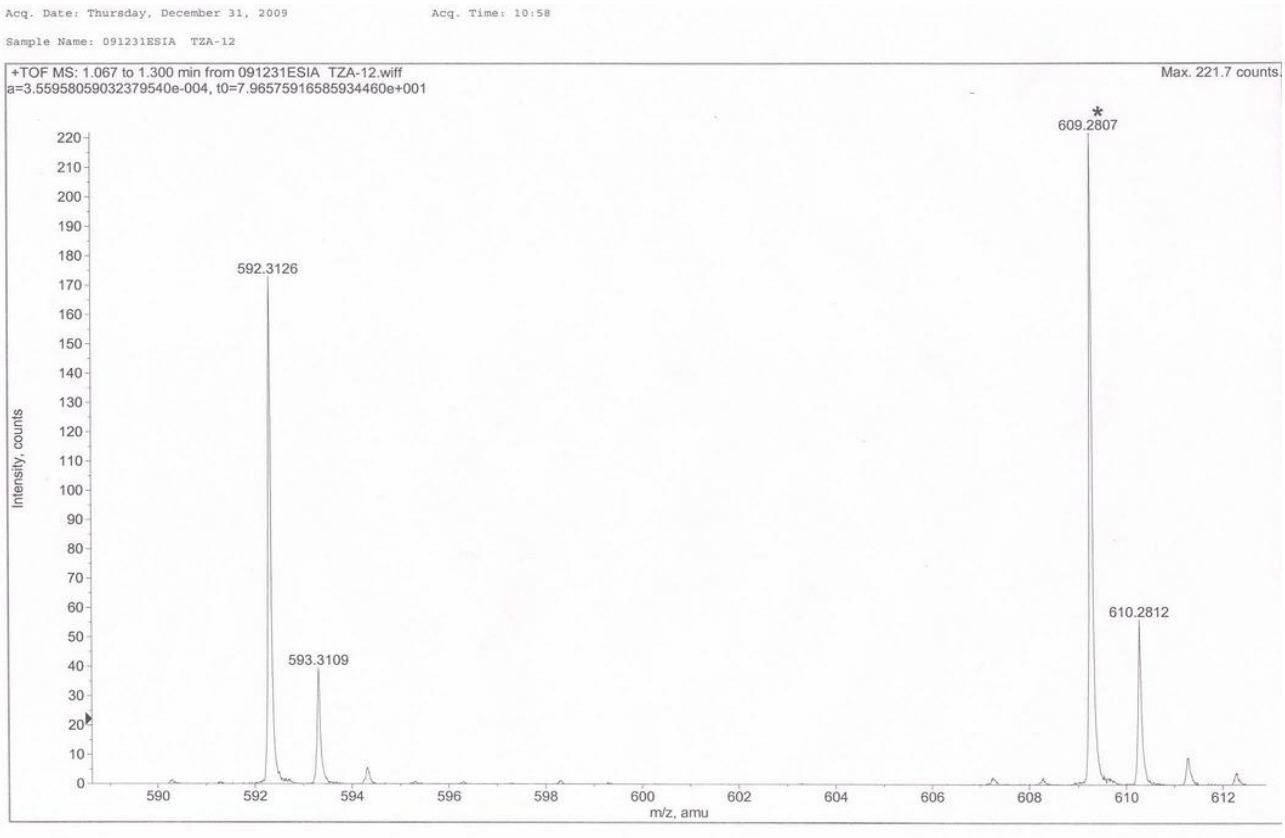
S44 The ROSEY spectrum of *epi*-Mauritine A *N*-oxide (4)



S45 The Positive FABMS of *epi*-Mauritine A *N*-oxide (4)



S46 The Positive HRESIMS of *epi*-Mauritine A *N*-oxide (4)



S46 The Positive HRESIMS of *epi*-Mauritine A *N*-oxide (4)

Acq. Date: Thursday, December 31, 2009 Acq. Time: 10:58

Sample Name: 091231ESIA TZA-12

Elemental composition calculator

Target m/z: +592.3126 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 091231ESIA TZA-12.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	5	5
8	Na	0	0
9	O	4	6
10	S	0	0

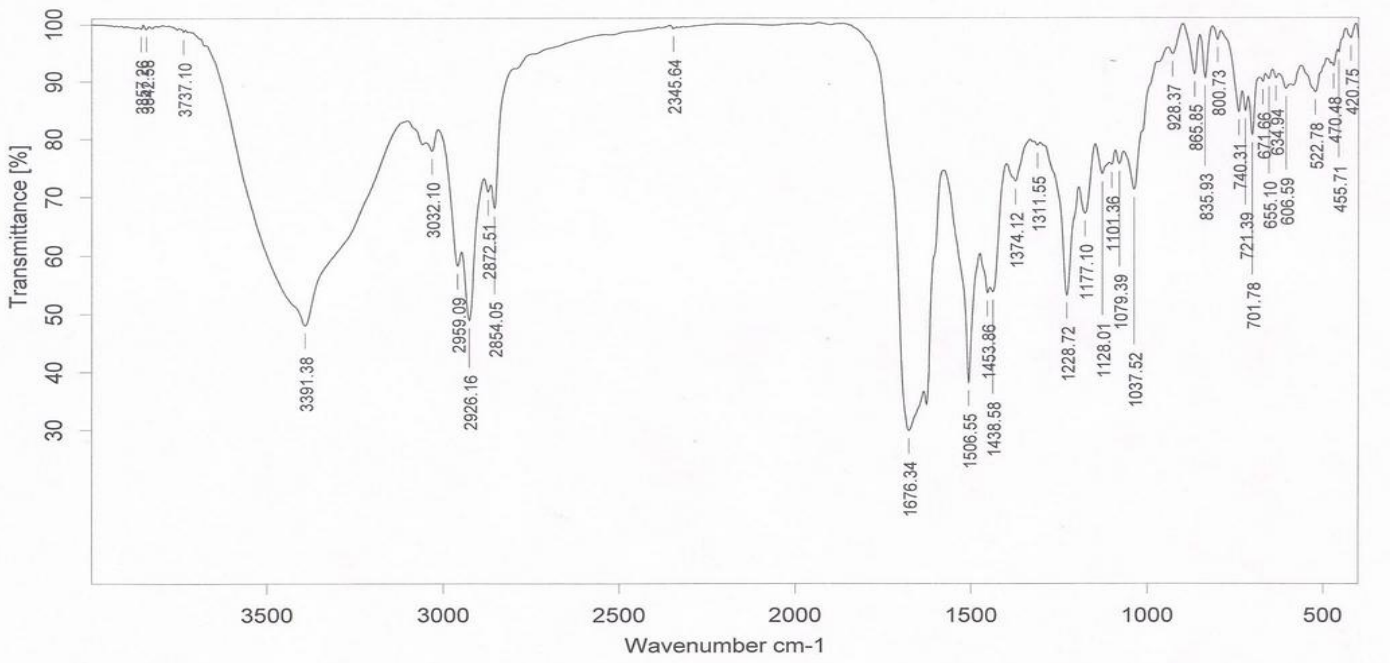
Acq. Date: Thursday, December 31, 2009 Acq. Time: 10:58

Sample Name: 091231ESIA TZA-12

	Elements	Min Number	Max Number
11	Si	0	0

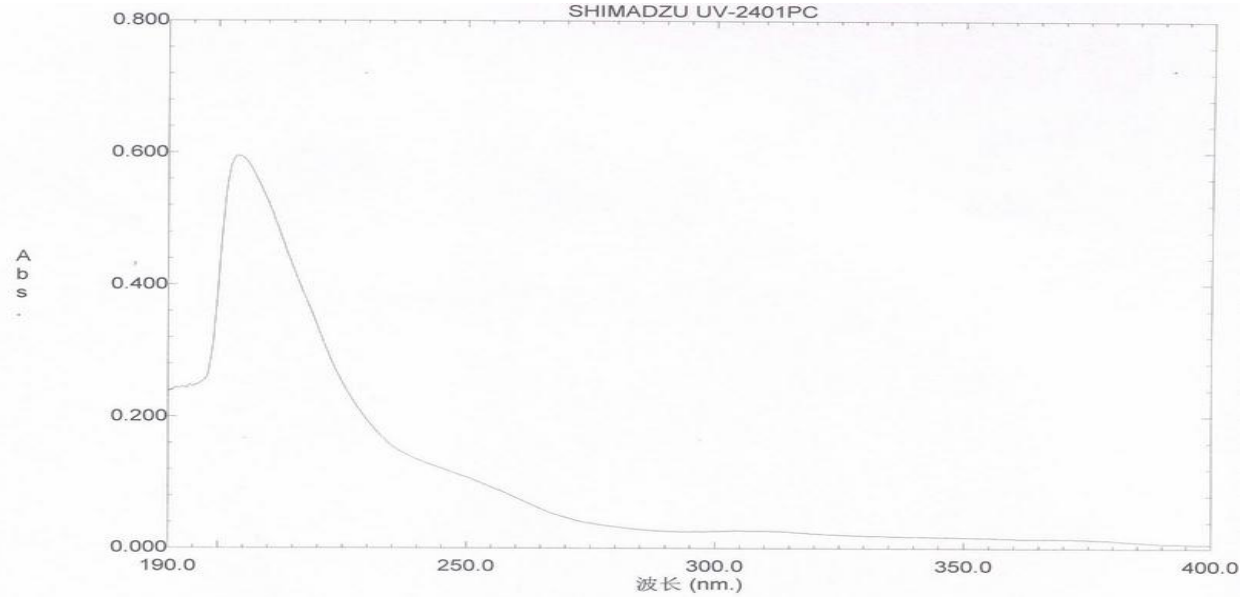
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C32 H42 N5 O6	592.3135	-0.9095	-1.5356	14.5

S47 The IR spectrum of *epi*-Mauritine A *N*-oxide (4)



Sample : TZA-12	Frequency Range : 399.271 - 3996.57	Measured on : 03/01/2010	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 100103IR2	Zerofilling : 2	Acquisition : Double Sided,For	

S48 The UV spectrum of *epi*-Mauritine A *N*-oxide (4)



文件名: TZA-12

创建于: 18:31 09-12-23
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 2.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	309.40	0.0265
2	204.00	0.5950

TZA-12

样品浓度：0.0128毫克/毫升
溶剂：甲醇

S49 The $[\alpha]_D$ of *epi*-Mauritine A *N*-oxide (4)

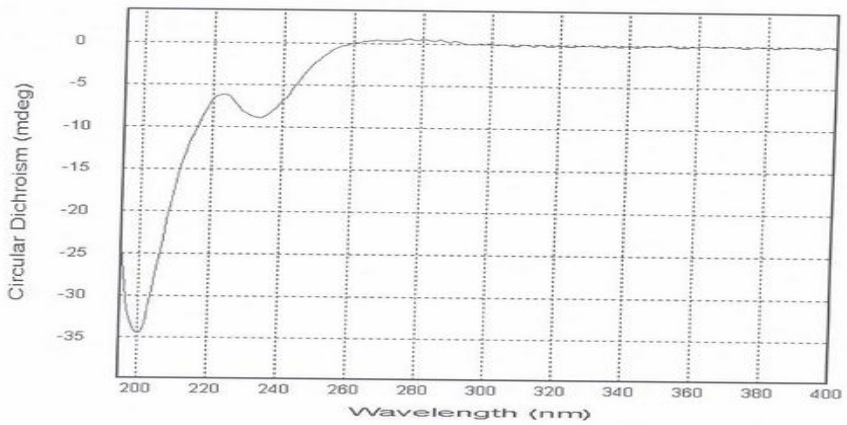
Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	2 (1/3)	Sp.Rot	-1163.0000	-0.5815 0.0000	24.3 50.00 Cell	Thu Jun 17 14:23:11 2010 0.00100g/mlMeOH TZA-12	Na 589nm	2 sec 10 sec
No.2	2 (2/3)	Sp.Rot	-1165.2000	-0.5826 0.0000	24.3 50.00 Cell	Thu Jun 17 14:23:24 2010 0.00100g/mlMeOH TZA-12	Na 589nm	2 sec 10 sec
No.3	2 (3/3)	Sp.Rot	-1163.4000	-0.5817 0.0000	24.3 50.00 Cell	Thu Jun 17 14:23:37 2010 0.00100g/mlMeOH TZA-12	Na 589nm	2 sec 10 sec

$-1163.866)^{\circ}$

S50 The CD spectrum of *epi*-Mauritine A *N*-oxide (4)



