Supporting Information

Structurally Diverse Alkaloids from the Seeds of *Peganum harmala*

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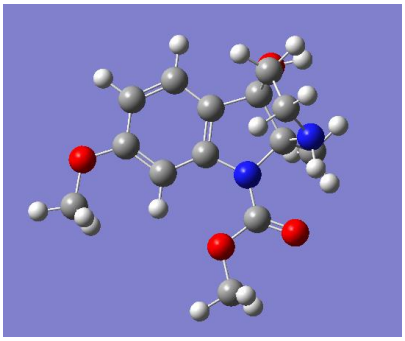
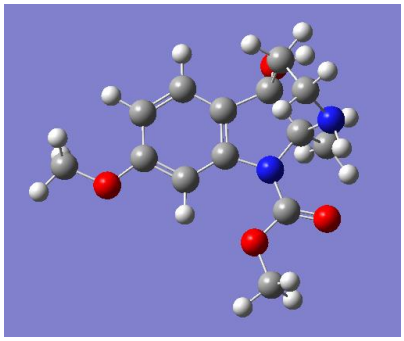
*E-mail: yangdz@purdue.edu

Content

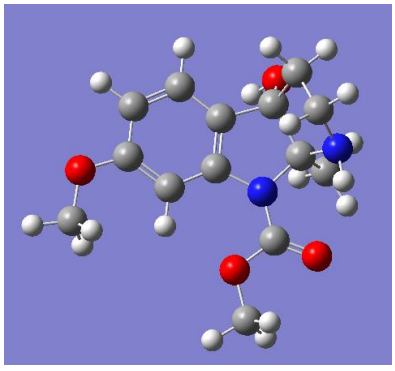
Figure S1 The main conformers for (2*S*,6*S*)-**1** obtained by conformational searching in CONFLEX software.



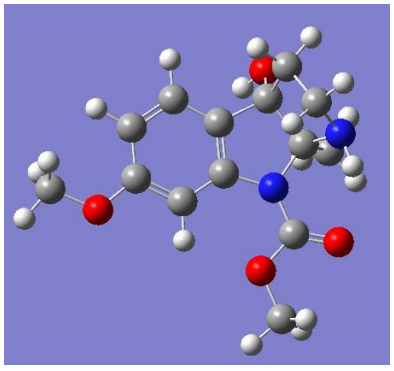
Con 1, 46.6 %



Con 2, 39.6 %

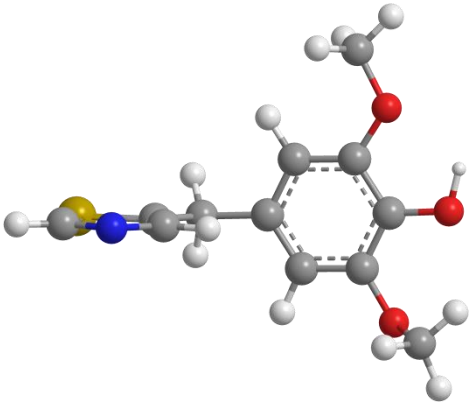


Con 3, 7.6 %

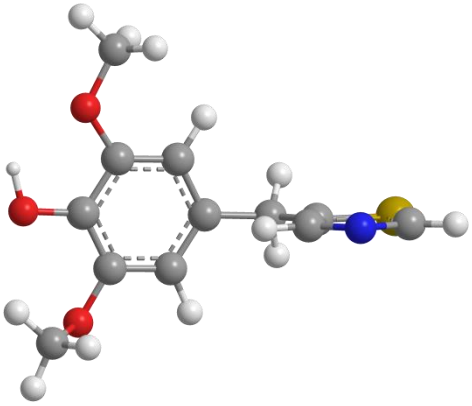


Con 4, 5.0

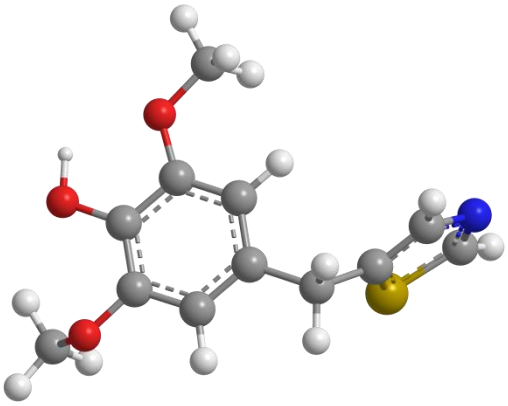
Figure S2. Lowest energy 3D conformers of **3a**.



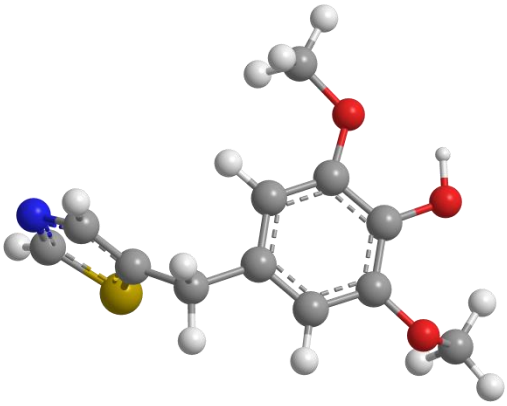
Con 1



Con 2

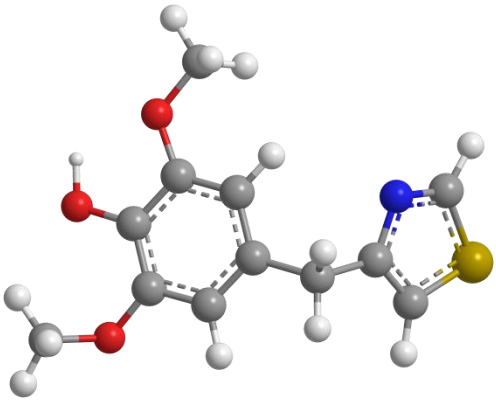


Con 3

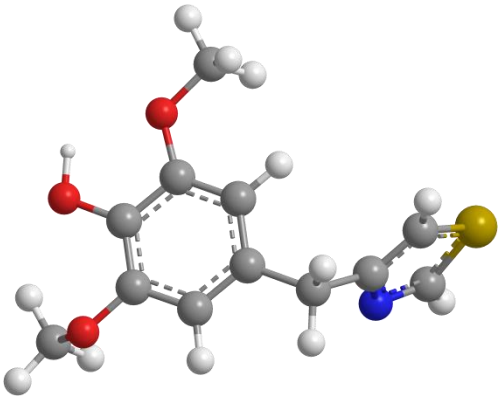


Con 4

Figure S3. Lowest energy 3D conformers of **3b**.



Con 1



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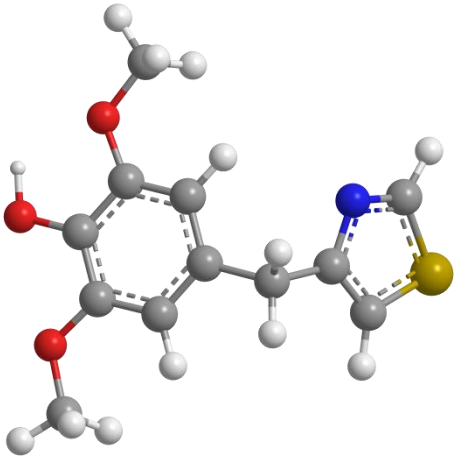

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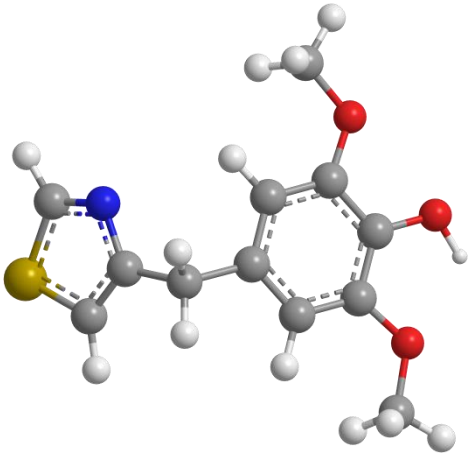
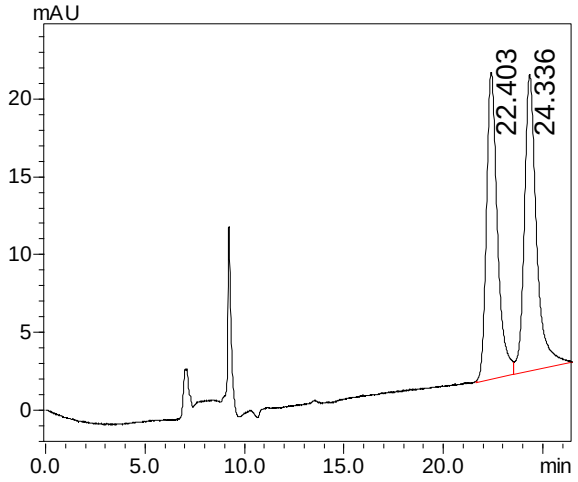


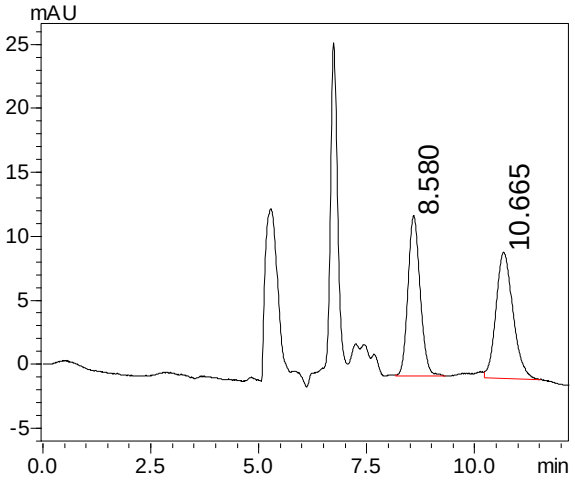
Con 4

Figure S4 The chiral HPLC separation chromatogram of peganine A (**1**)



Peak No.	Time	Area	Area %	Plate number	Tailing	Resolution
1	22.403	753257	48.2142	8852.740	1.480	--
2	24.336	809056	51.7858	9204.738	1.370	1.965

Figure S5 The chiral HPLC separation chromatogram of peganine B (**2**)



Peak No.	Time	Area	Area %	Plate number	Tailing	Resolution
1	8.580	247883	48.1066	4287.745	1.143	--
2	10.665	267396	51.8934	3628.523	1.169	3.383

Figure S6 The ^{1}H NMR spectrum of peganine A (**1**) in DMSO-d_6 (400 MHz)

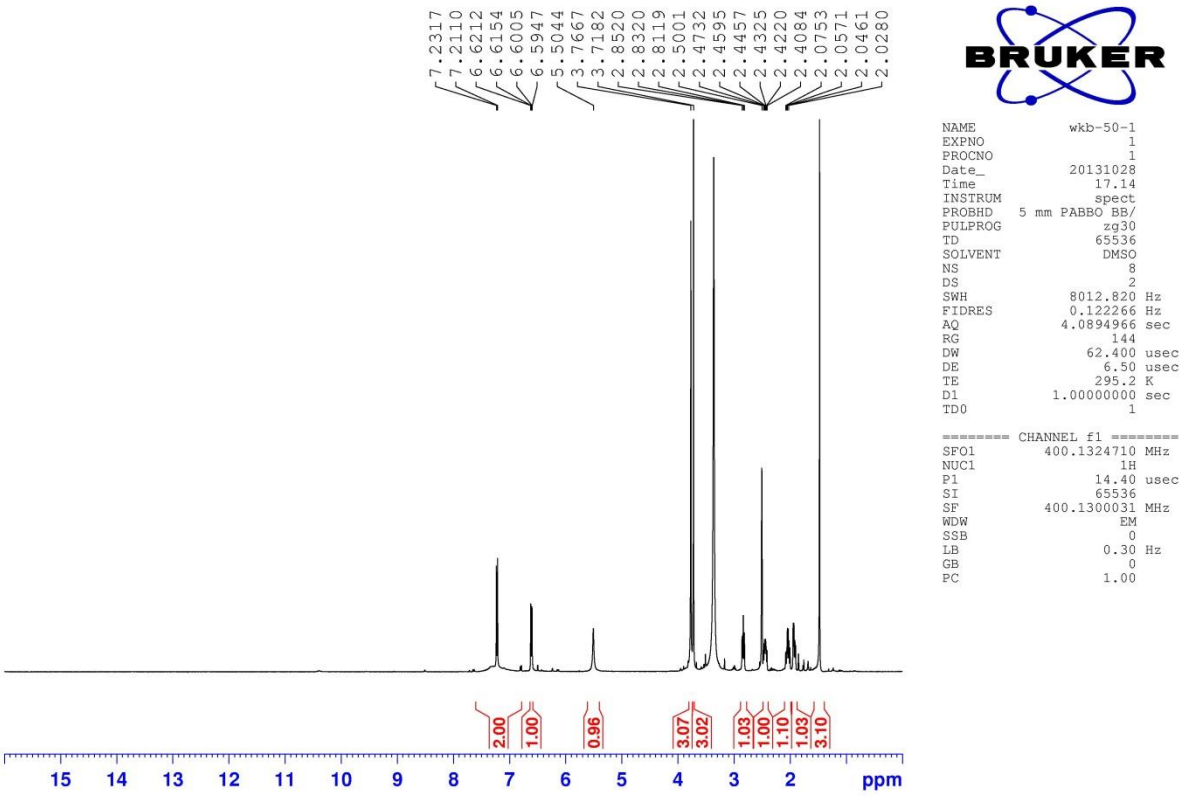


Figure S7 The ^{13}C NMR spectrum of peganine A (**1**) in DMSO-d_6 (100 MHz)