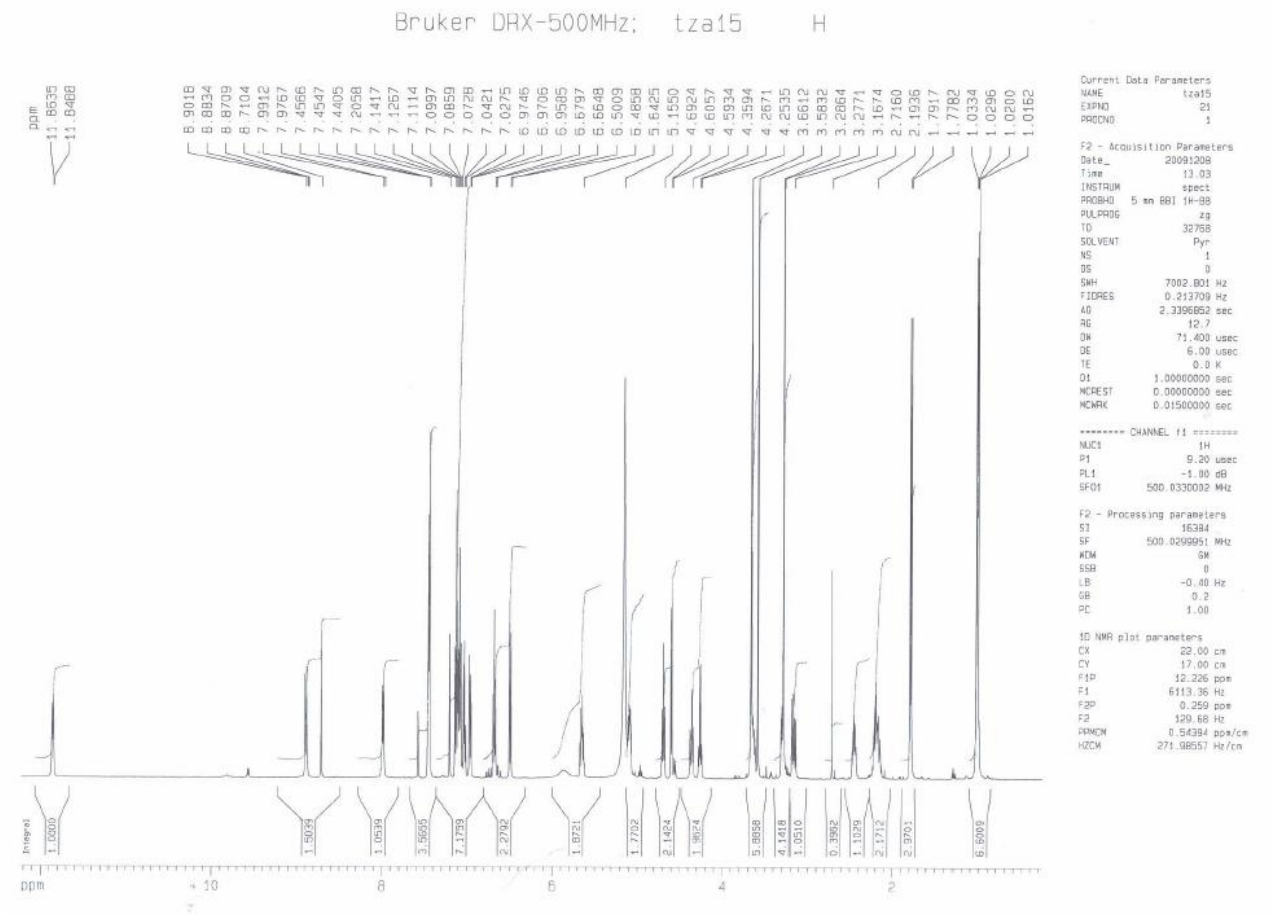
File: CD TZA-12-1mm(195-400)0008.dsx
ProBinaryX
Attributes :
- Time Stamp :Thu Dec 16 15:49:53 2010

- File ID : {9E4B3D56-D716-4b56-811A-59206833EFA2}
- Is CFR Compliant : false
- Original unaltered data

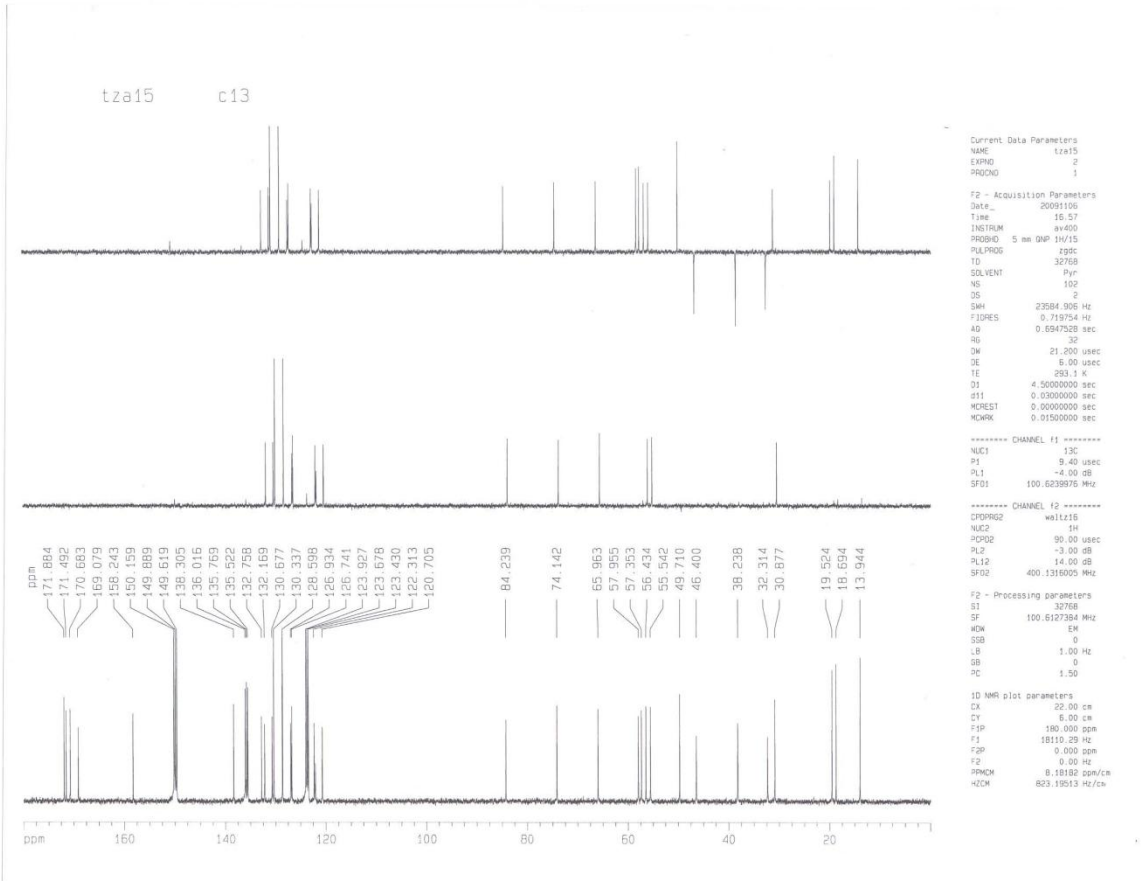
Remarks:
- HV (CDDC channel): 0 v
- Time per point: 1 s
- Description: Sample 1
- Concentration: 0.0180mg/ml MeOH
- Pathlength: 1 mm

Settings:
- Time-per-point: 1s (25us x 40000)
- Wavelength: 195nm - 400nm
- Step Size: 1nm
- Bandwidth: 1nm

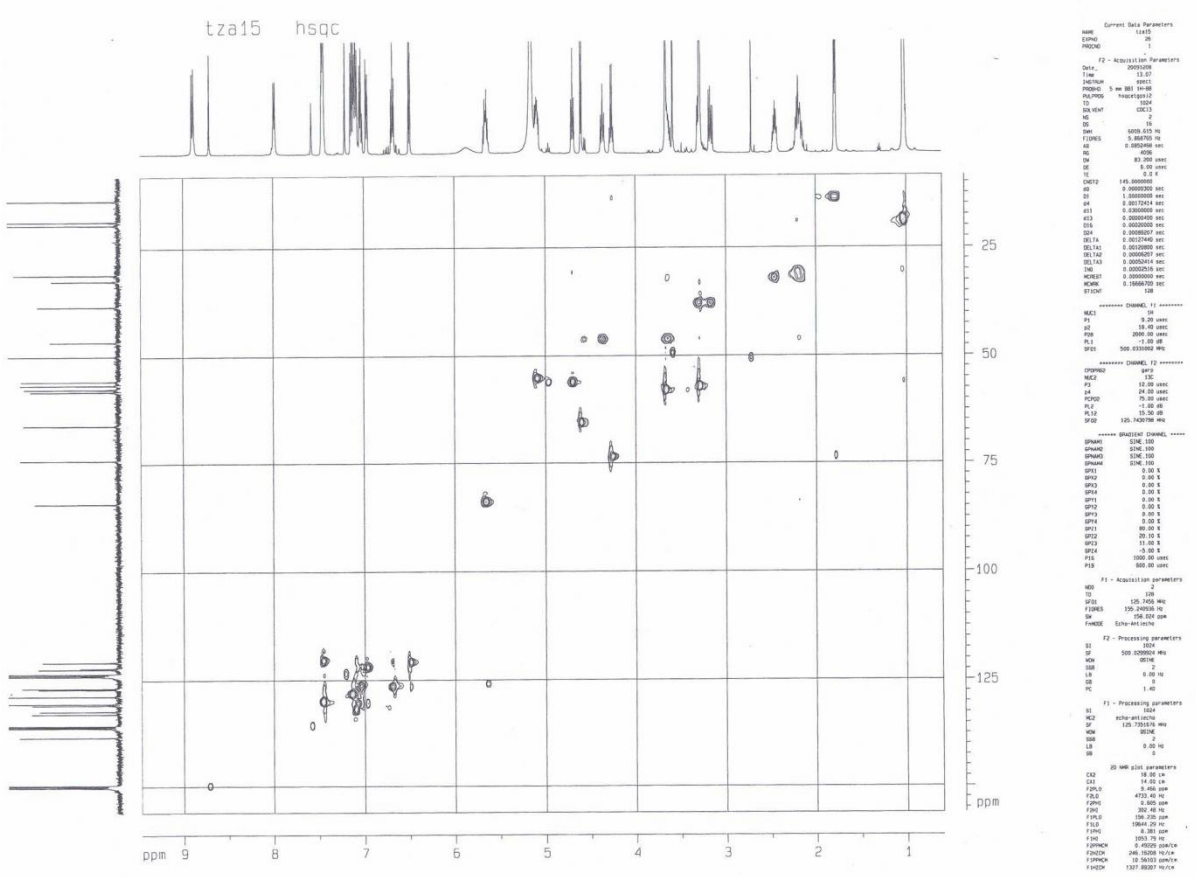
S51 The ^{1}H NMR spectrum of Mauritine A *N*-oxide (5) in C_5H_5N



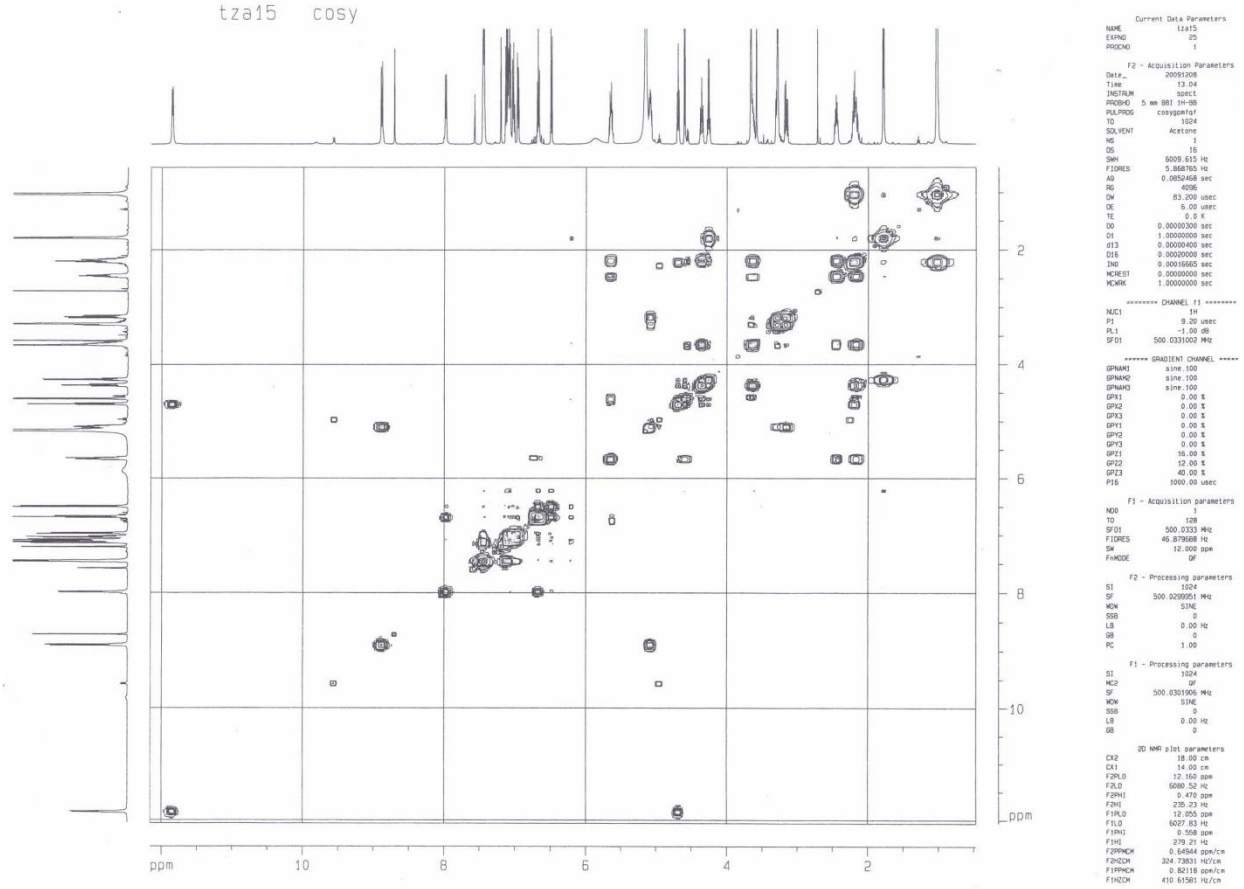
S52 The ^{13}C NMR spectrum of Mauritine A *N*-oxide (5) in C_5H_5N