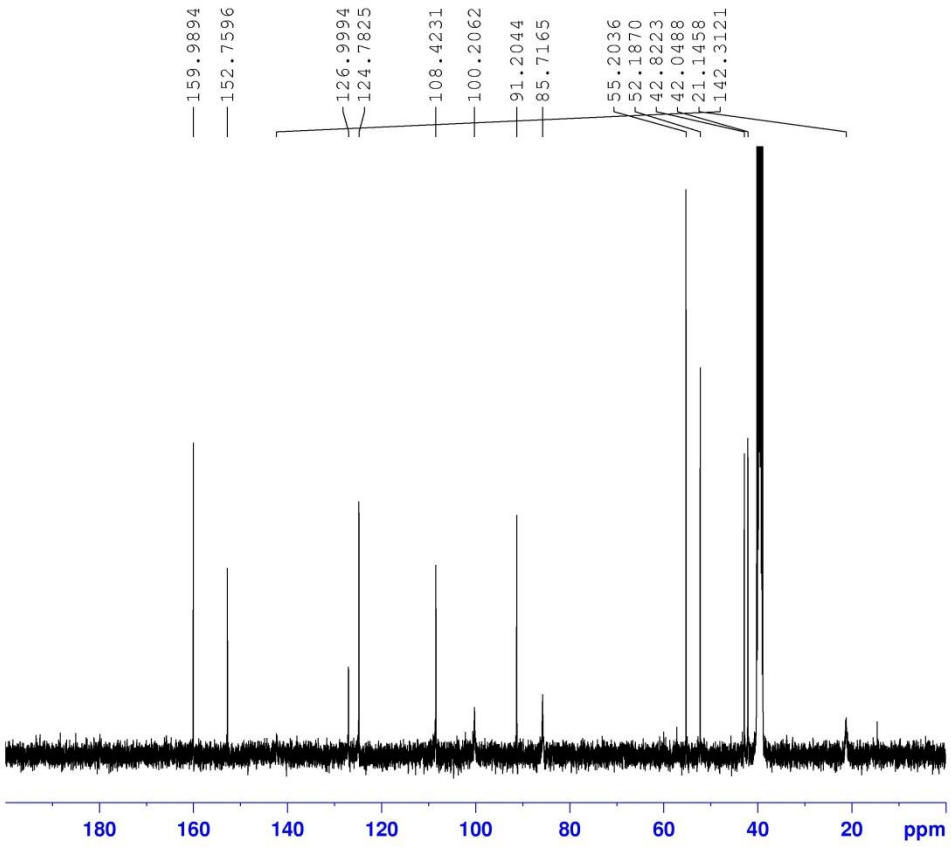


Figure S8 The HSQC spectrum of peganine A (**1**) in DMSO-d_6 (600 MHz)

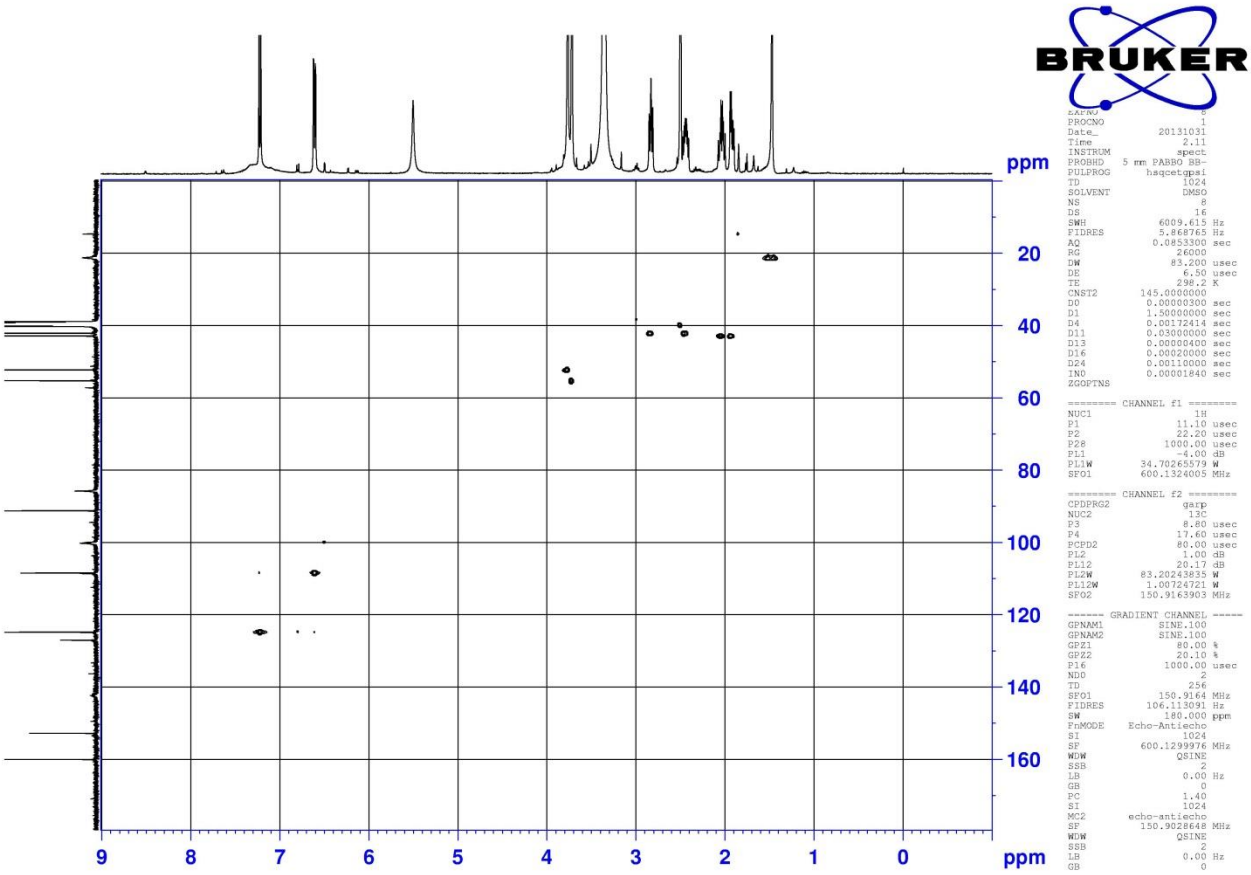


Figure S9 The HMBC spectrum of peganine A (**1**) in DMSO-d_6 (600 MHz)

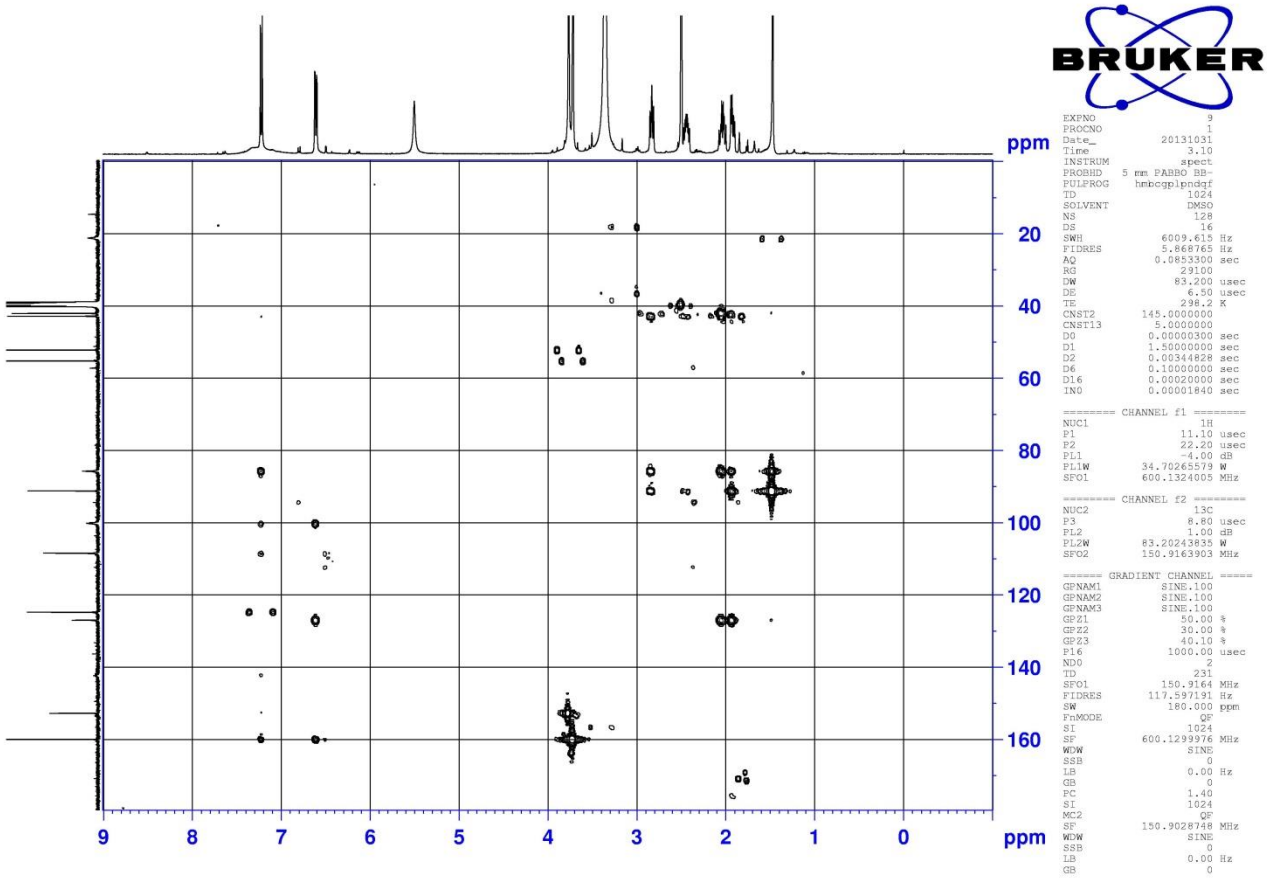
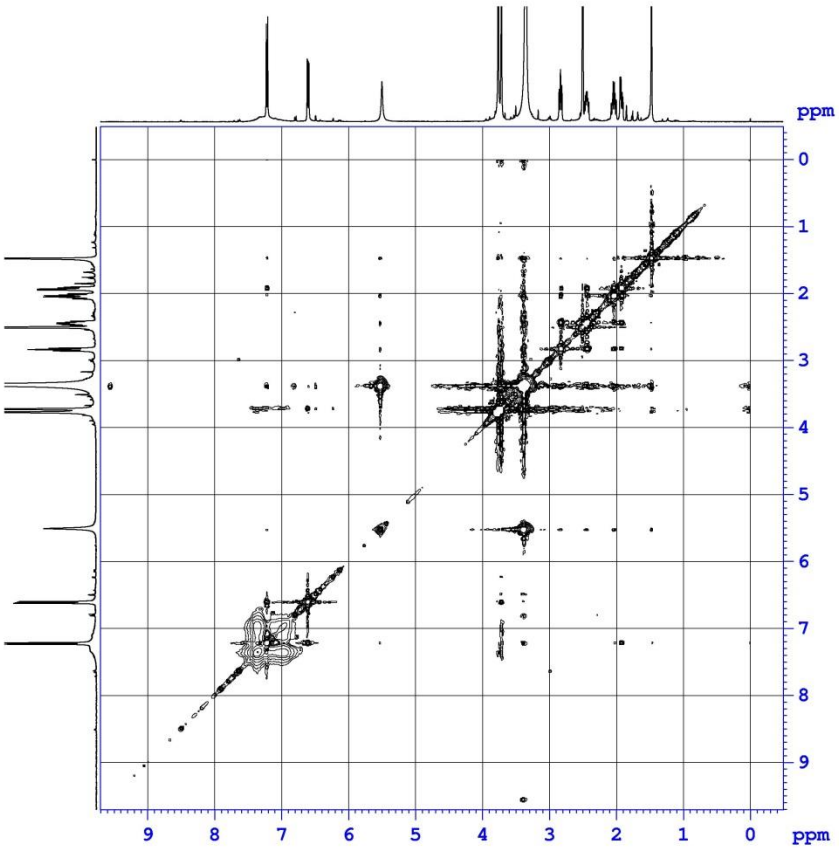