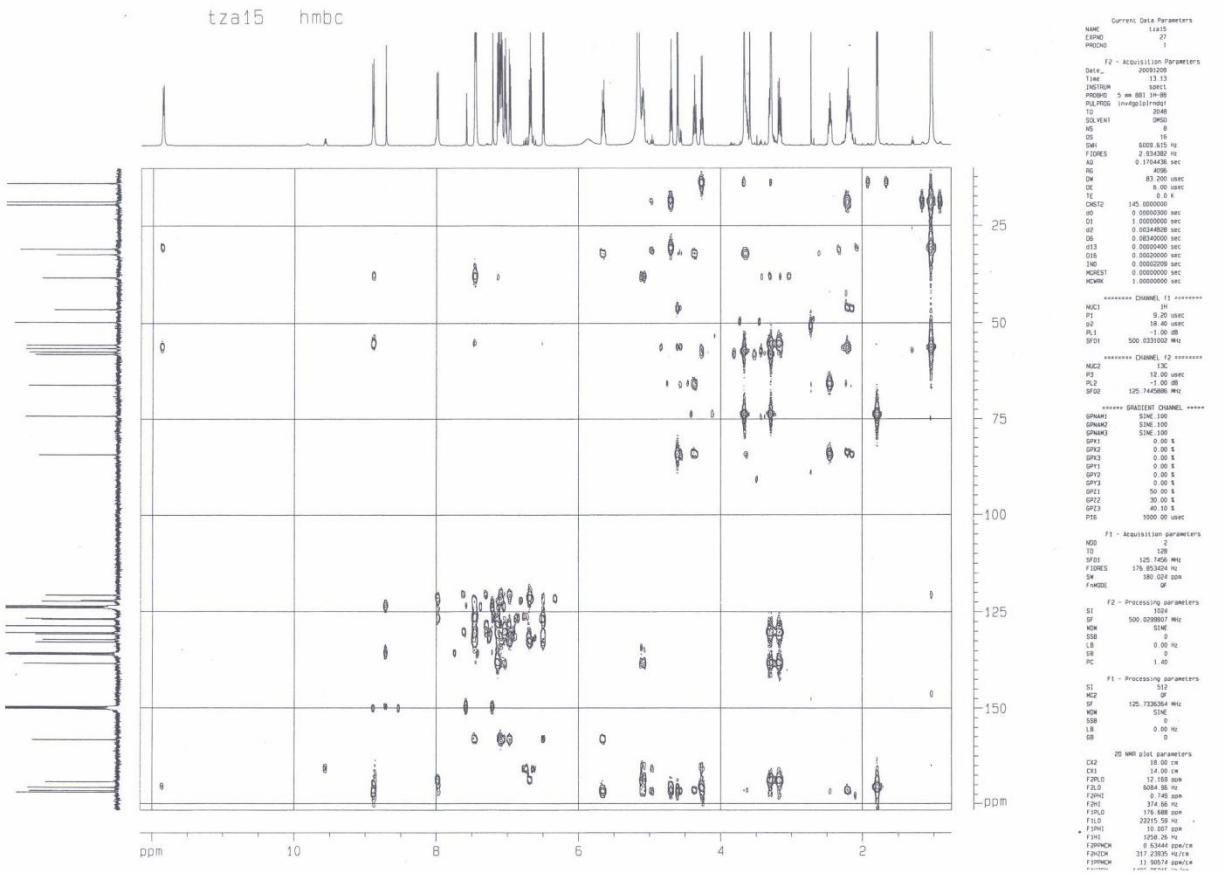
S53 The HSQC spectrum of Mauritine A *N*-oxide (5)



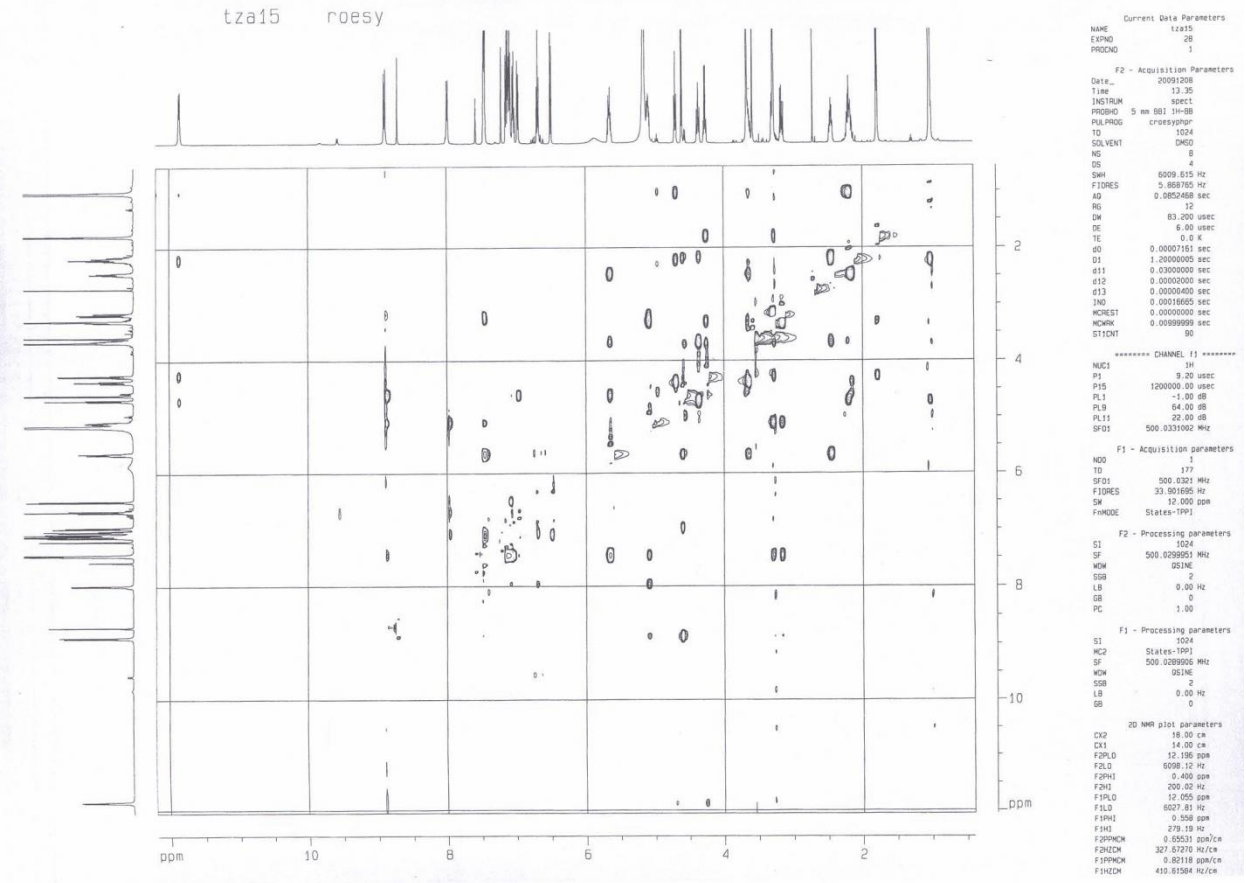
S54 The COSY spectrum of Mauritine A *N*-oxide (5)



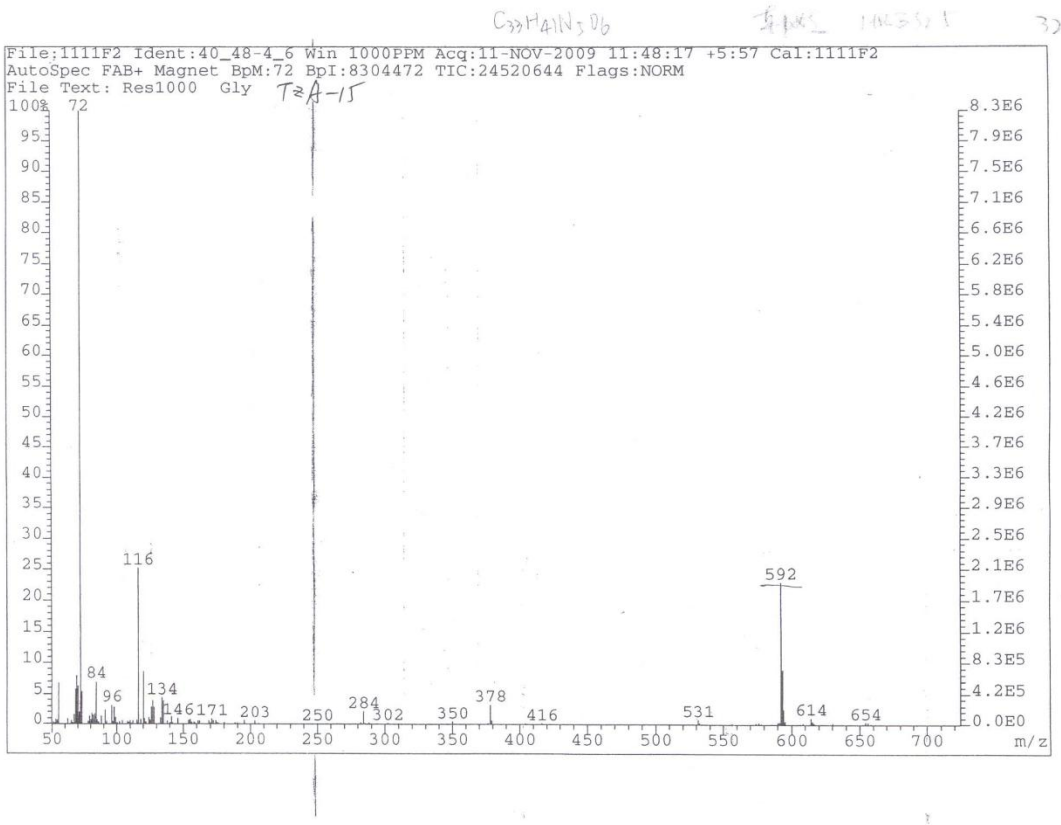
S55 The HMBC spectrum of Mauritine A *N*-oxide (5)



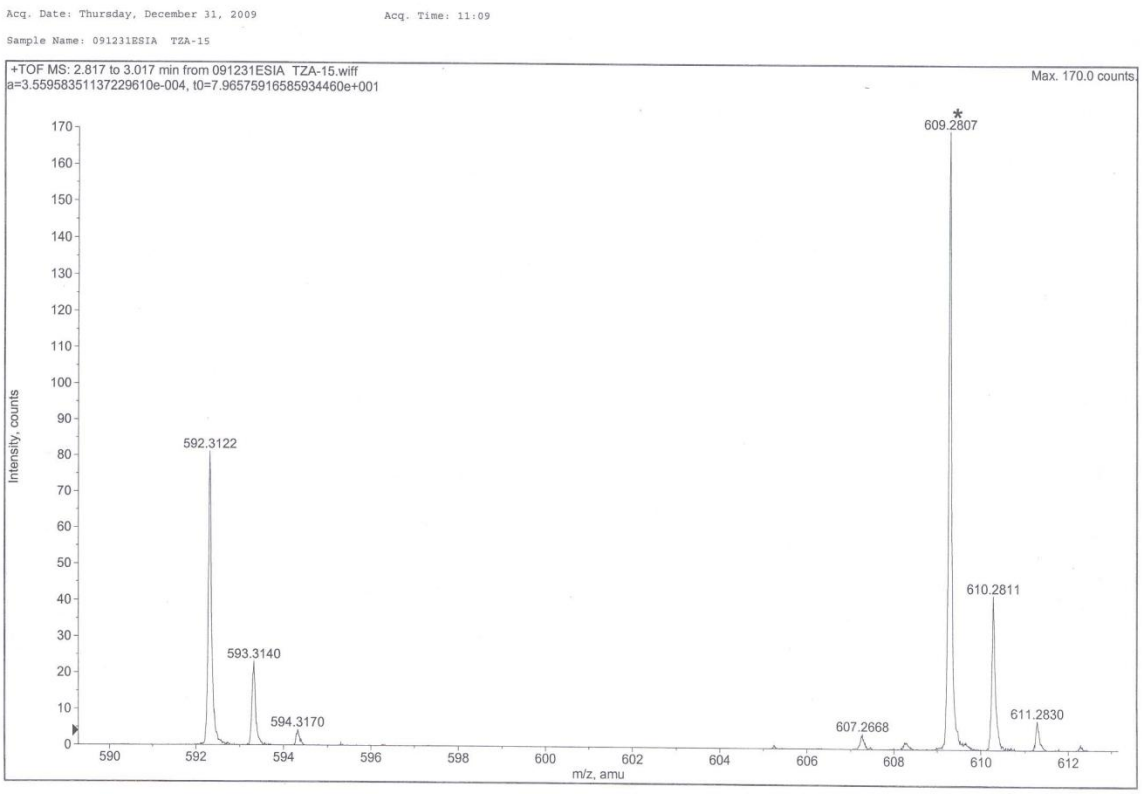
S56 The ROSEY spectrum of Mauritine A *N*-oxide (5)



S57 The Positive FABMS spectrum of Mauritine A *N*-oxide (5)



S58 The Positive HRESIMS spectrum of Mauritine A *N*-oxide (5)



S58 The Positive HRESIMS spectrum of Mauritine A *N*-oxide (5)

Acq. Date: Thursday, December 31, 2009 Acq. Time: 11:09

Sample Name: 091231ESIA TZA-15

Elemental composition calculator

Target m/z: +592.3122 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 091231ESIA TZA-15.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	5	5
8	Na	0	0
9	O	4	6
10	S	0	0

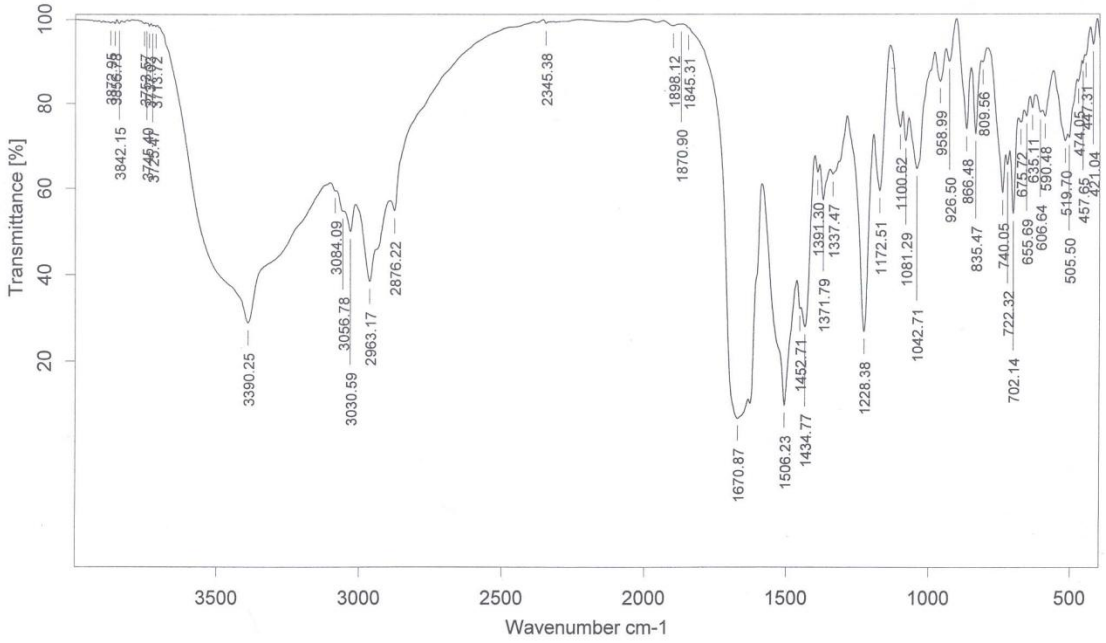
Acq. Date: Thursday, December 31, 2009 Acq. Time: 11:09

Sample Name: 091231ESIA TZA-15

	Elements	Min Number	Max Number
11	Si	0	0

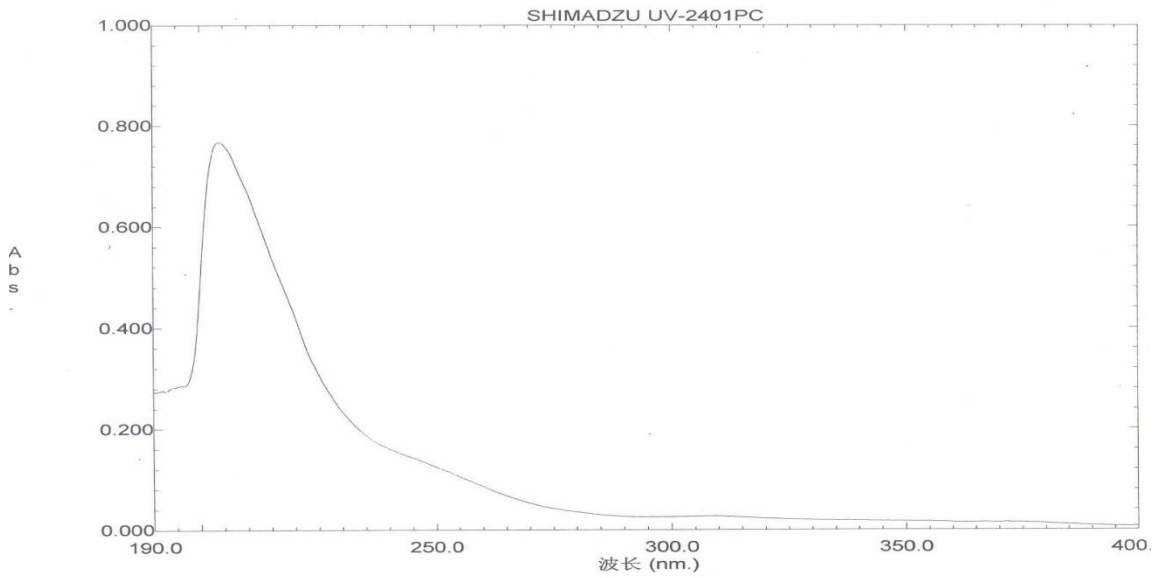
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C32 H42 N5 O6	592.3135	-1.3095	-2.2109	14.5

S59 The IR spectrum of Mauritine A *N*-oxide (5)



Sample : TZA-15	Frequency Range : 399.271 - 3996.57	Measured on : 03/01/2010	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 100103IR3	Zerofilling : 2	Acquisition : Double Sided,For	

S60 The UV spectrum of Mauritine A *N*-oxide (5)



S61 The $[\alpha]_D$ of Mauritine A *N*-oxide (5)

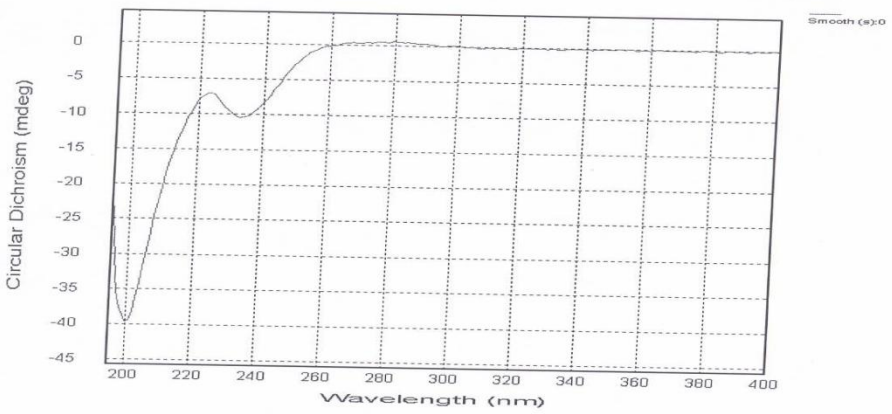
Optical rotation measurement

Model : P-1020 (A060460638)

No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	1 (1/3)	Sp.Rot	-377.0000	-0.1885 0.0000	23.9 50.00 Cell	Thu Jun 17 14:03:11 2010 0.00100g/mlMeOH TZA-15	Na 589nm	2 sec 10 sec
No.2	1 (2/3)	Sp.Rot	-377.0000	-0.1885 0.0000	23.8 50.00 Cell	Thu Jun 17 14:03:24 2010 0.00100g/mlMeOH TZA-15	Na 589nm	2 sec 10 sec
No.3	1 (3/3)	Sp.Rot	-375.8000	-0.1879 0.0000	23.9 50.00 Cell	Thu Jun 17 14:03:38 2010 0.00100g/mlMeOH TZA-15	Na 589nm	2 sec 10 sec

-376.6000°

S62 The CD of Mauritine A *N*-oxide (5)



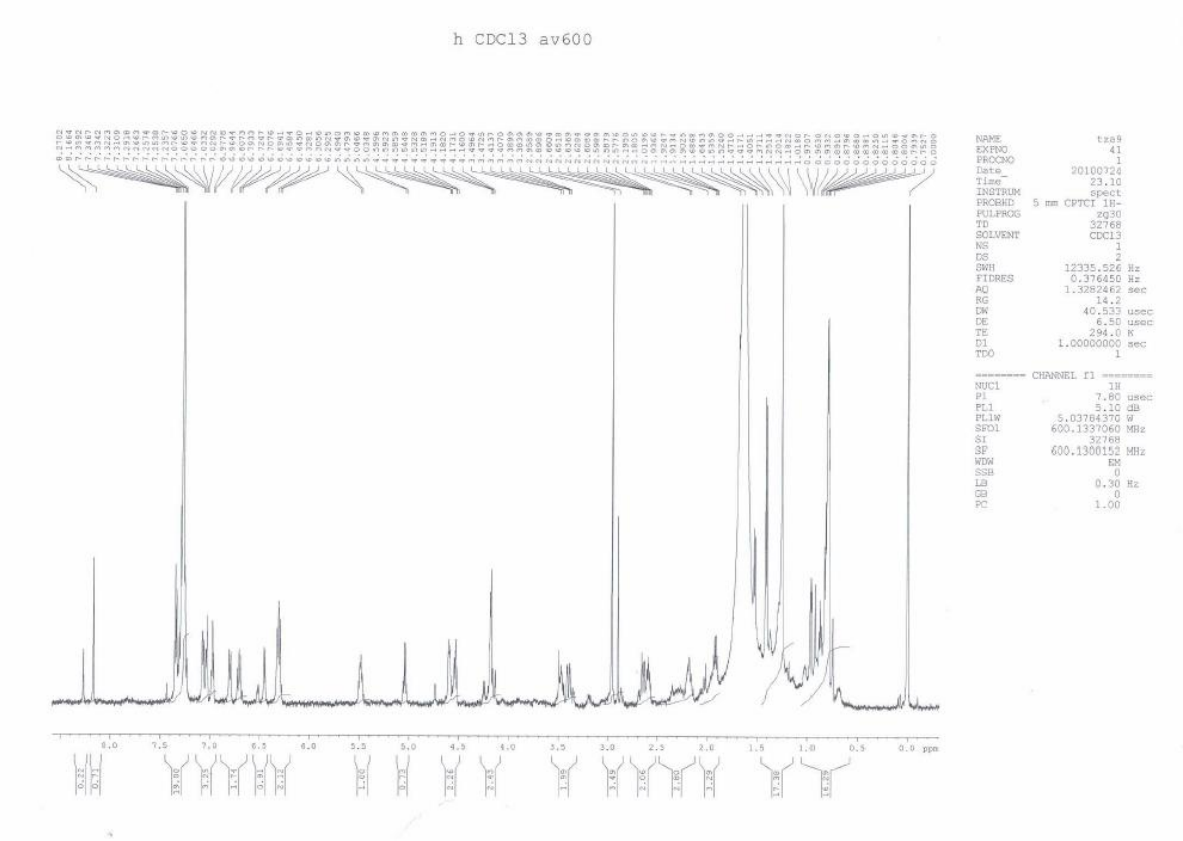
File: CD TZA-15-1mm(195-400)0007.dsx
ProBinaryX
Attributes :
- Time Stamp :Thu Dec 16 15:37:55 2010

- File ID : {272C0D10-A7FB-456b-A87B-C2E2F1E77FF3}
- Is CFR Compliant : false
- Original unaltered data

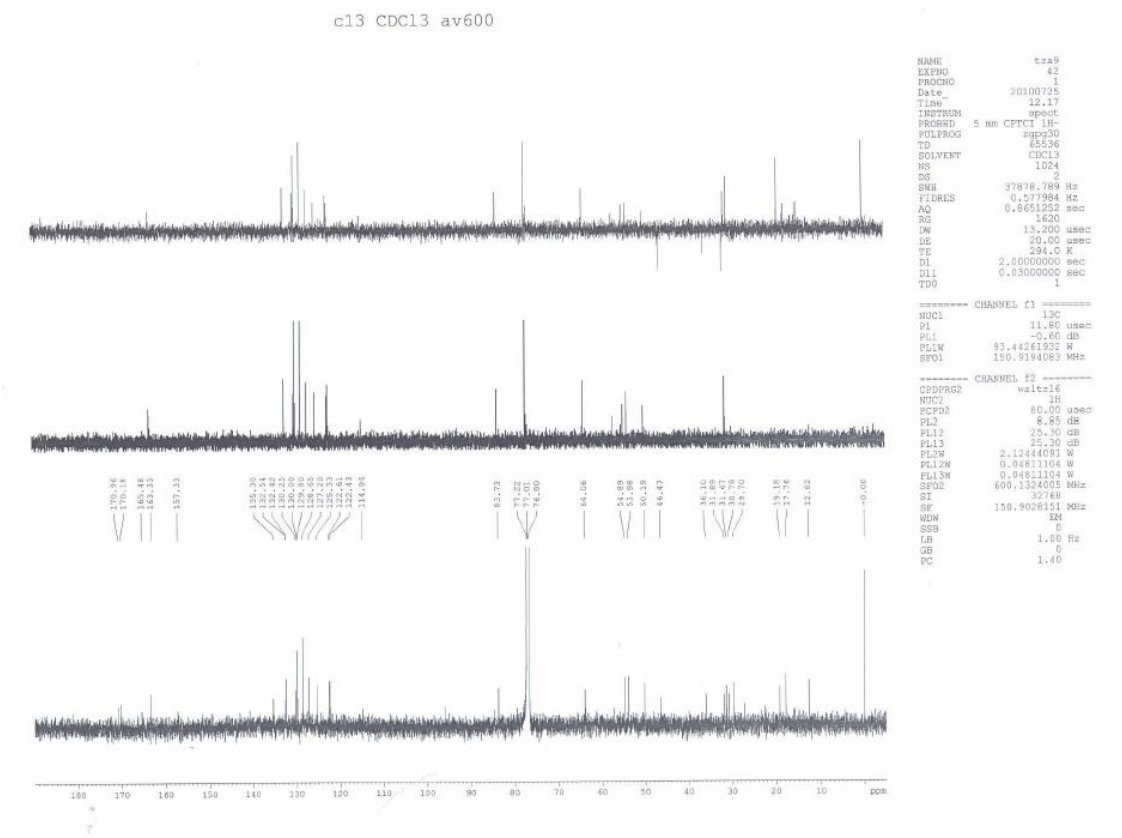
Remarks:
- HV (CDDC channel): 0 v
- Time per point: 1 s
- Description: Sample 1
- Concentration: 0.0200mg/ml MeOH
- Pathlength: 1 mm

Settings:
- Time-per-point: 1s (25us x 40000)
- Wavelength: 195nm - 400nm
- Step Size: 1nm
- Bandwidth: 1nm