Figure S10 The NOESY spectrum of peganine A (**1**) in DMSO-d_6 (600 MHz)



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SOLVENT	DMSO
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DS	4
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FIDRES	5.868765 Hz
AQ	0.0853300 sec
RG	114
DW	83.200 usec
DE	6.50 usec
TE	289.8 K
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D1	2.00000000 sec
D8	0.60000002 sec
IN0	0.00016640 sec
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P1	11.10 usec
PL1	-4.00 dB
PL1W	34.70265579 W
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ND0	1
TD	256
SFO1	600.133 MHz
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SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	States-TPPI
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

Figure S11 The HRESIMS spectrum of peganine A (**1**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name	D:\Data\20131121\WKB-50_1-b,6_01_2222.d	Acquisition Date	11/21/2013 10:18:30 AM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	WKB-50	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

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Formula, max.							
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Estimate Carbon	yes						

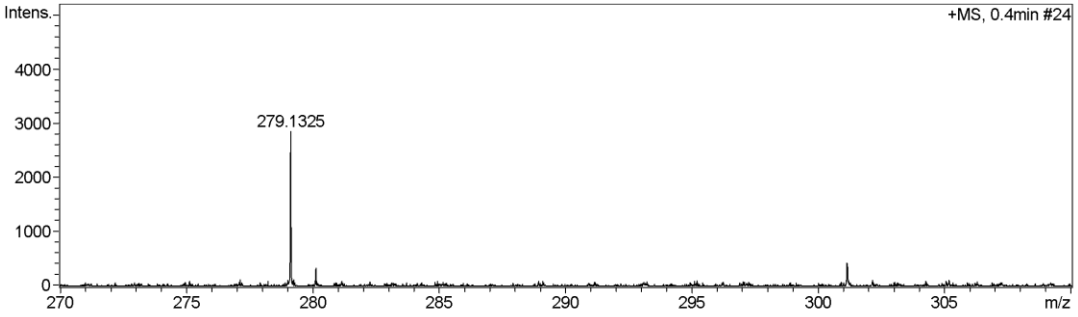

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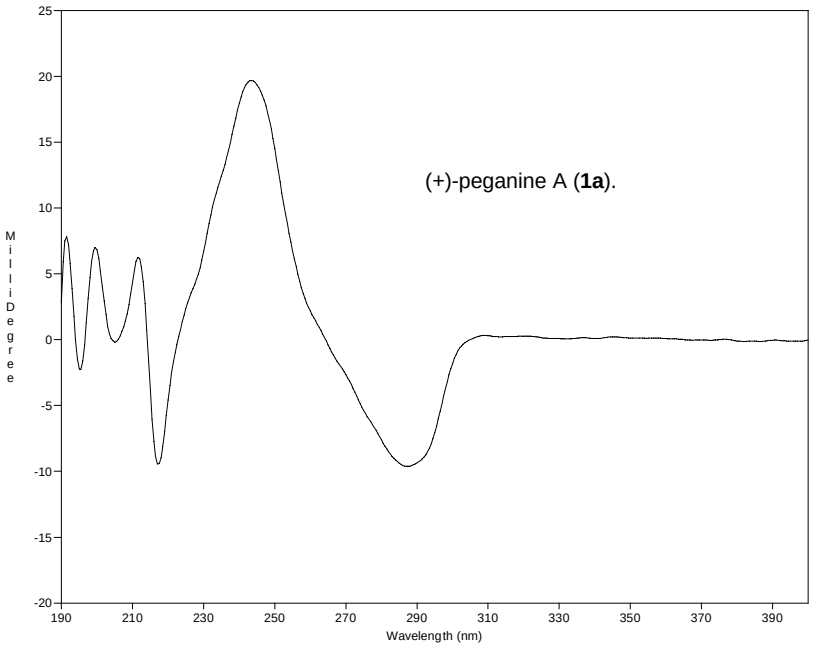
Figure S12 The ECD spectrum of (+)-peganine A (**1a**) and (**–**)-peganine A (**1b**)



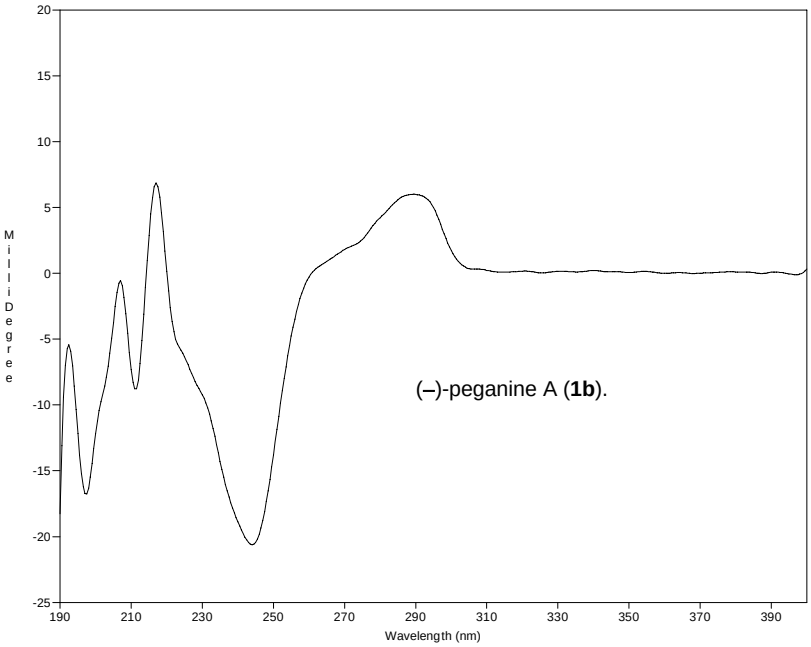


Figure S13 The ^{1}H NMR spectrum of peganine B (**2**) in DMSO-d_6 (400 MHz)

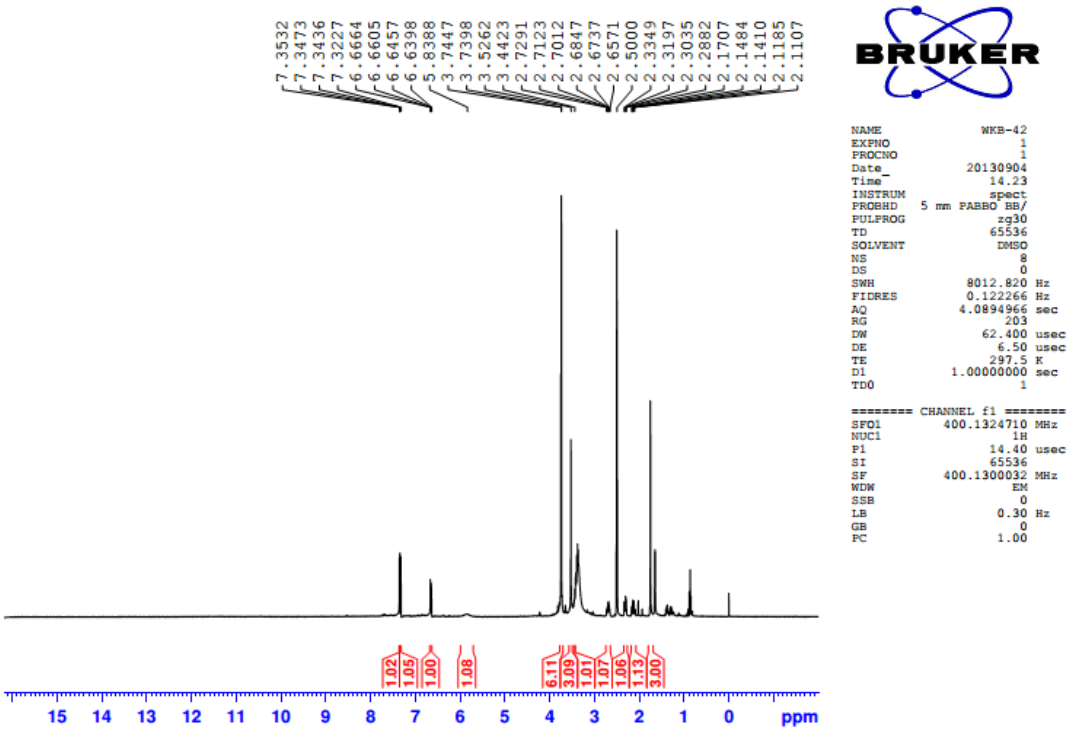


Figure S14 The ^{13}C NMR spectrum of peganine B (**2**) in DMSO-d_6 (100 MHz)

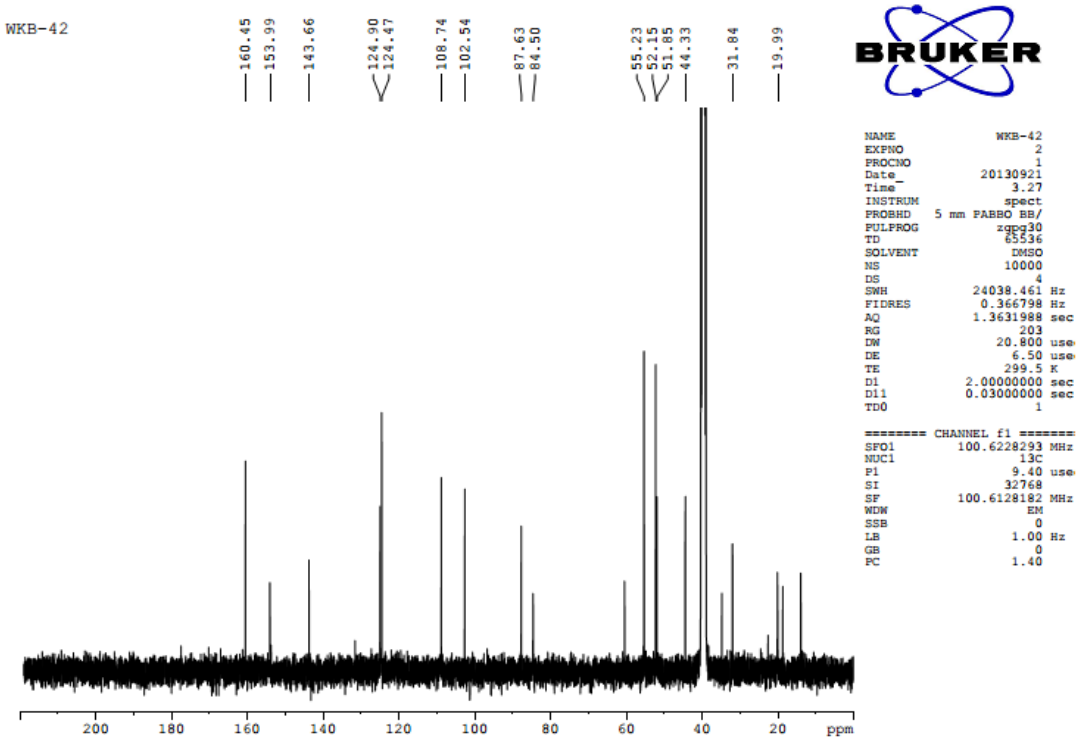


Figure S15 The HSQC spectrum of peganine B (**2**) in DMSO-d_6 (600 MHz)

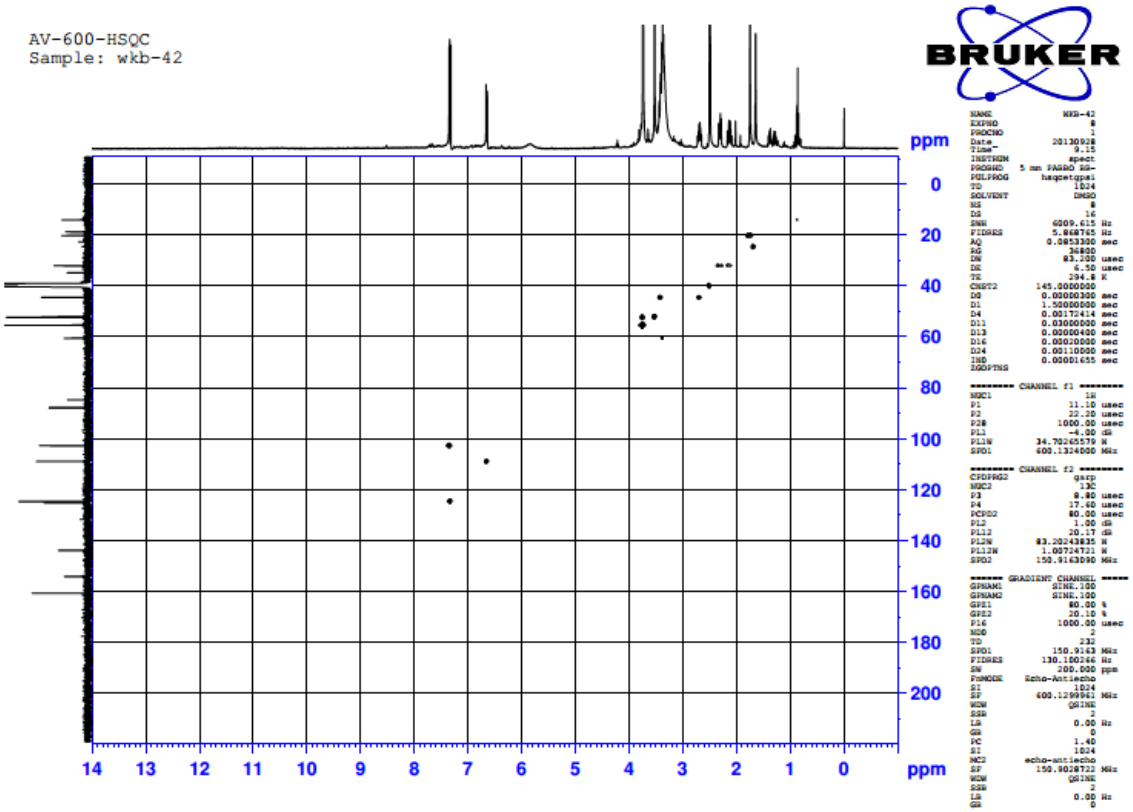


Figure S16 The HMBC spectrum of peganine B (**2**) in DMSO-d_6 (600 MHz)

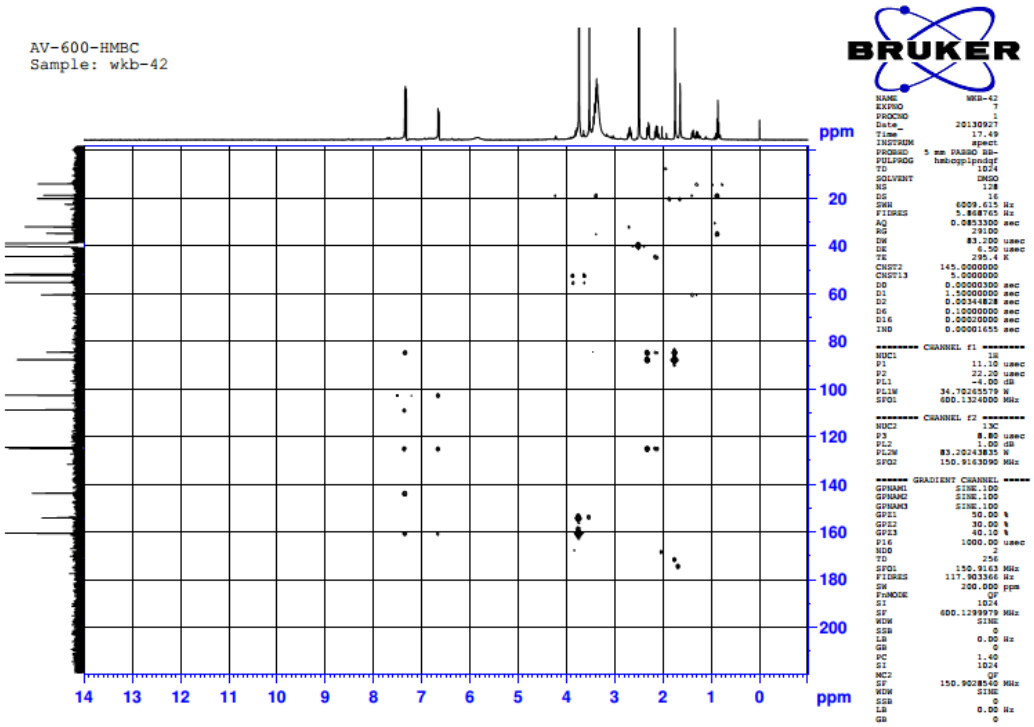
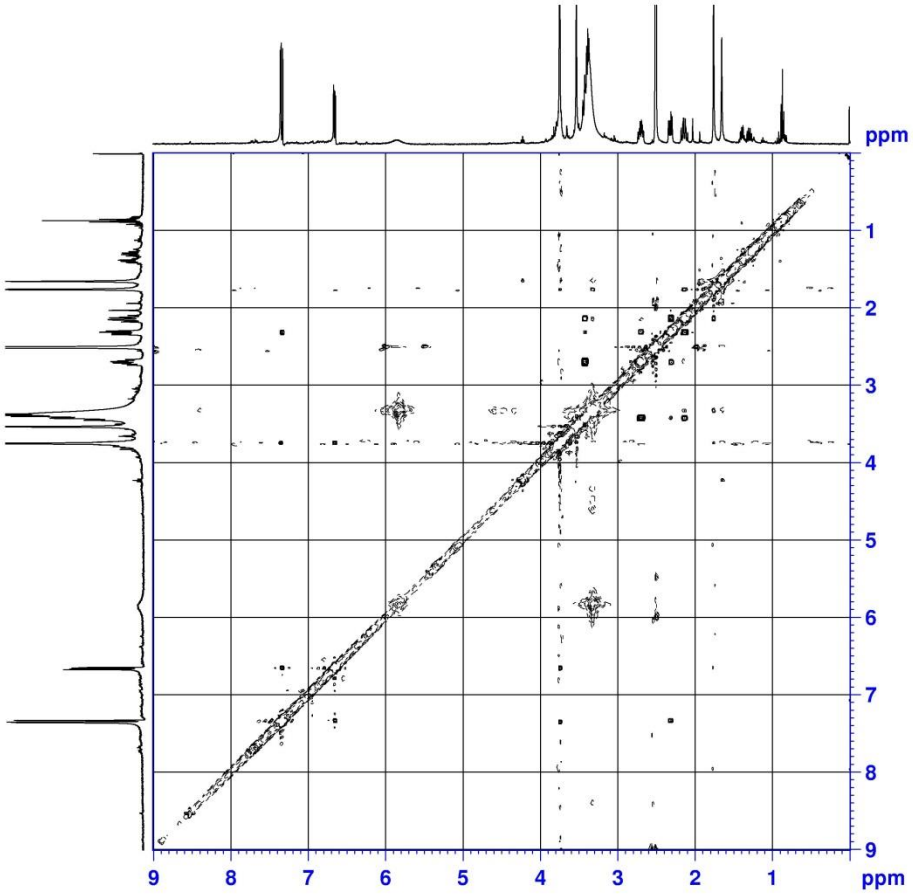


Figure S17 The NOESY spectrum of peganine B (**2**) in DMSO-d_6 (600 MHz)



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SOLVENT	DMSO
NS	4
DS	4
SWH	6009.615 Hz
FIDRES	5.868765 Hz
AQ	0.0853300 sec
RG	256
DW	83.200 usec
DE	6.50 usec
TE	298.2 K
D0	0.00006907 sec
D1	2.00000000 sec
D8	0.60000002 sec
IN0	0.00016640 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	11.10 usec
PL1	-4.00 dB
PL1W	34.70265579 W
SFO1	600.1324005 MHz
ND0	1
TD	256
SFO1	600.1324 MHz
FIDRES	23.475023 Hz
SW	10.014 ppm
FnMODE	States-TPPI
SI	1024
SF	600.1299980 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	States-TPPI
SF	600.1299958 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

Figure S18 The HRESIMS spectrum of peganine B (**2**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

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Method	ldj_bga_jh.m	Operator	Bruker Customer
Sample Name	WKB-42	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

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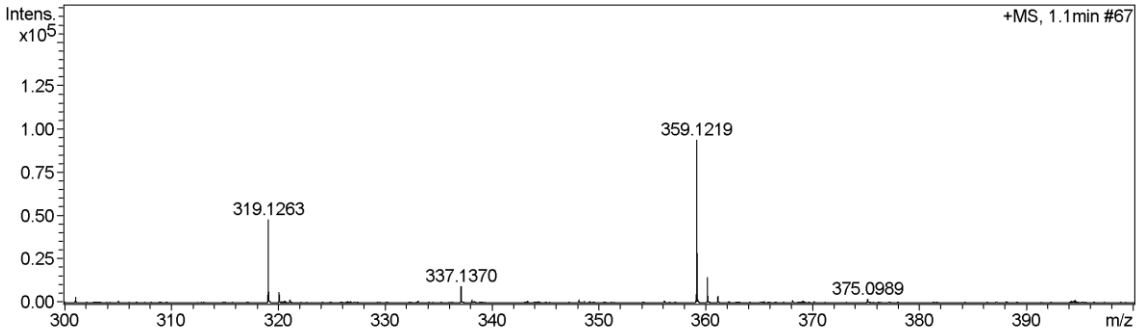
Formula, max.							
Measured m/z	359.122	Tolerance	10	mDa	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



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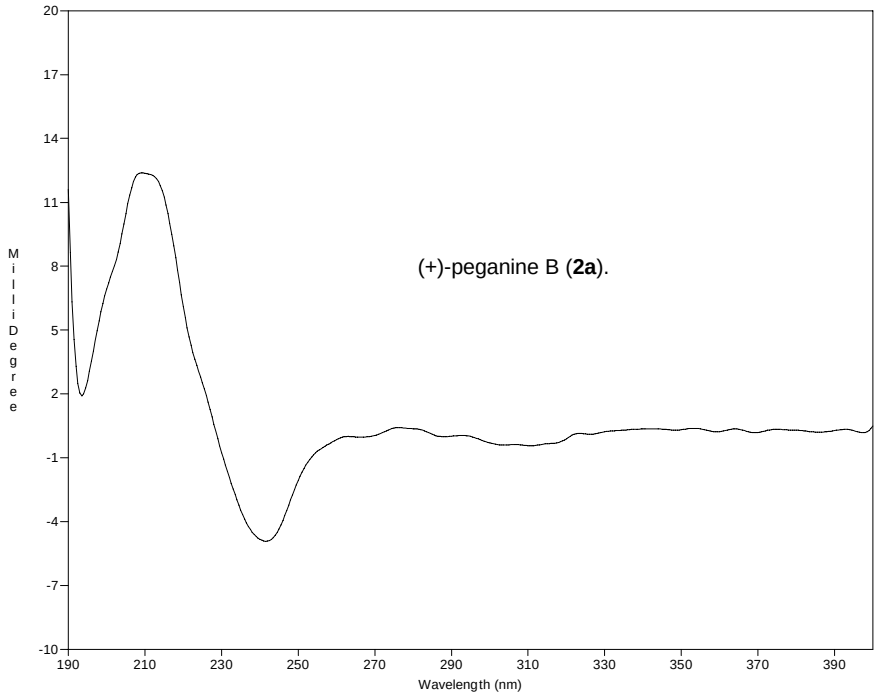
C 16 H 20 N 2 Na 1 O 6	0.018	359.1214	-1.41	-0.94	-0.51	7.50	ok	even

Figure S19 The ECD spectrum of (+)-peganine B (**2a**) and (**–**)-peganine B (**2b**)



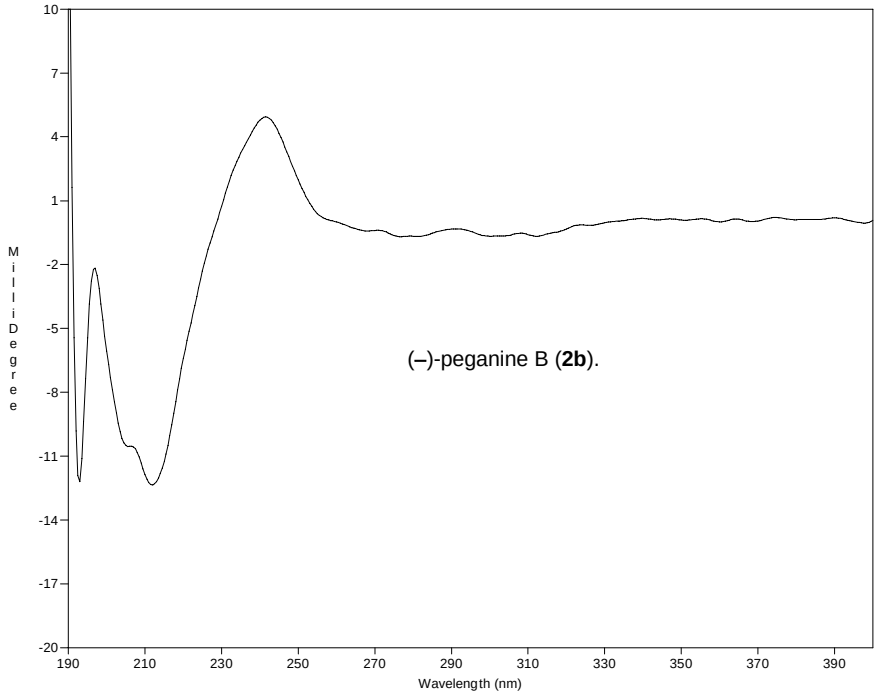


Figure S20 The ^{1}H NMR spectrum of peganumal A (**3**) in DMSO-d_6 (600 MHz)