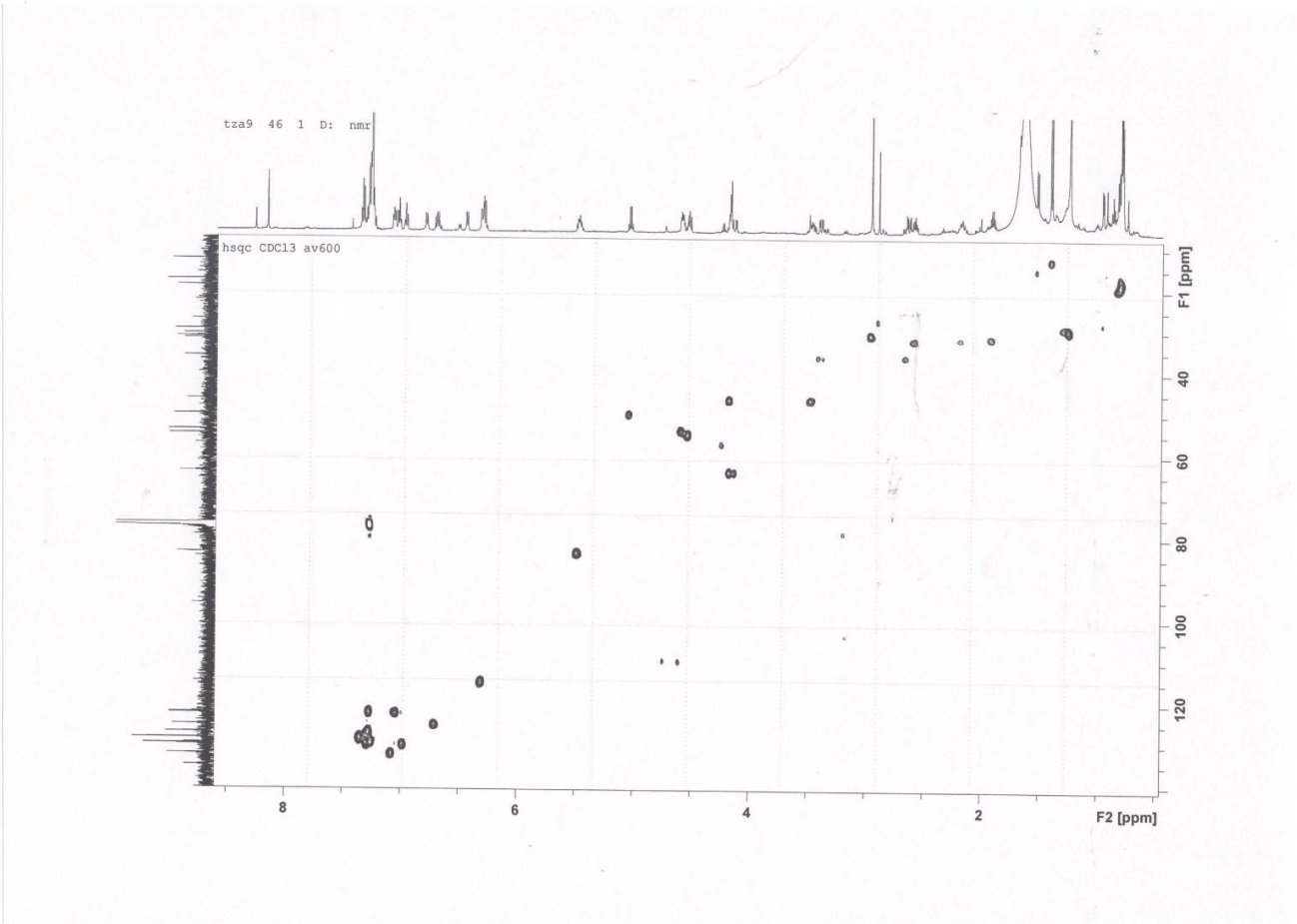
S63 The ^{1}H NMR spectrum of Apetaline C (6) in $CDCl_3$



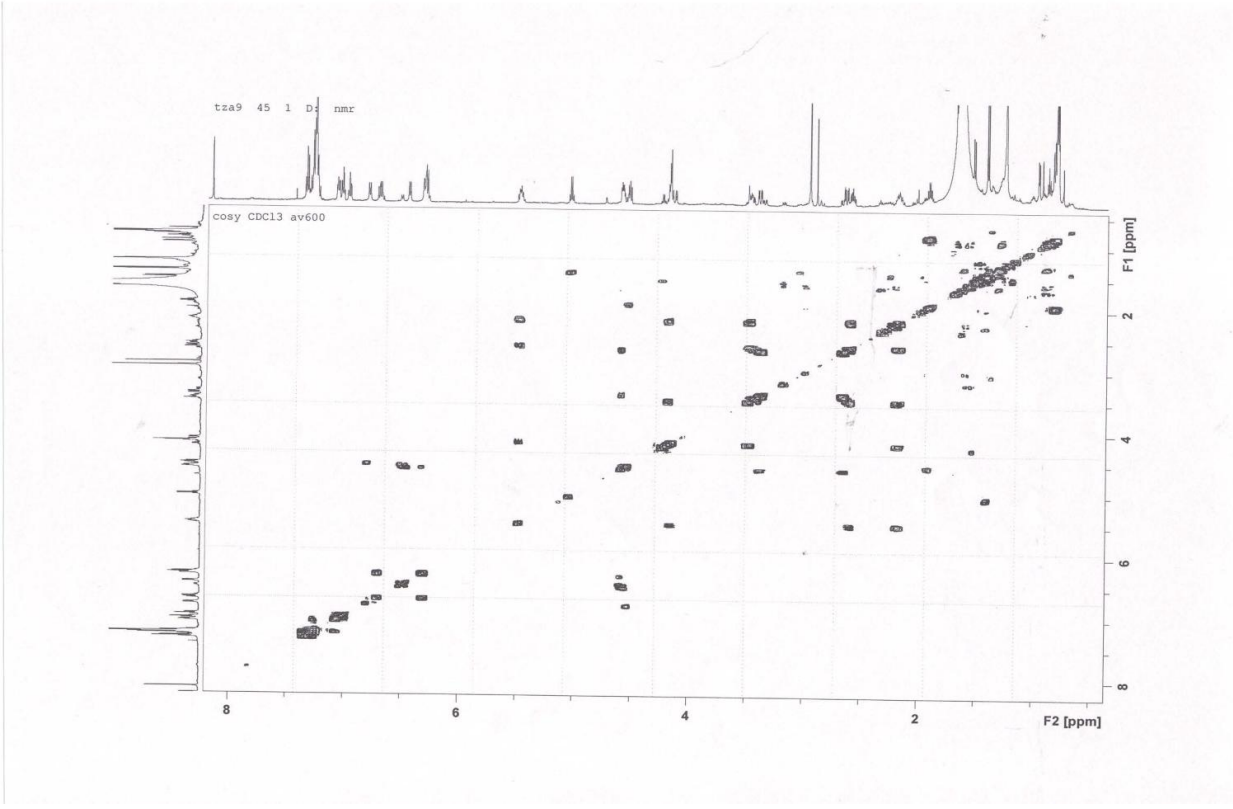
S64 The ^{13}C NMR spectrum of Apetaline C (6) in $CDCl_3$



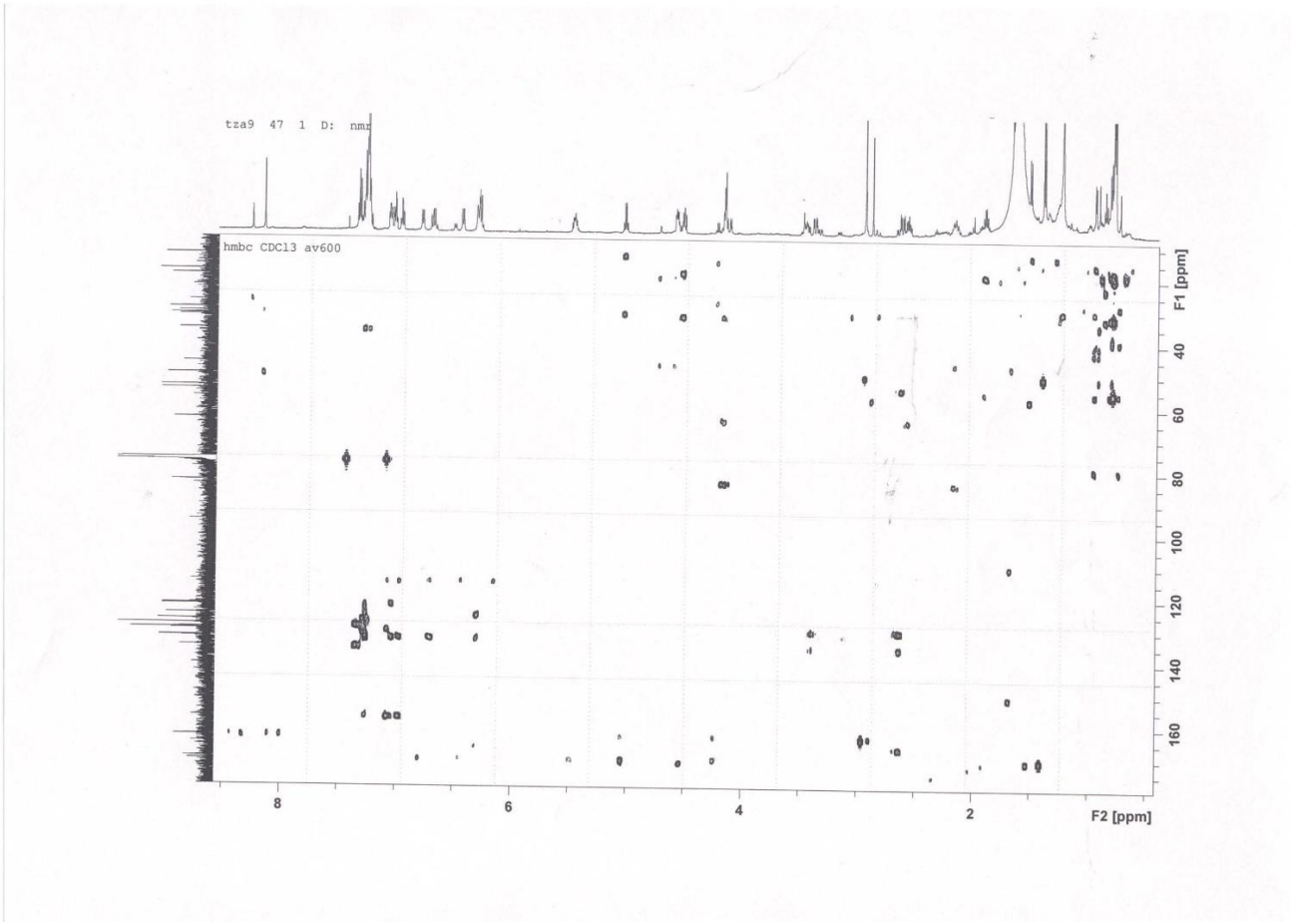
S65 The HSQC spectrum of Apetaline C (6)



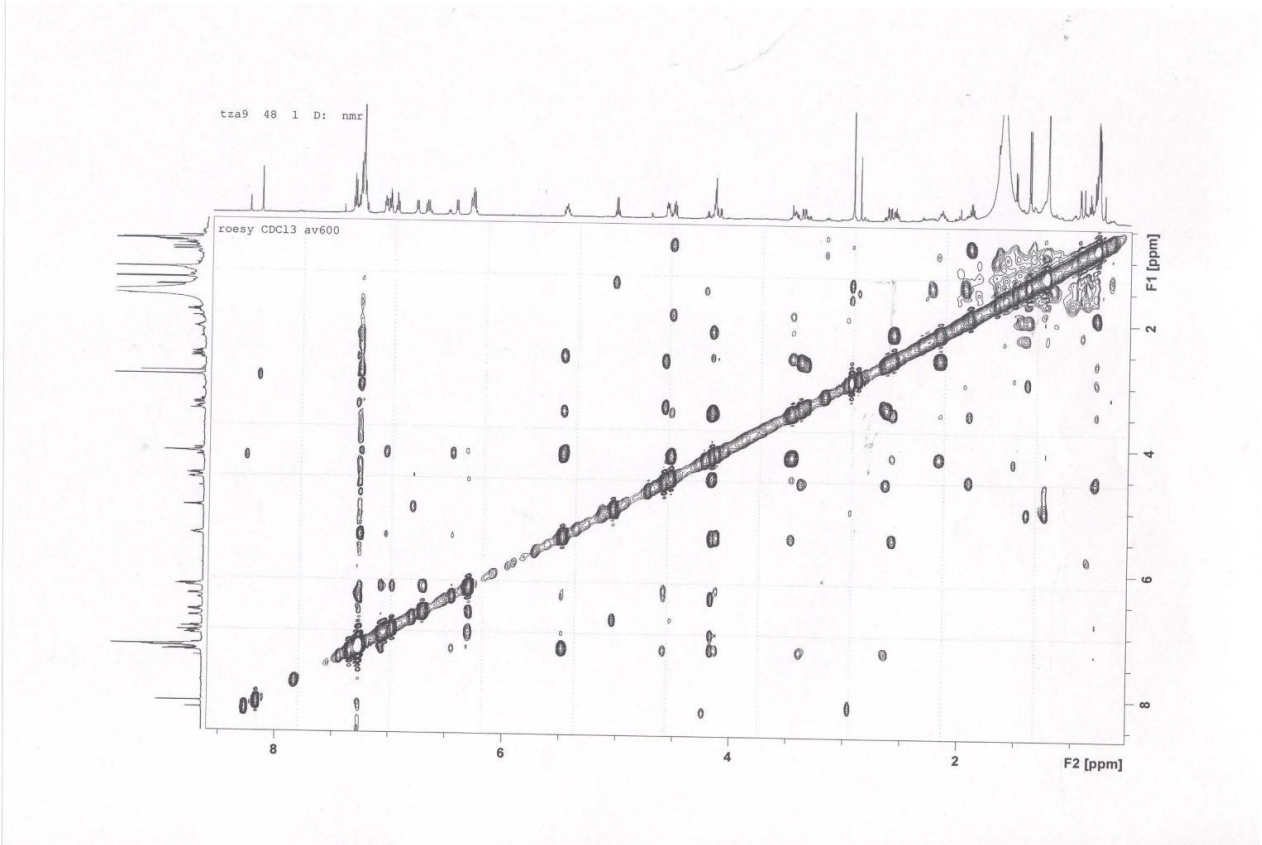
S66 The ^{1}H-^{1}H COSY spectrum of Apetaline C (6)