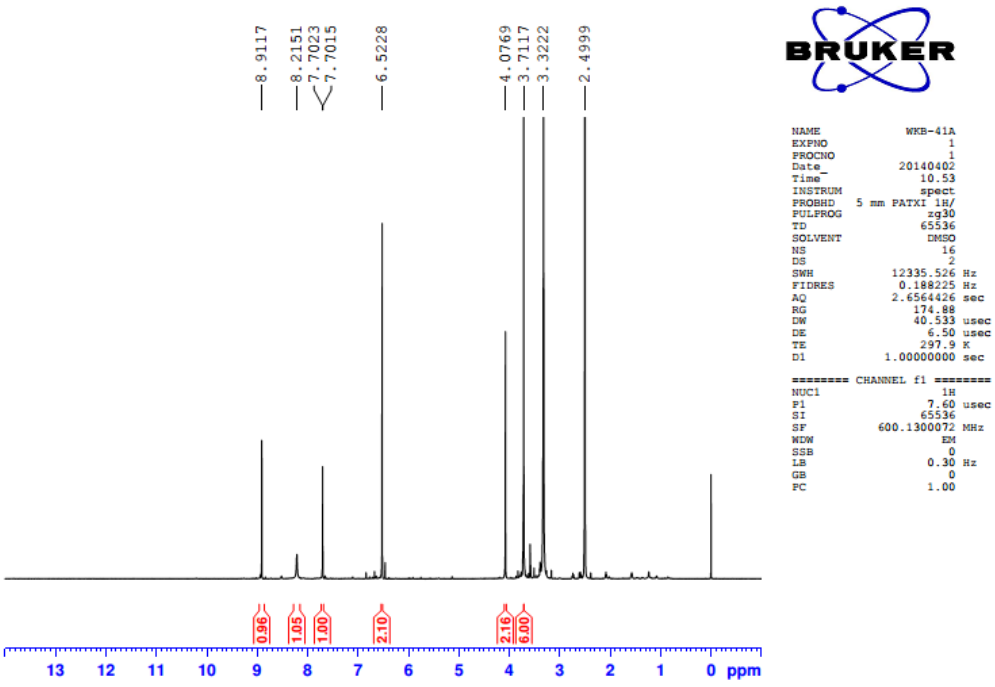


Figure S21 The ^{13}C NMR spectrum of peganumal A (**3**) in DMSO-d_6 (150 MHz)

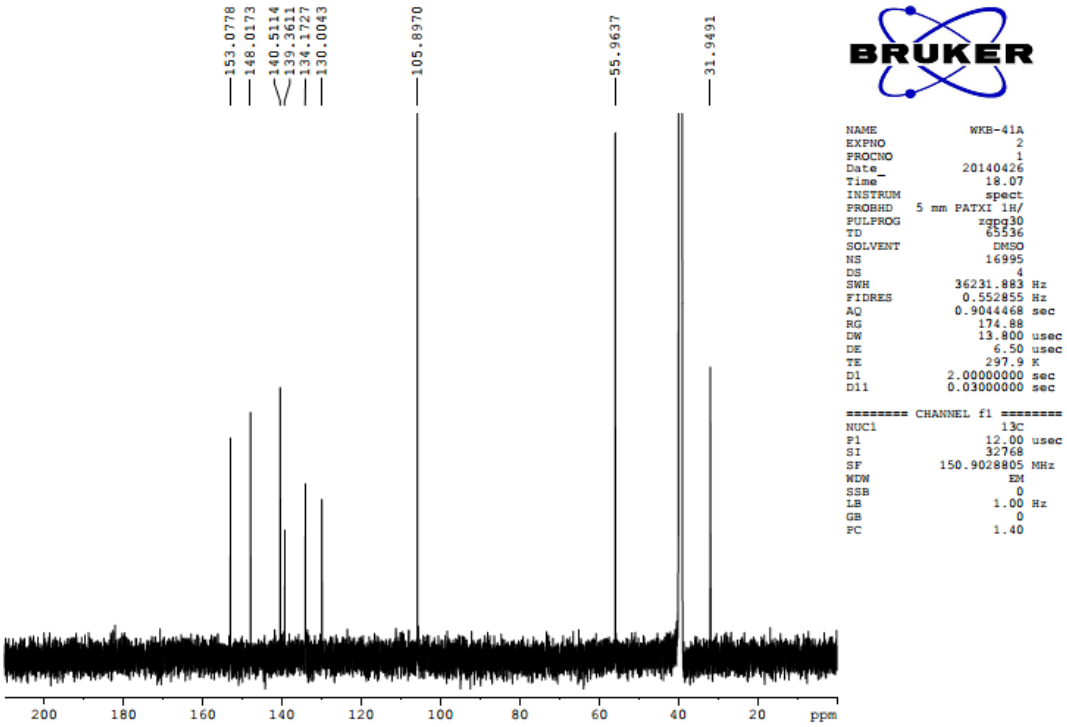
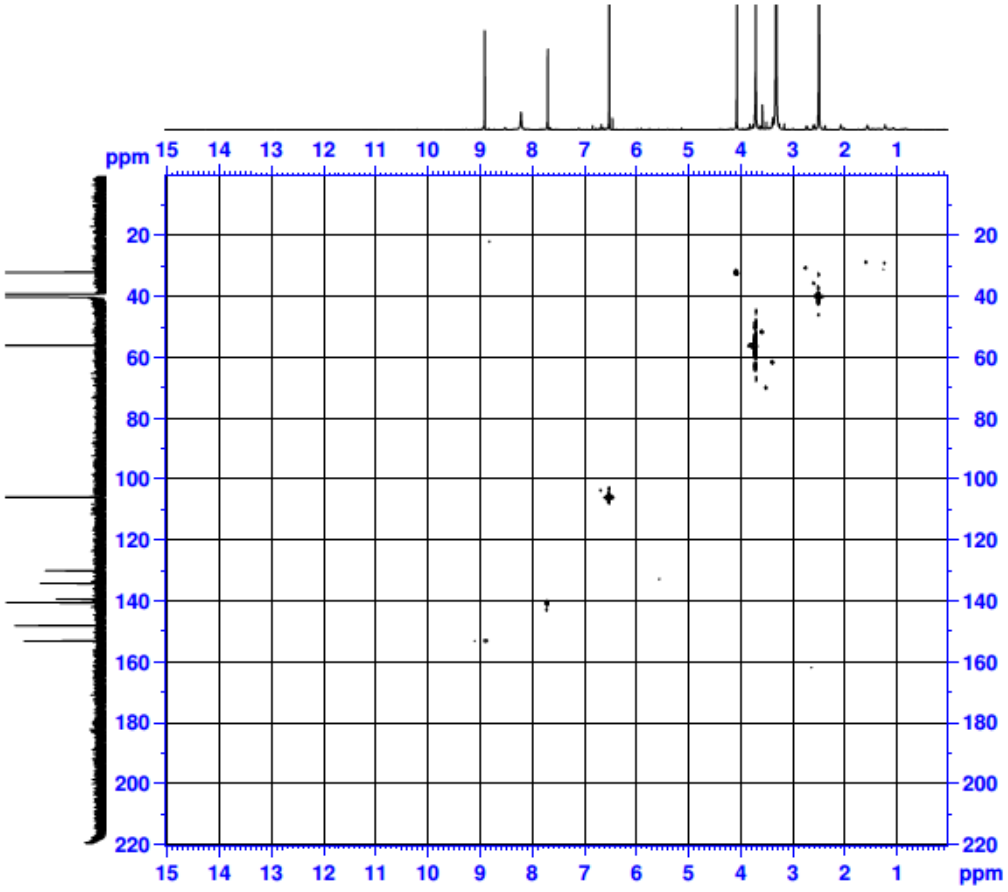


Figure S22 The HSQC spectrum of peganumal A (**3**) in DMSO-d_6 (600 MHz)

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PROCNO                  1
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PULPROG       hsqcetgpsi
TD                   1024
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NS                      8
DS                     16
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FIDRES          7.042518 Hz
AQ              0.0710473 sec
RG                 174.88
DW                 69.333 usec
DE                   6.50 usec
TE                 298.0 K
CNST2         145.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D4              0.00172414 sec
D11             0.03000000 sec
D13             0.00000400 sec
D16             0.00020000 sec
D24             0.00000000 sec
IN0             0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
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P2                  15.20 usec
P28               1000.00 usec
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TD                    256
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SW                180.000 ppm
FnMODE      Echo-Antiecho
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SF            600.1300023 MHz
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LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2         echo-antiecho
SF            150.9028659 MHz
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SSB                     2
LB                   0.00 Hz
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Figure S23 The HMBC spectrum of peganumal A (**3**) in DMSO-d_6 (600 MHz)

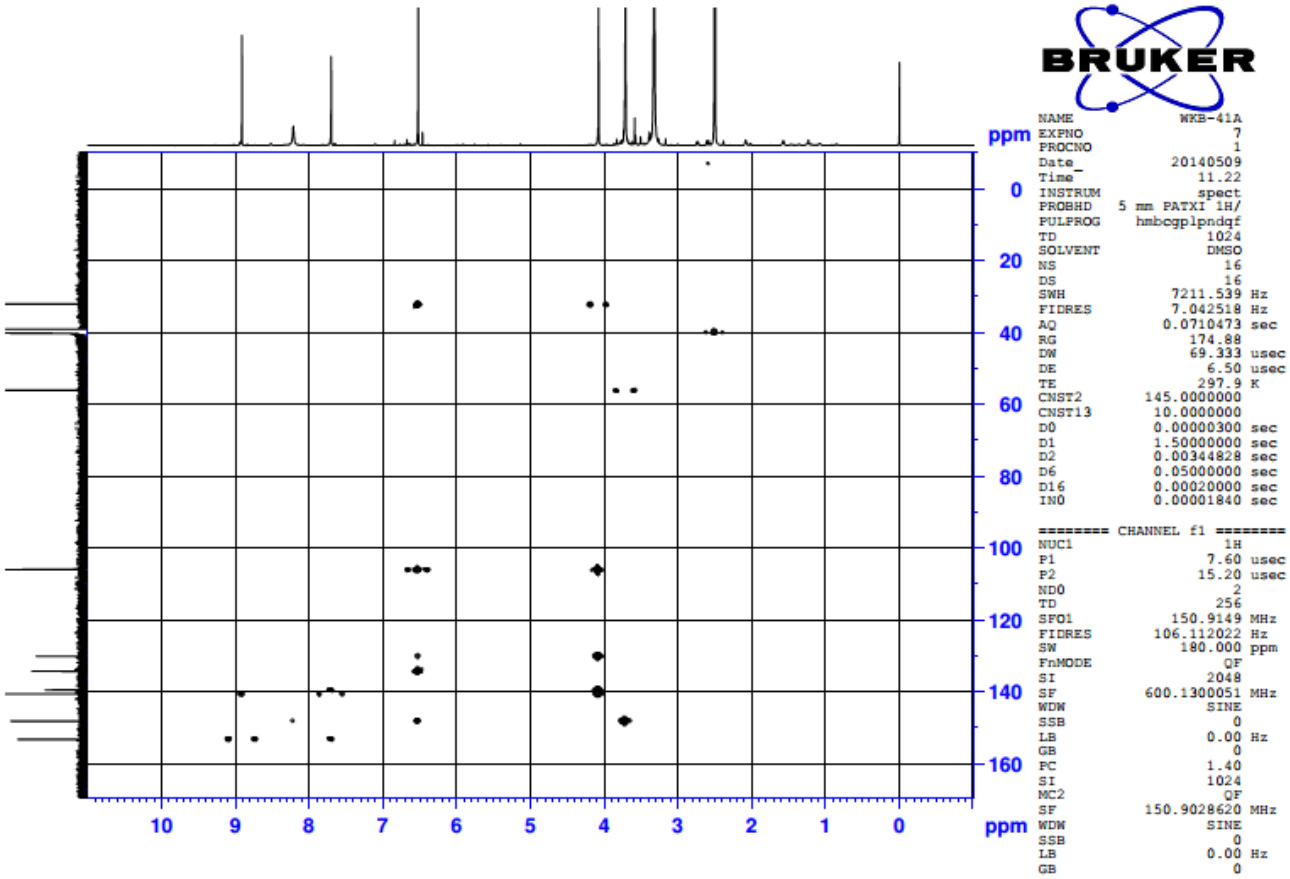

Figure S24 The HRESIMS spectrum of peganumal A (**3**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

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Comment			

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

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Formula, max.							
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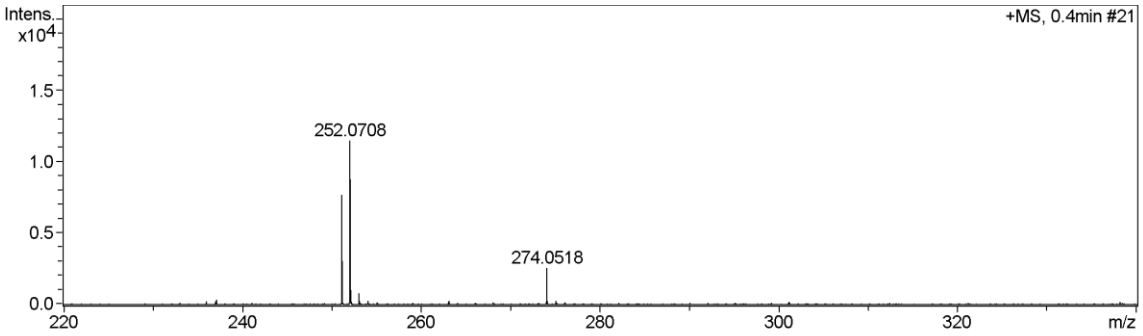
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 12 H 13 N 1 Na 1 O 3 S 1	0.048	274.0508	-3.44	-3.64	-0.94	6.50	ok	even

Figure S25 The ^{1}H NMR spectrum of peganumal B (**4**) in DMSO-d_6 (400 MHz)

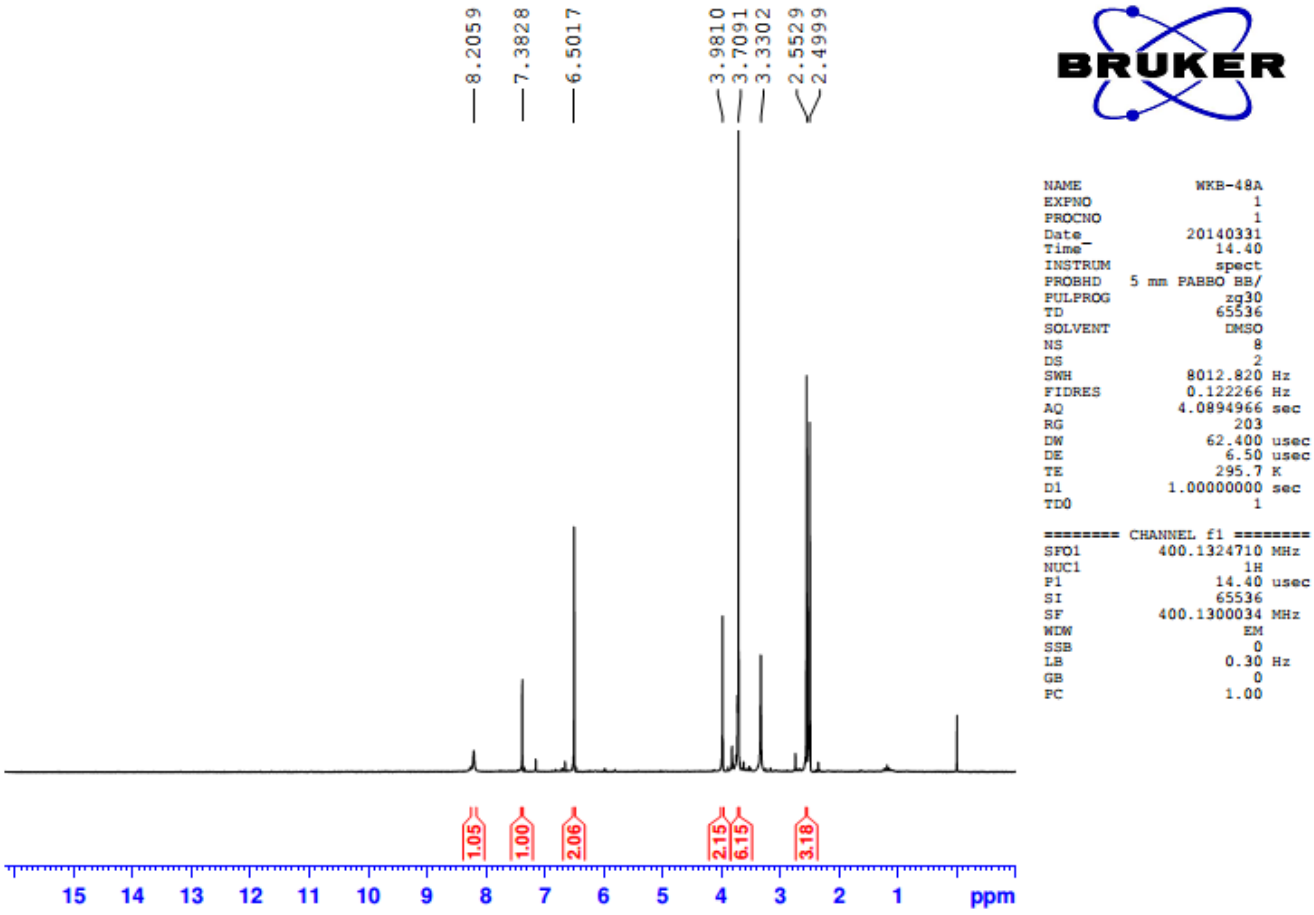


Figure S26 The ^{13}C NMR spectrum of peganumal B (**4**) in DMSO-d_6 (100 MHz)

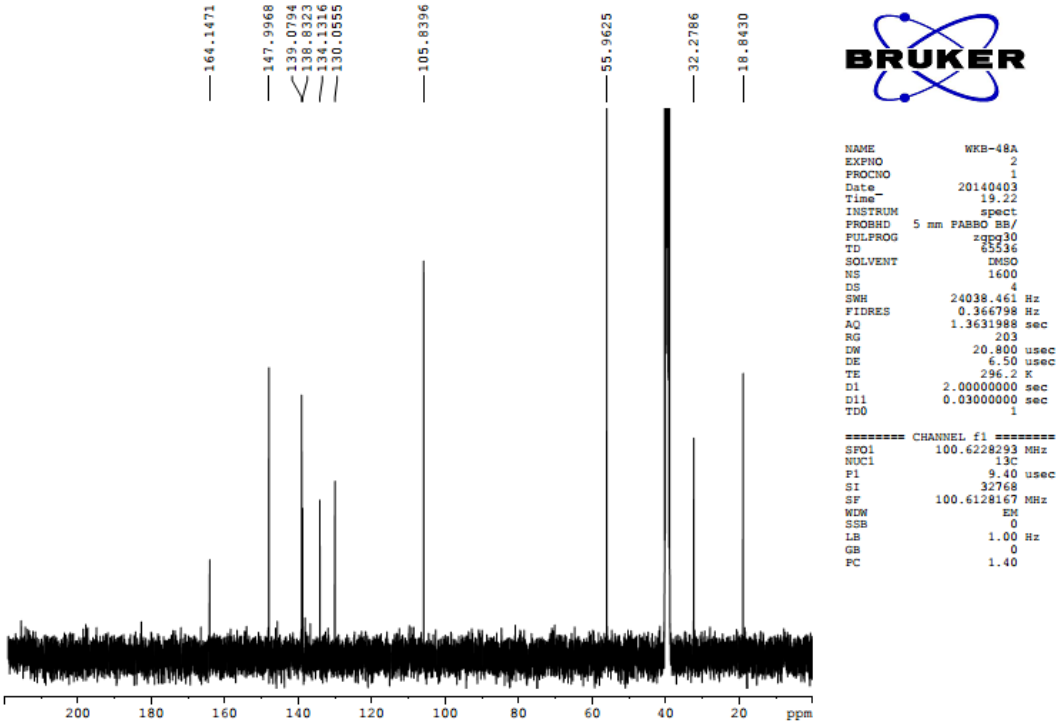


Figure S27 The HSQC spectrum of peganumal B (**4**) in DMSO-d_6 (600 MHz)

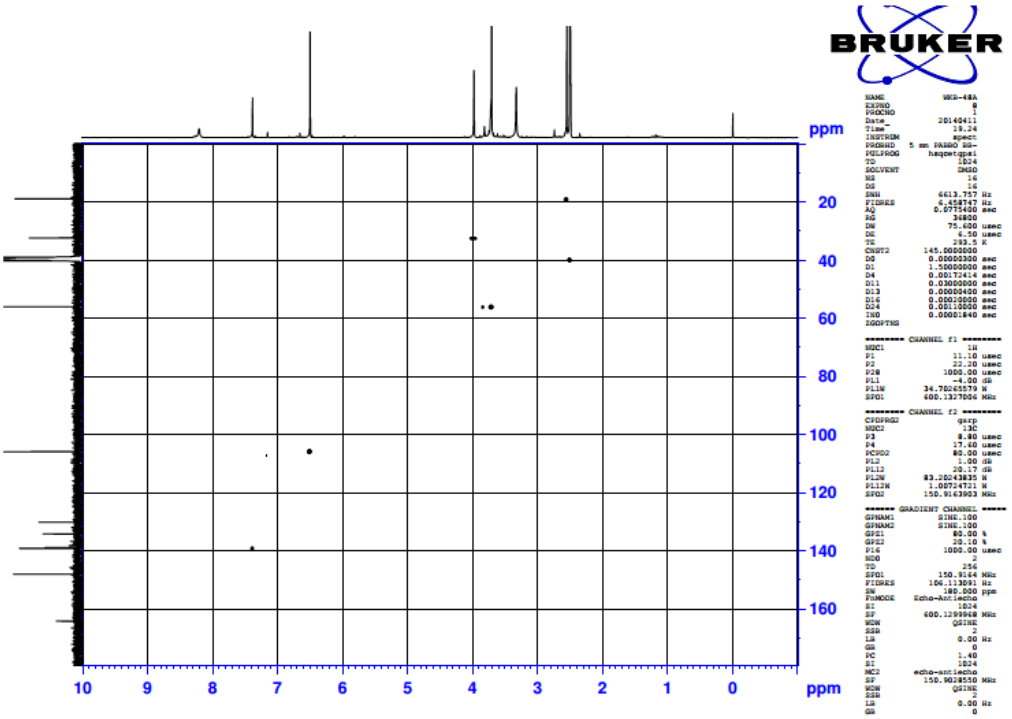


Figure S28 The HMBC spectrum of peganumal B (**4**) in DMSO-d_6 (600 MHz)

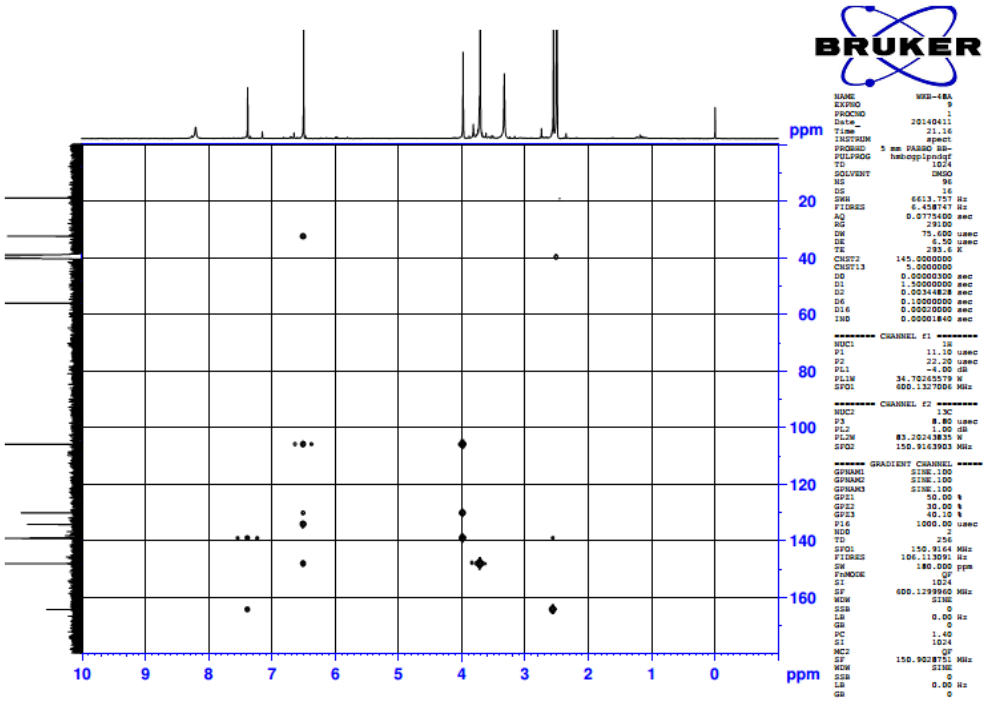


Figure S29 The HRESIMS spectrum of peganumal B (**4**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