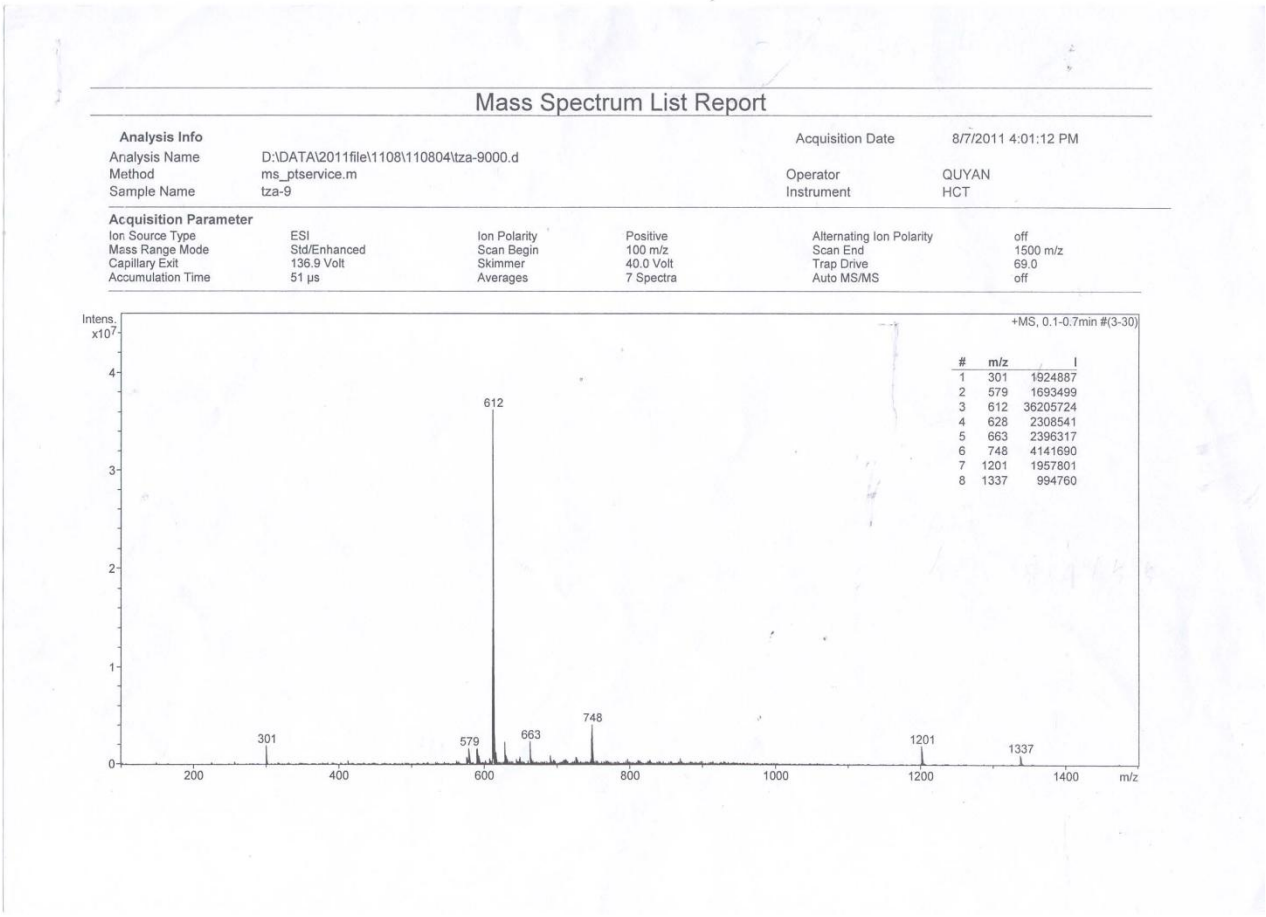
S67 The HMBC spectrum of Apetaline C (6)



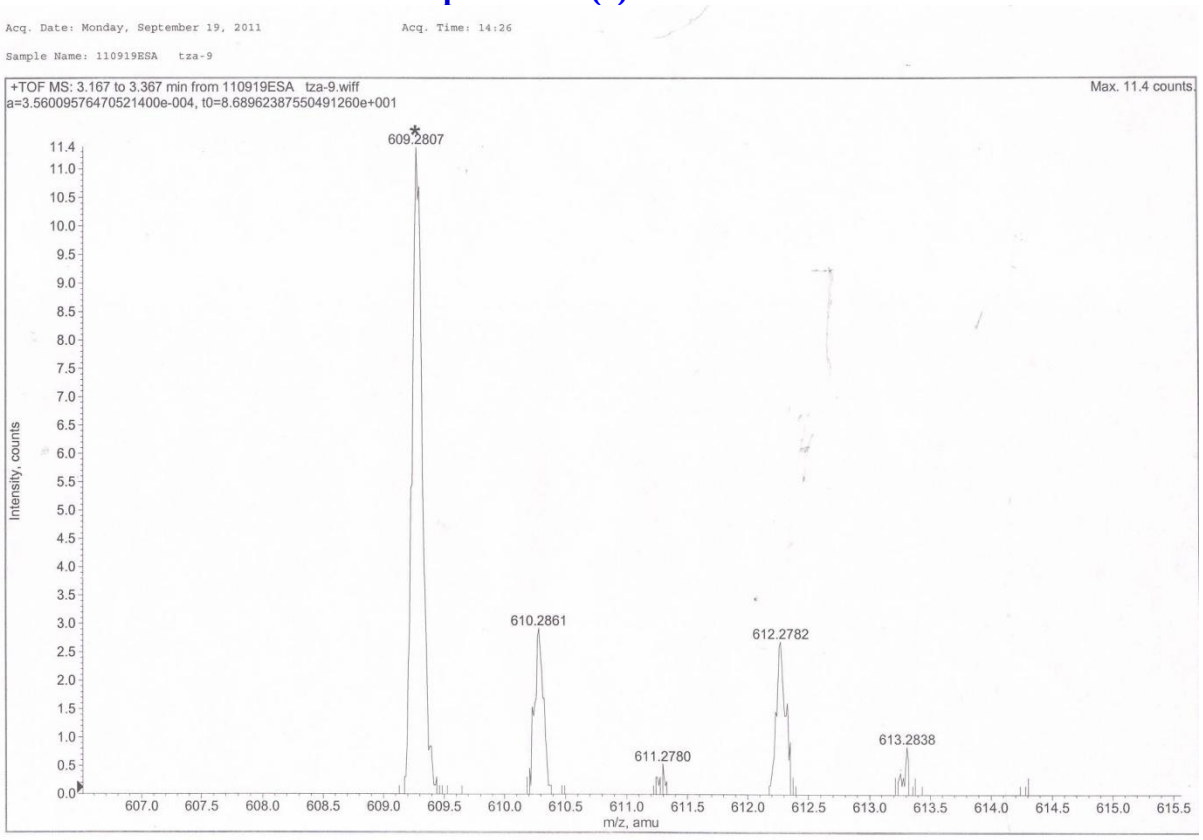
S68 The ROSEY spectrum of Apetaline C (6)



S69 The Positive ESIMS of Apetaline C (6)



S70 The Positive HRESIMS of Apetaline C (6)



S70 The Positive HRESIMS of Apetaline C (6)

Acq. Date: Monday, September 19, 2011 Acq. Time: 14:26

Sample Name: 110919ESA tza-9

Elemental composition calculator

Target m/z: +612.2782 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 110919ESA tza-9.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	I	0	0
7	K	0	0
8	N	5	5
9	Na	1	1
10	O	3	6

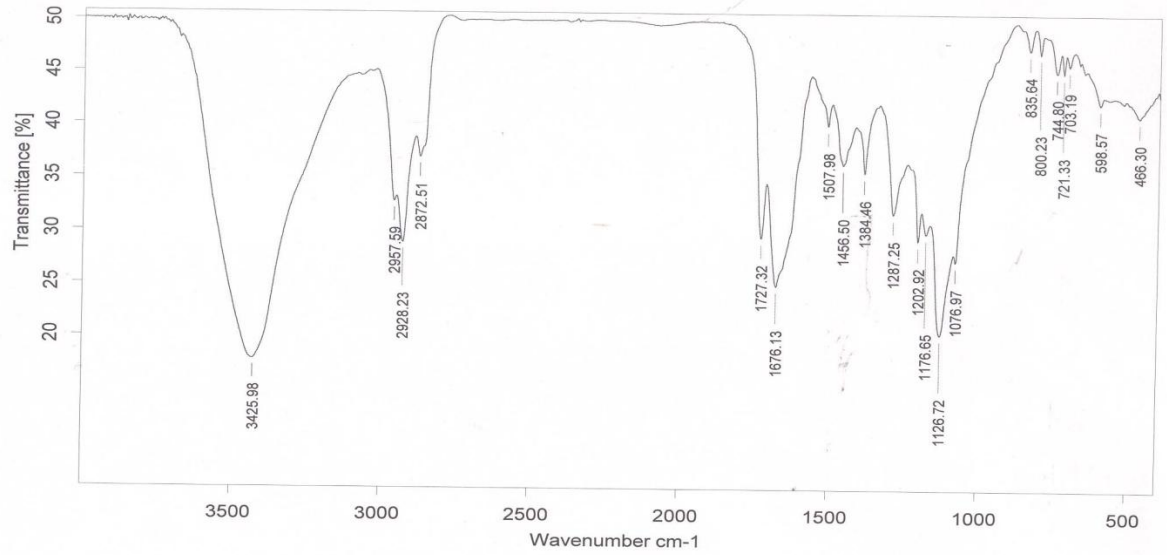
Acq. Date: Monday, September 19, 2011 Acq. Time: 14:26

Sample Name: 110919ESA tza-9

	Elements	Min Number	Max Number
11	P	0	0
12	Pt	0	0
13	S	0	0
14	Si	0	0

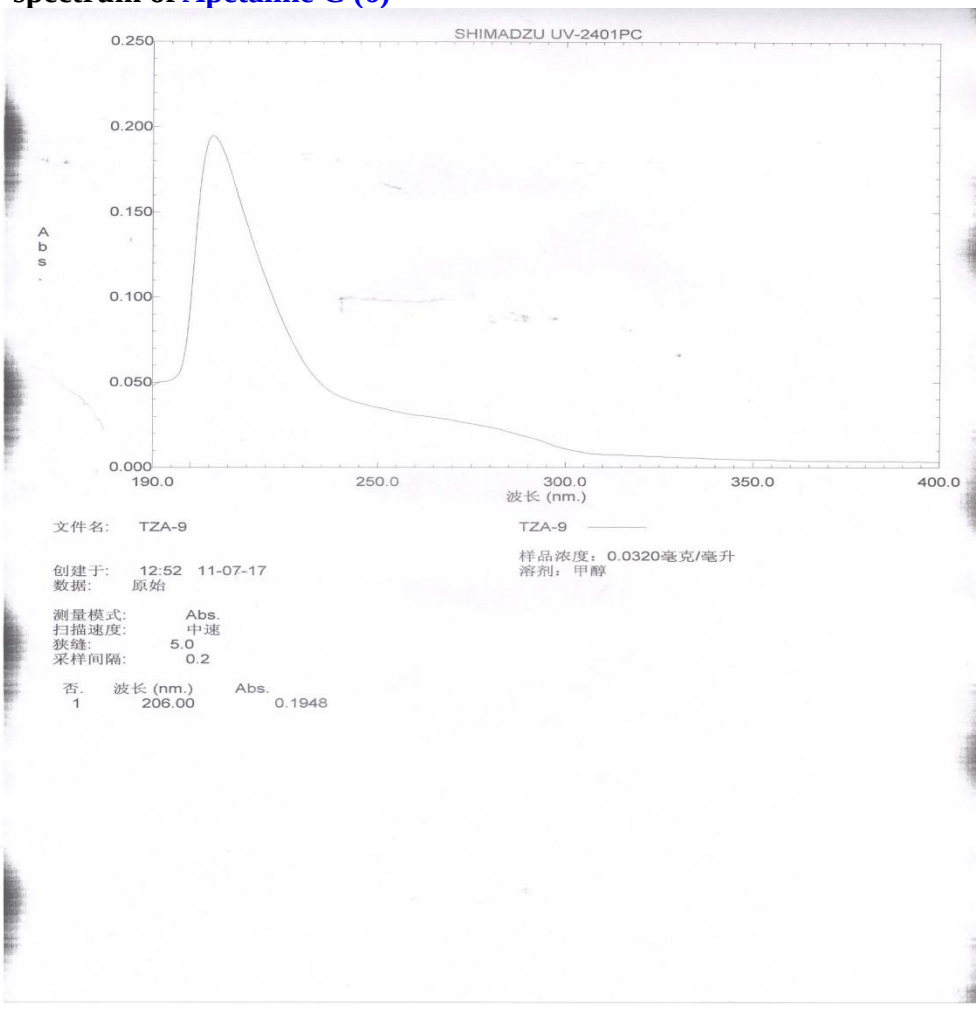
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C32 H39 N5 O6 Na	612.2798	-1.6041	-2.6199	15.5

S71 The IR spectrum of Apetaline C (6)



Sample : tza-9	Frequency Range : 399.246 - 3996.32	Measured on : 31/08/2011	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 110831IR0	Zerofilling : 2	Acquisition : Double Sided,For	

S72 The UV spectrum of Apetaline C (6)



S73 The $[\alpha]_D$ of Apetaline C (6)