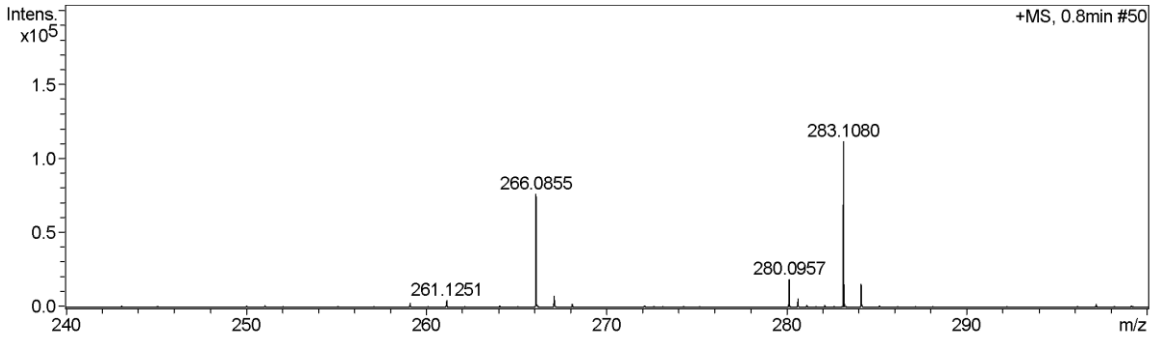
Analysis Name	D:\Data\20140430CEYANG\WKB-48A_1-a,3_01_3262.d	Acquisition Date	4/30/2014 2:06:24 PM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	WKB-48A	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C13H15N1O3S1H						
Formula, max.							
Measured m/z	266.086	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	yes	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 13 H 16 N 1 O 3 S 1	0.036	266.0845	-3.50	-5.40	-0.93	6.50	ok	even

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Figure S30 The ^{1}H NMR spectrum of pegaharmine F (**5**) in DMSO-d_6 (600 MHz)

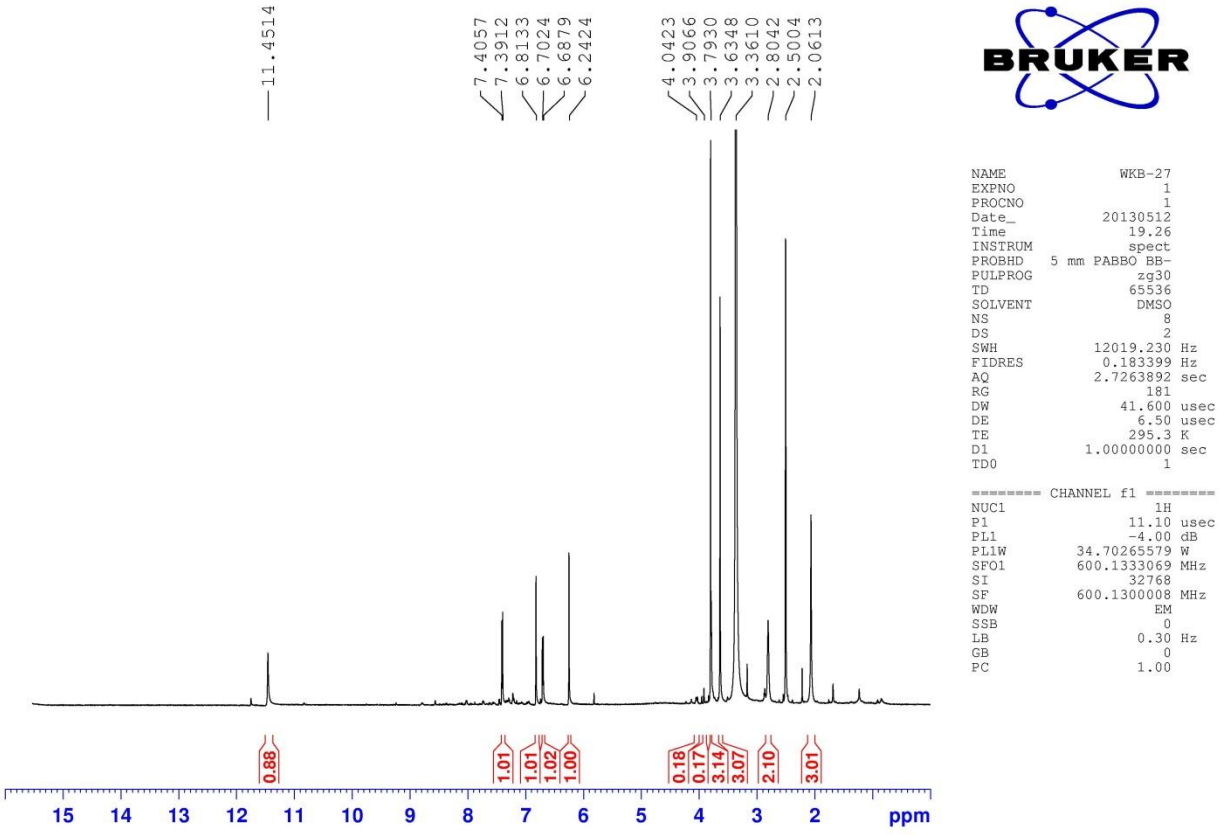


Figure S31 The ^{13}C NMR spectrum of pegaharmine F (**5**) in DMSO-d_6 (100 MHz)

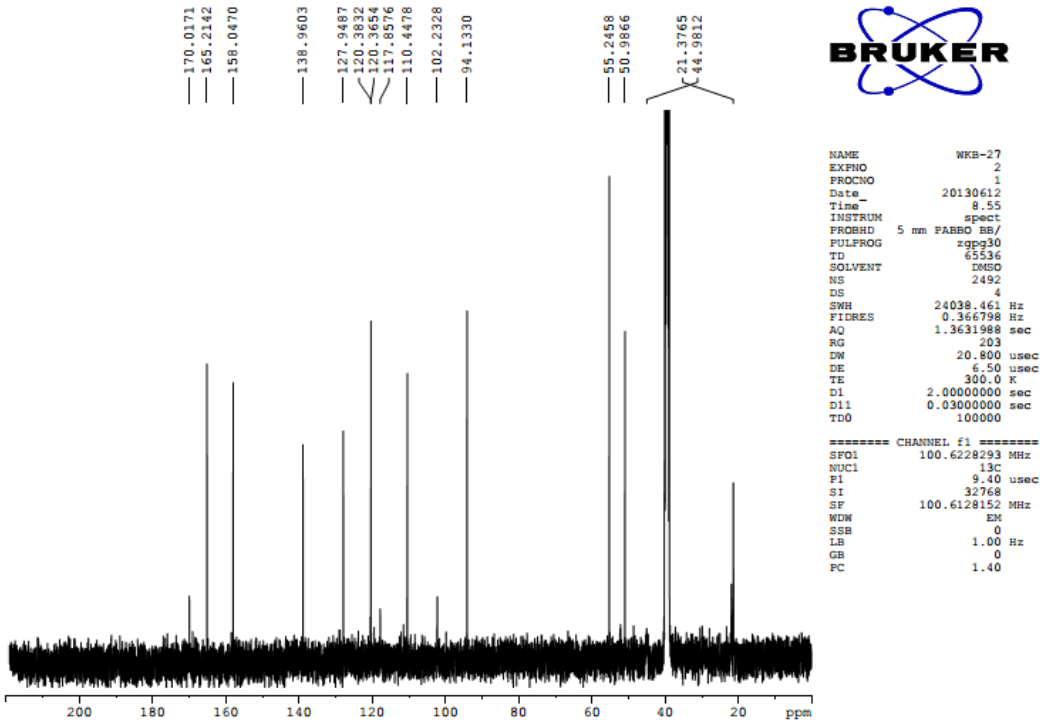


Figure S32 The HSQC spectrum of pegaharmine F (**5**) in DMSO-d_6 (600 MHz)

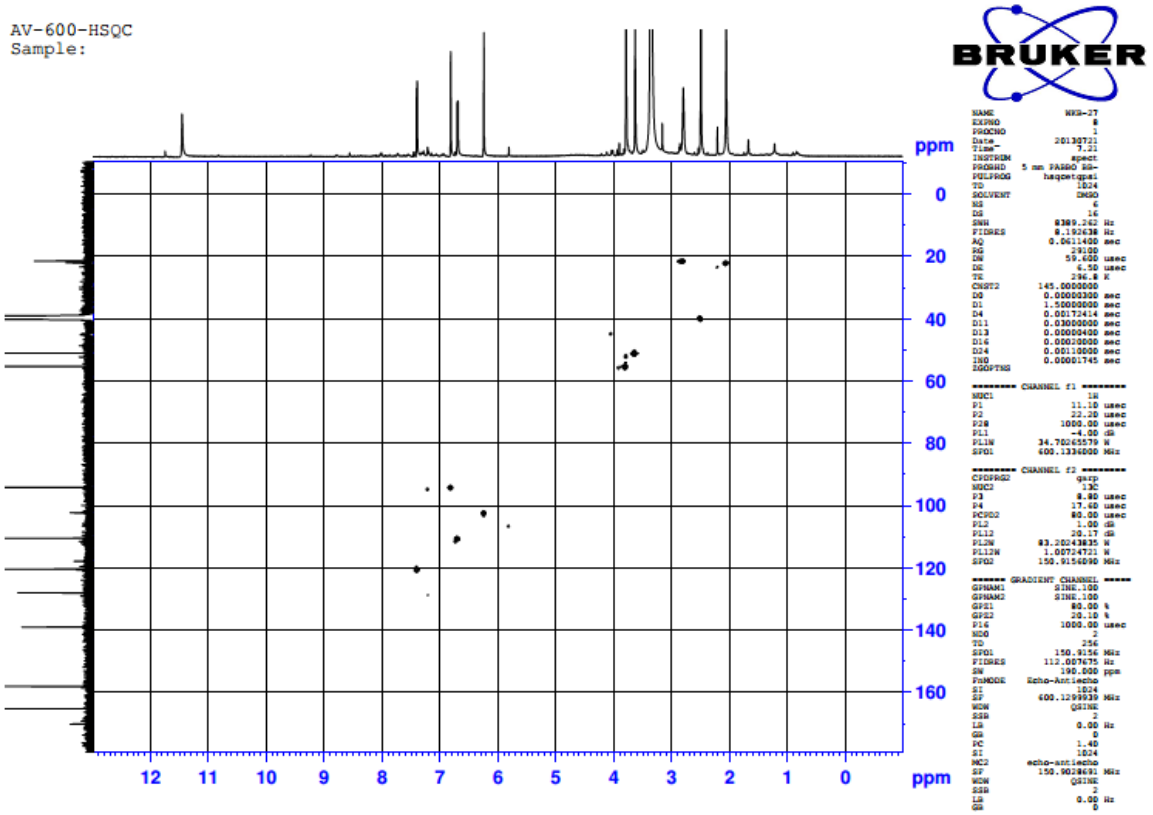


Figure S33 The HMBC spectrum of pegaharmine F (**5**) in DMSO-d_6 (600 MHz)

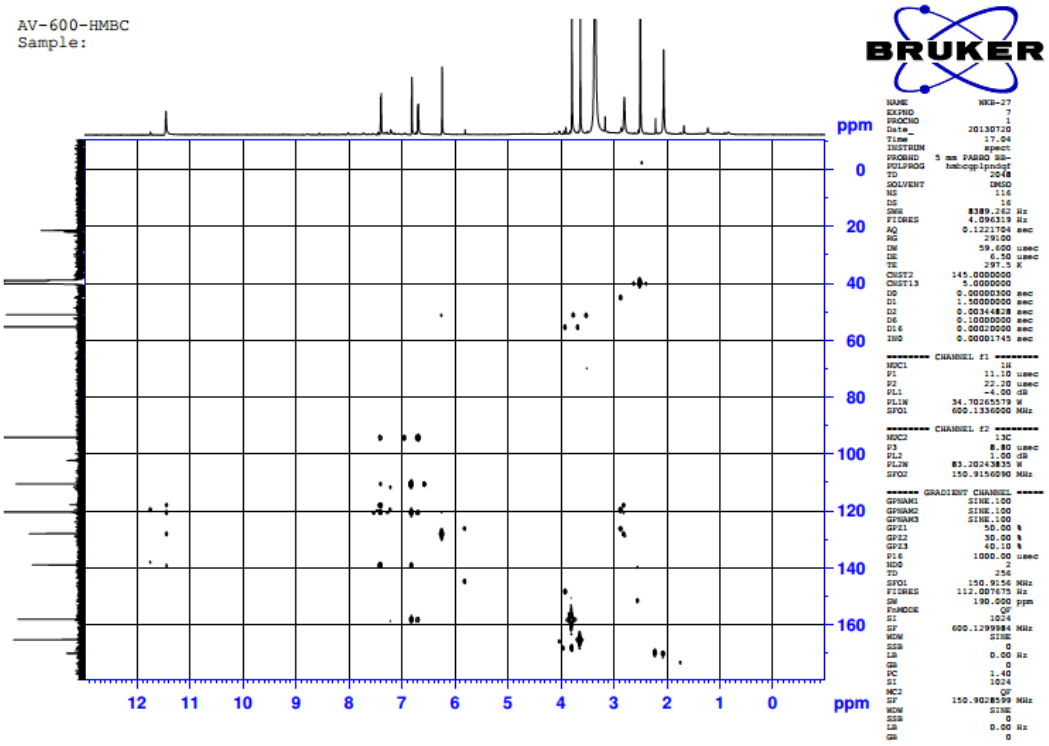


Figure S34 The HRESIMS spectrum of pegaharmine F (**5**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