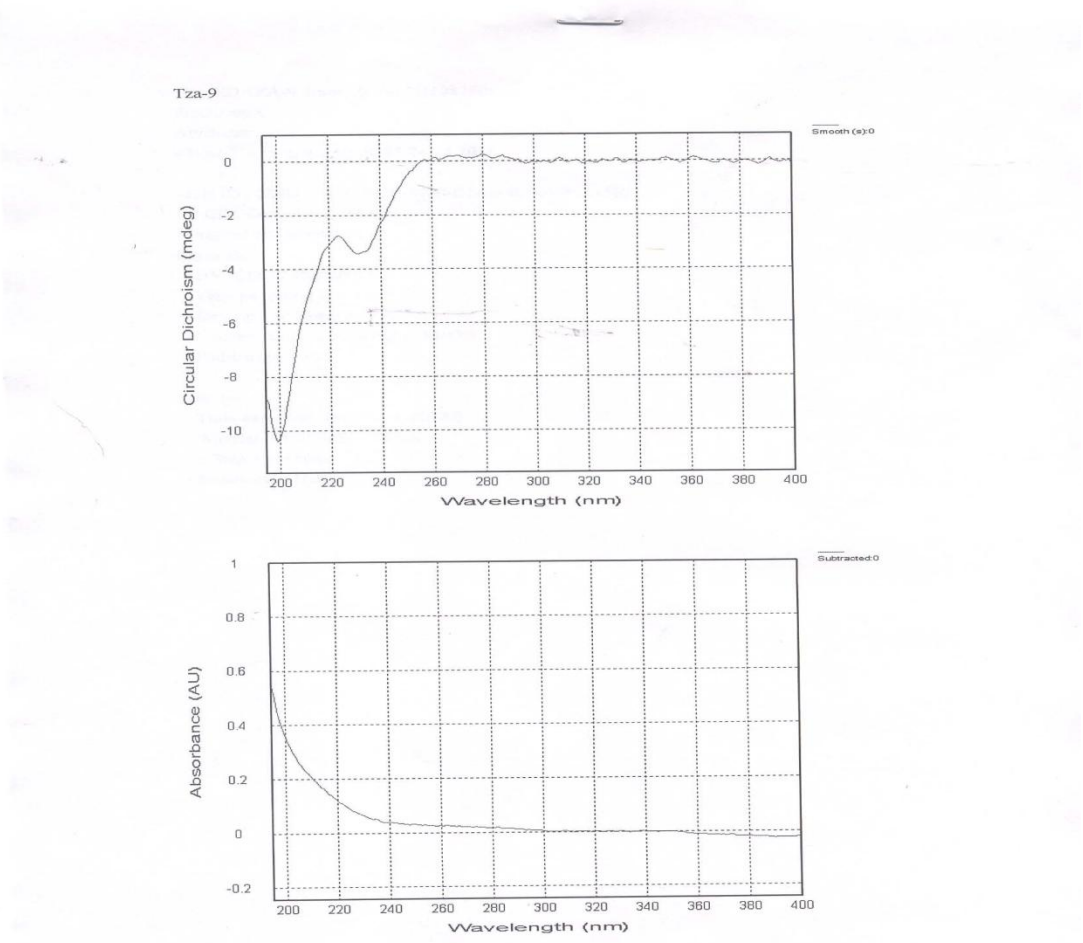
Optical rotation measurement

Model : P-1020 (A060460638)

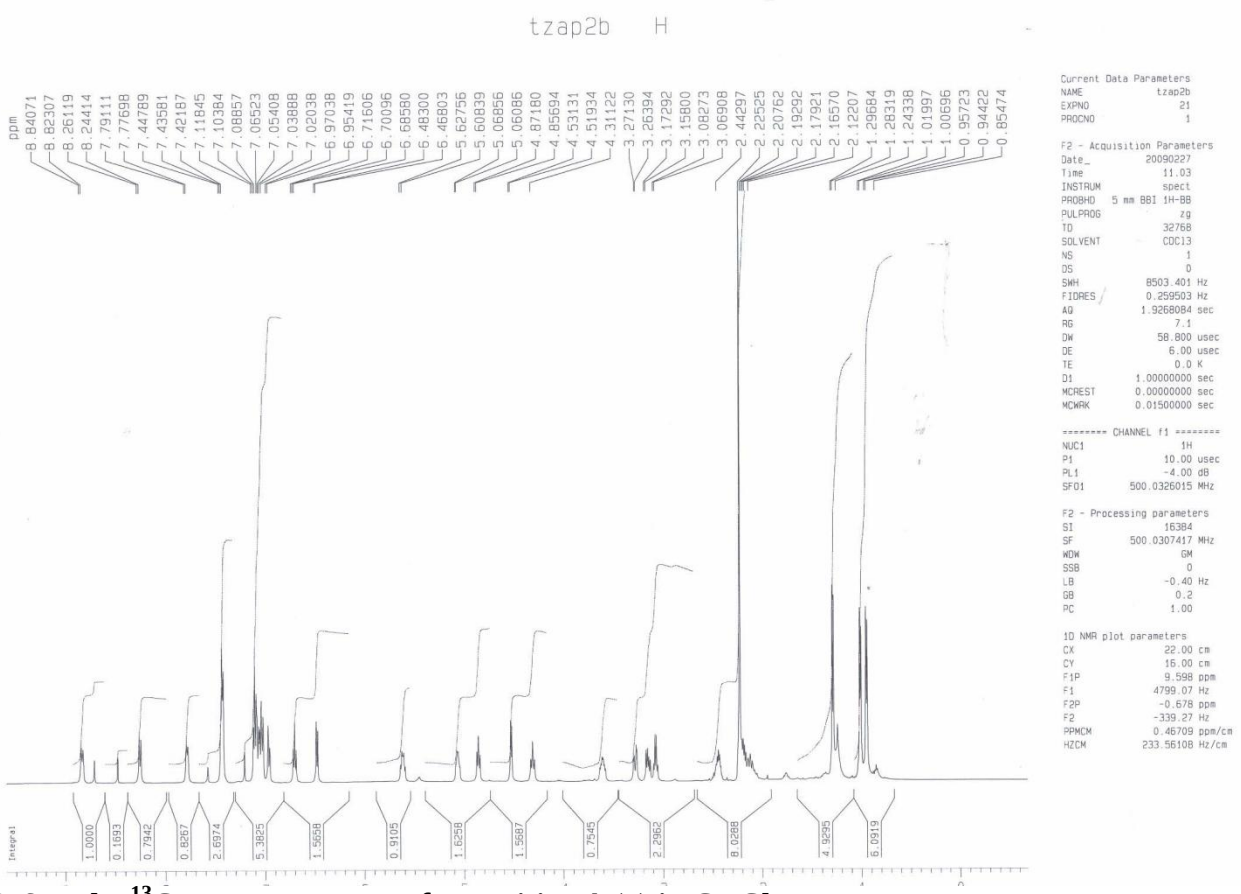
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	10 (1/3)	Sp.Rot	-30.8000	-0.0154 0.0000	24.5 50.00 Cell	Sat Aug 27 12:00:51 2011 0.00100g/mlMeOH TZA-9	Na 589nm	2 sec 10 sec
No.2	10 (2/3)	Sp.Rot	-28.4000	-0.0142 0.0000	24.4 50.00 Cell	Sat Aug 27 12:01:04 2011 0.00100g/mlMeOH TZA-9	Na 589nm	2 sec 10 sec
No.3	10 (3/3)	Sp.Rot	-30.2000	-0.0151 0.0000	24.4 50.00 Cell	Sat Aug 27 12:01:17 2011 0.00100g/mlMeOH TZA-9	Na 589nm	2 sec 10 sec

$-29.8000°$

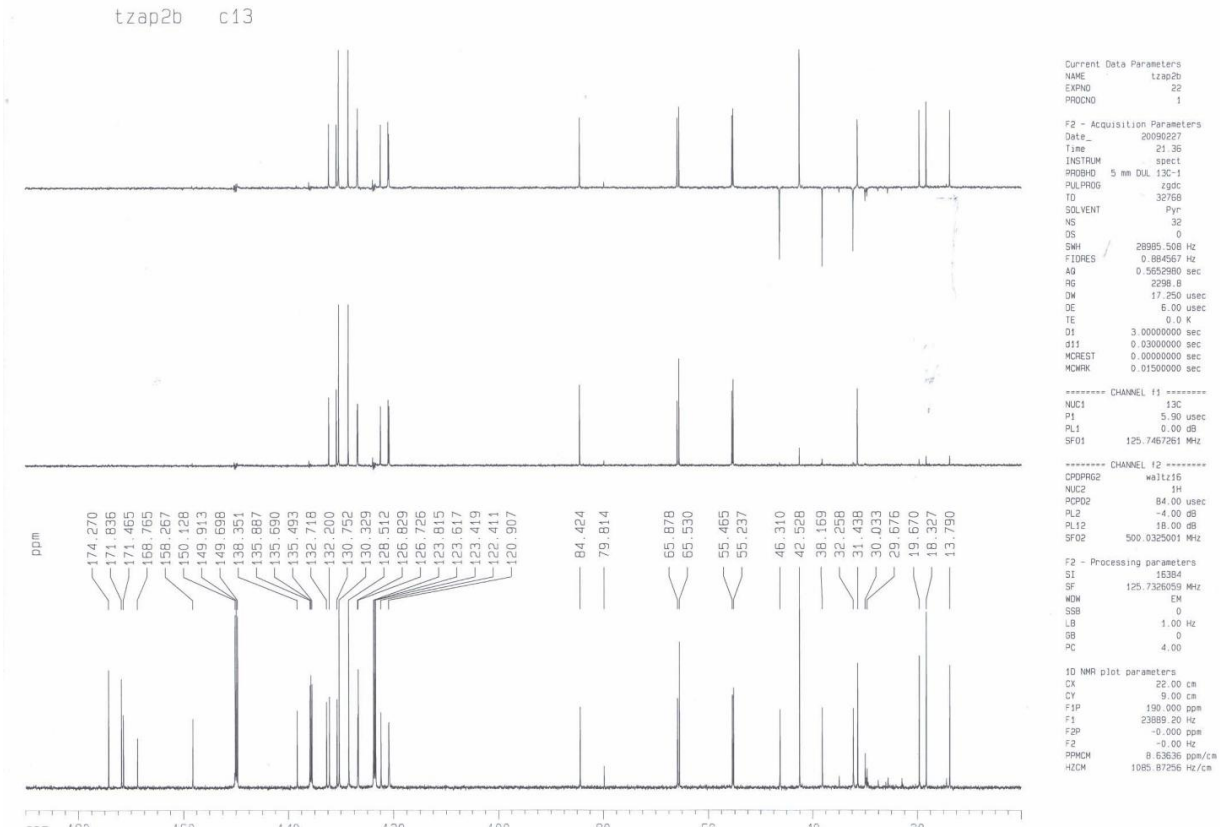
S74 The CD spectrum of Apetaline C (6)



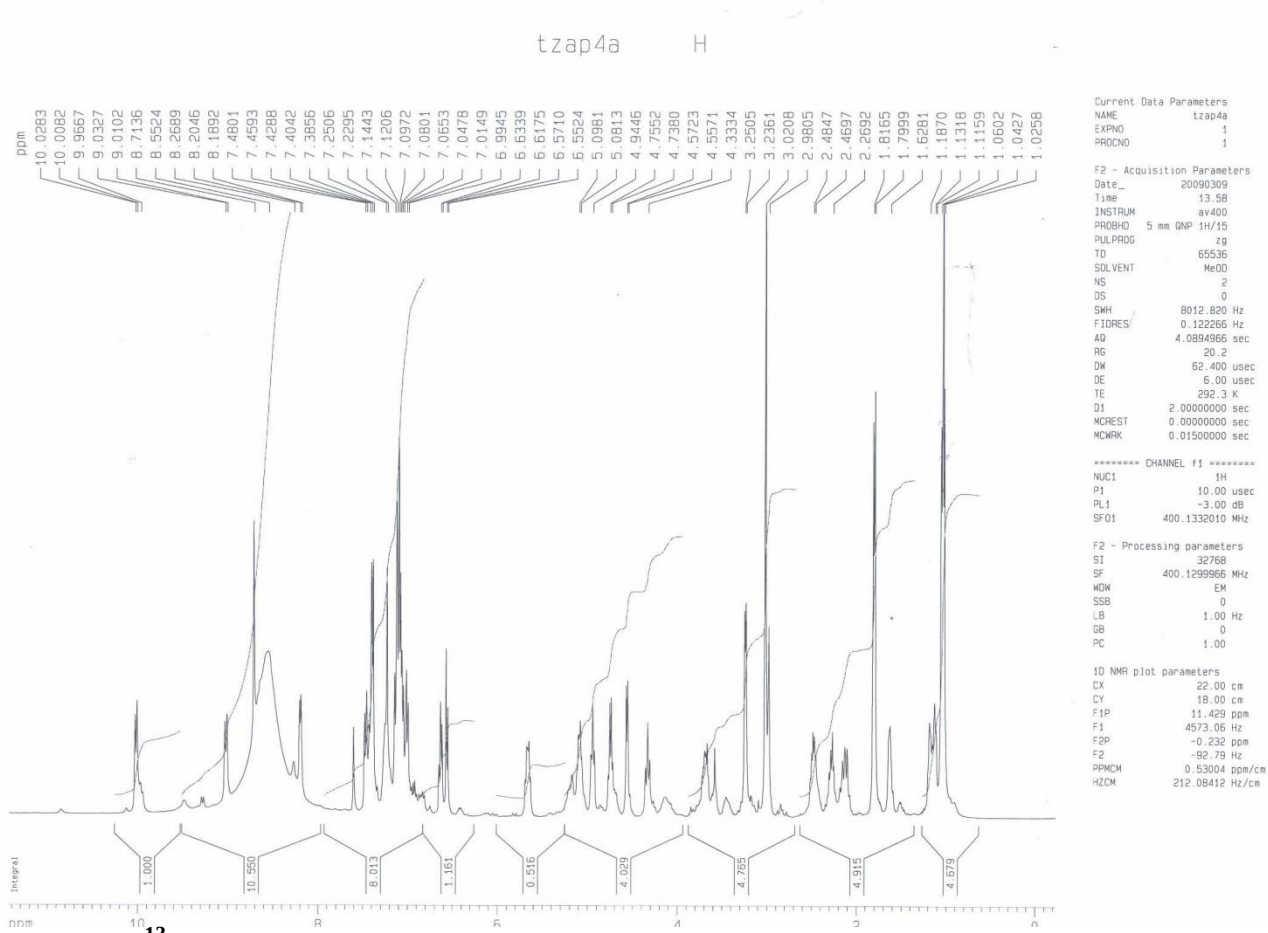
S75 The ^{1}H NMR spectrum of Mauritine A (7) in $CDCl_3$



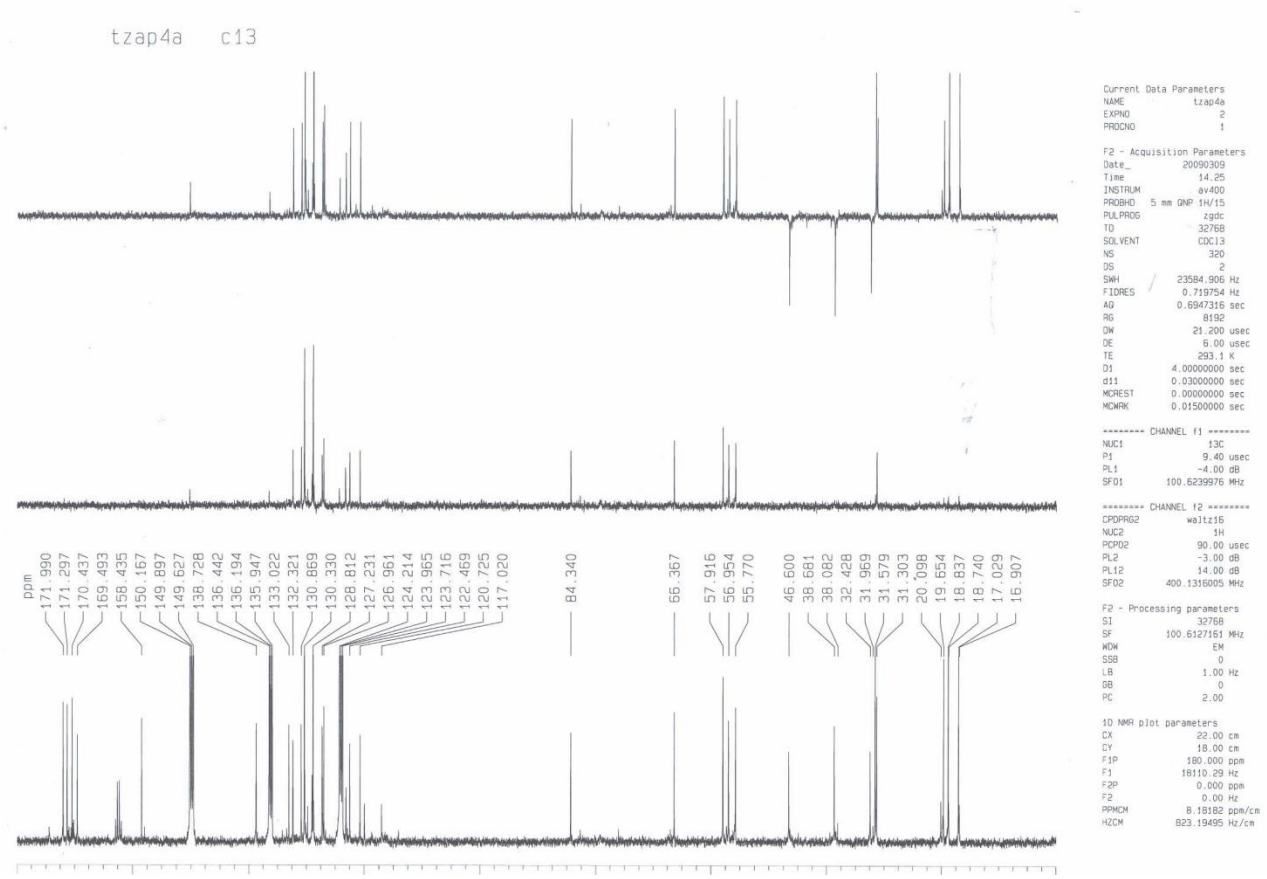
S76 The ^{13}C NMR spectrum of Mauritine A (7) in $CDCl_3$



S77 The ^{1}H NMR spectrum of Mauritine F (8) in $CDCl_3$



S78 The ^{13}C NMR spectrum of Mauritine F (8) in $CDCl_3$



S79 Retention time of standard amino acids and the hydrolysates of 1-8

Amino Acid	Rt/min	Compounds	Configuration	Rt/min
L-Phe	55.81	**1**	L-Phe, L-Val	56.01, 45.22
D-Phe	30.02	**2**	L-Phe, L-Val	56.21, 47.62
L-Val	44.51	**3**	L-Phe, L-Val, D-N,N(CH_3)$_2$-Ala	56.72, 44.24, 27.66
D-Val	62.73	**4**	L-Phe, L-Val	56.12, 43.65
L-N(CH_3)-Ala	33.21	**5**	L-Phe, L-Val	53.04, 44.76
D-N(CH_3)-Ala	48.25	**6**	L-Phe, L-Val	56.13, 45.60
L-N,N(CH_3)$_2$-Ala	38.57	**7**	L-Phe, L-Val, L-N,N(CH_3)$_2$-Ala	55.91, 44.63, 38.17
D-N,N(CH_3)$_2$-Ala	27.55	**8**	L-Phe, L-Val, L-N(CH_3)-Ala	55.22, 45.43, 33.38

S80 ^{1}H and ^{13}C NMR data of 7-8

No.	**7** [b,*]		**7** [c,#]		**8** [c,*]		**8** [b,#]	
	δ_C, mult.	δ_H (J in Hz)	δ_C, mult.	δ_H (J in Hz)	δ_C, mult.	δ_H (J in Hz)	δ_C, mult.	δ_H (J in Hz)
1	120.9, CH	6.48, d, (7.5)	115.1, CH	6.25, d, (7.7)	123.1, CH	6.56, d, (6.9)	114.7, CH	6.29, d, (7.9)
2	126.8, CH	6.70, t, (7.5)	125.3, CH	6.64, m	127.2, CH	6.63, t, (6.9)	125.3, CH	6.70, dd, (10.4, 7.9)
3		7.78, d, (7.5)		6.32, d, (10.3)		8.20, d, (6.9)		6.33, d, (10.4)
4	168.8, qC		166.5, qC		169.5, qC		166.4, qC	
5	55.2, CH	5.06, m	54.0, CH	4.55, m	55.8, CH	5.09, m	54.0, CH	4.60, m
6		8.83, d, (8.8)		6.45, d, (8.5)		9.02, d, (9.0)		6.42, d, (8.4)
7	171.8, qC		170.3, qC		171.3, qC		170.4, qC	
8	65.9, CH	4.53, d, (6.0)	64.1, CH	4.12, d, (5.7)	66.4, CH	4.56, d, (6.1)	64.1, CH	4.15, d, (6.1)
9	84.4, CH	5.62, m	83.6, CH	5.44, m	84.3, CH	5.66, m	83.6, CH	5.50, dt, (10.2, 6.1)
11	158.3, qC		157.3, qC		158.4, qC		157.3, qC	
12	122.4, CH	6.96, d, (8.1)	122.5, CH	6.98, m	122.5, CH	6.98-7.15$^\Theta$	122.6, CH	7.04, dd, (8.2, 2.4)
13	130.8, CH	7.03$^\Theta$	130.2, CH	6.91, d, (8.2)	130.9, CH	6.98-7.15$^\Theta$	130.2, CH	6.95, dd, (8.2, 1.4)
14	132.7, qC		132.4, qC		133.0, qC		132.4, qC	
15	132.2, CH	7.06$^\Theta$	132.3, CH	7.01, d, (8.5)	132.3, CH	6.98-7.15$^\Theta$	132.4, CH	7.06, dd, (9.2, 1.4)
16	120.9, CH	7.44$^\Theta$	122.2, CH	7.24$^\Theta$	120.7, CH	7.47, d, (8.3)	122.3, CH	7.20-7.30$^\Theta$
17	38.2, CH_2	3.15, dd, (13.7, 7.5)	36.1, CH_2	2.64, dd, (14.0, 5.4)	38.7, CH_2	3.00, d, (16.1)	36.0, CH_2	2.66, dd, (14.1, 5.3)
		3.28, dd, (13.7, 3.8)		3.32, m		3.24, d, (5.8)		3.41, dd, (14.1, 4.1)
18	138.4, qC		135.6, qC		138.7, qC		135.5, qC	
19	130.3, CH	7.43, d, (7.3)	130.0, CH	7.26$^\Theta$	130.3, CH	7.39, d, (7.4)	130.1, CH	7.32, d, (7.1)
20	128.5, CH	7.10, t, (7.3)	128.4, CH	7.19$^\Theta$	128.8, CH	6.98-7.15$^\Theta$	128.5, CH	7.20-7.30$^\Theta$
21	126.7, CH	7.06$^\Theta$	127.0, CH	7.22$^\Theta$	127.0, CH	6.98-7.15$^\Theta$	127.1, CH	7.20-7.30$^\Theta$
22	128.5, CH	7.10, t, (7.3)	128.4, CH	7.19$^\Theta$	128.8, CH	6.98-7.15$^\Theta$	128.5, CH	7.20-7.30$^\Theta$
23	130.3, CH	7.43, d, (7.3)	130.0, CH	7.26$^\Theta$	130.3, CH	7.39, d, (7.4)	130.1, CH	7.32, d, (7.1)
24	32.3, CH_2	2.12, m	31.9, CH_2	2.14, m	32.4, CH_2	2.27, m	31.9, CH_2	2.19, m
		2.44, m		2.45, m		2.48, m		2.58, m
25	46.3, CH_2	3.61, m	46.4, CH_2	3.44, m	46.6, CH_2	3.67, m	46.4, CH_2	3.47, m
		4.31, t, (9.3)		4.20, t, (9.2)		4.33, t, (9.3)		4.57, m
27	171.5, qC		171.4, qC		170.4, qC		171.4, qC	
28	55.5, CH	4.86, t, (8.2)	54.7, CH	4.46, t, (8.1)	57.0, CH	4.94, t, (7.9)	54.2, CH	4.20, dd, (12.0, 8.9)
29	31.4, CH	2.19, m	29.6, CH	1.94, m	31.3, CH	2.13, m	31.2, CH	1.97, dq, (12.0, 6.7)
30	19.7, CH_3	1.01, d, (6.5)	19.2, CH_3	0.83, d, (6.8)	18.8, CH_3	1.05, d, (6.9)	19.2, CH_3	0.86, d, (6.7)
31	18.3, CH_3	0.95, d, (6.5)	17.9, CH_3	0.81, d, (6.8)	17.0, CH_3	1.03, d, (6.9)	17.6, CH_3	0.84, d, (6.7)
32		8.25, d, (8.2)		7.75, d, (8.6)		10.02, d, (7.9)		7.79, d, (8.9)
33	174.3, qC		174.2, qC		172.0, qC		175.1, qC	
34	65.5, CH	3.08, q, (6.8)	64.7, CH	3.02, m	57.9, CH	4.75, q, (6.7)	60.5, CH	3.12, q, (6.9)
35	13.8, CH_3	1.29, d, (6.8)	12.2, CH_3	1.23, d, (7.0)	19.7, CH_3	1.81, d, (6.7)	19.9, CH_3	1.35, d, (6.9)
37	42.5, CH_3	2.23, s	42.3, CH_3	2.30, s	31.6, CH_3	3.02, s	35.2, CH_3	2.48, s
38	42.5, CH_3	2.23, s	42.3, CH_3	2.30, s				

[b] Recorded at 125/500 MHz, [c] Recorded at 100/400 MHz. [*] Recorded at pyridine-d_5, [#] Recorded at chloroform-d_1, [Θ] overlapped.

S81 Figure 1. Key ^{1}H-^{1}H COSY, HMBC and selected ROESY correlations of compounds **1**–**6**

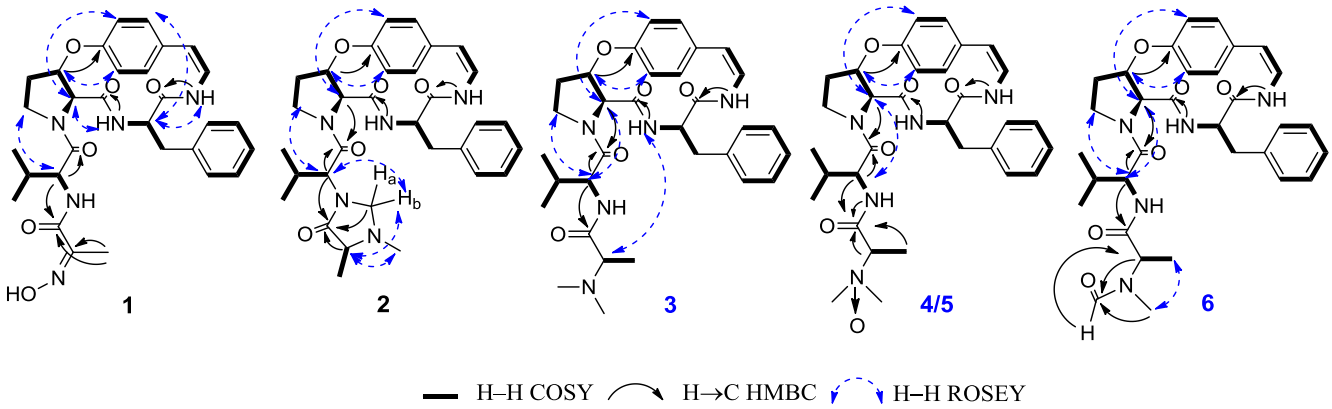


Figure 1. Key ^{1}H-^{1}H COSY, HMBC and selected ROESY correlations of compounds **1**–**6**