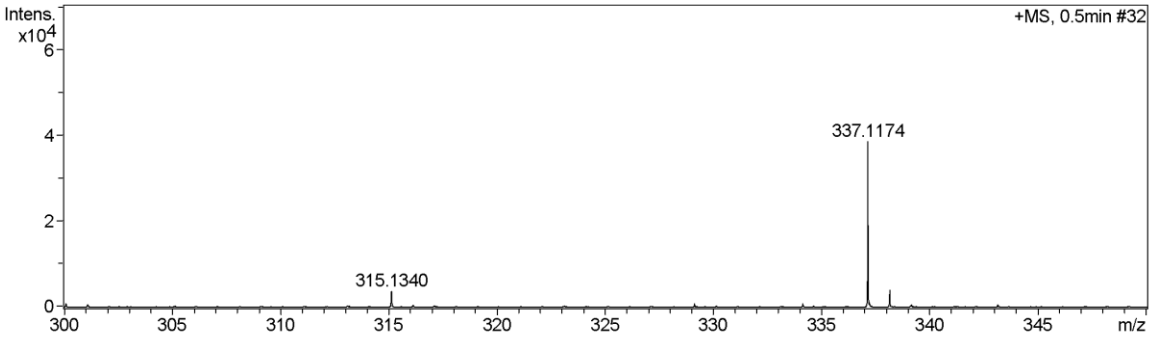
Analysis Name	D:\Data\20140605ceyang\wkb-27_1-a,3_01_3453.d	Acquisition Date	6/6/2014 9:00:50 AM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	wkb-27	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C17H18N2O4Na						
Formula, max.							
Measured m/z	337.117	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 17 H 18 N 2 Na 1 O 4	0.054	337.1159	-4.55	-3.09	-1.53	9.50	ok	even

Figure S35 The ^{1}H NMR spectrum of pegaharmine G (**6**) in DMSO-d_6 (600 MHz)

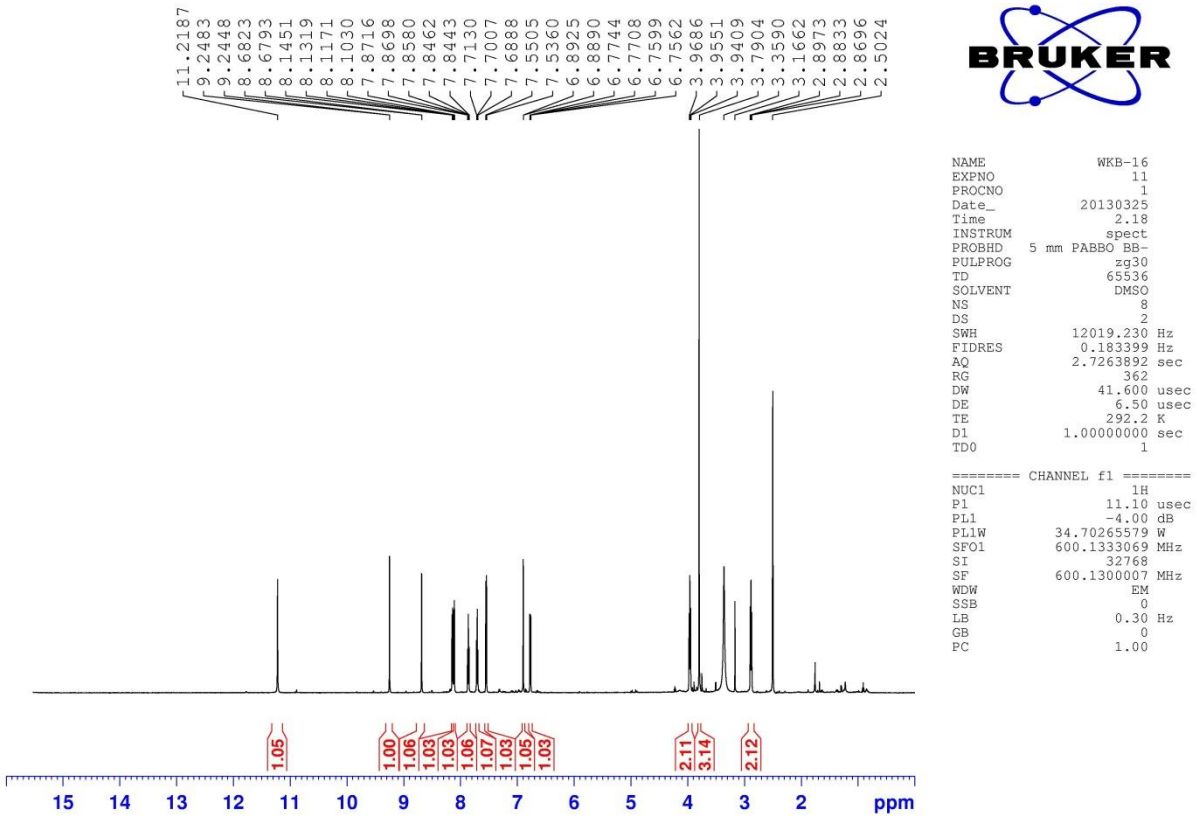
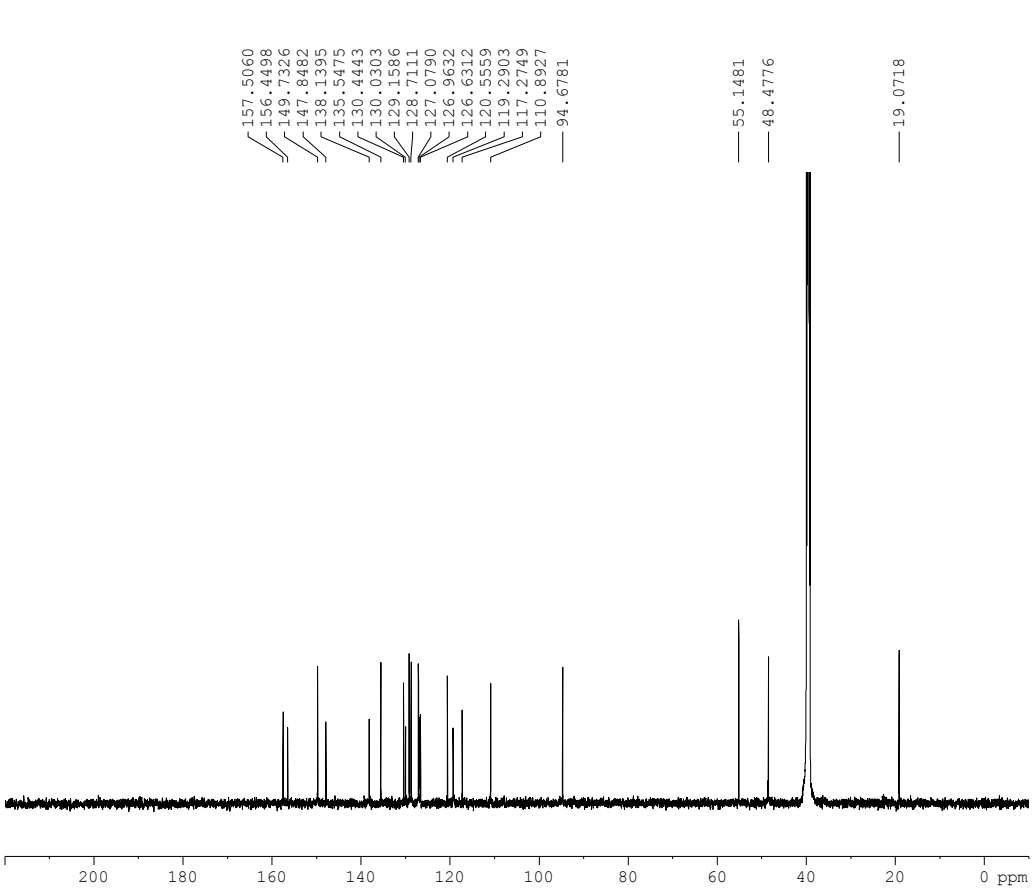


Figure S36 The ^{13}C NMR spectrum of pegaharmine G (**6**) in DMSO-d_6 (150 MHz)



BRUKER

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EXPNO                   2
PROCNO                  1
Date_            20130304
Time                20.47
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT               DMSO
NS                    4011
DS                       2
SWH             45454.547 Hz
FIDRES           0.693581 Hz
AQ              0.7209570 sec
RG                   20600
DW                  11.000 usec
DE                    6.50 usec
TE                   673.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    6.00 usec
PL1                   1.00 dB
PL1W          83.20243835 W
SFO1         150.9178993 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                 - 4.00 dB
PL12                13.16 dB
PL13                16.00 dB
PL2W          34.70265579 W
PL12W          0.66736388 W
PL13W          0.34702653 W
SFO2         600.1324005 MHz
SI                   32768
SF           150.9028748 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
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Figure S37 The HSQC spectrum of pegaharmine G (**6**) in DMSO-d_6 (600 MHz)

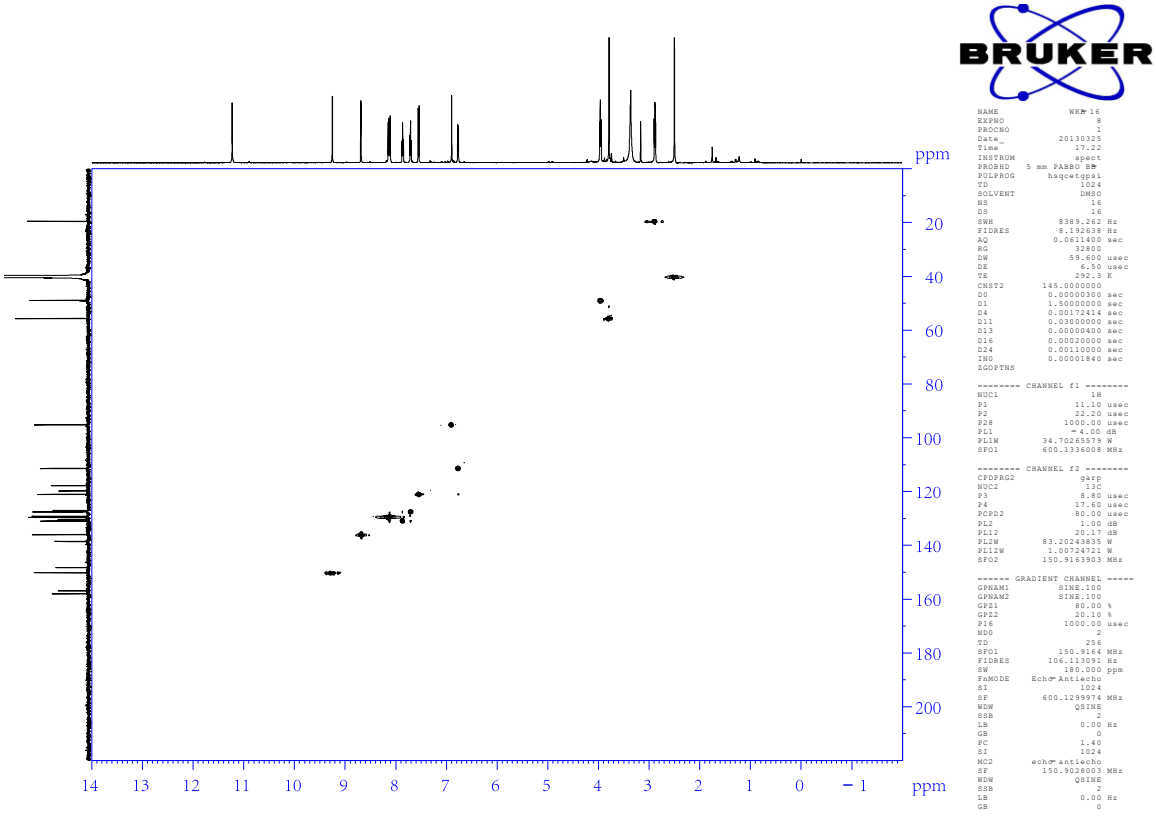


Figure S38 The HMBC spectrum of pegaharmine G (**6**) in DMSO-d_6 (600 MHz)

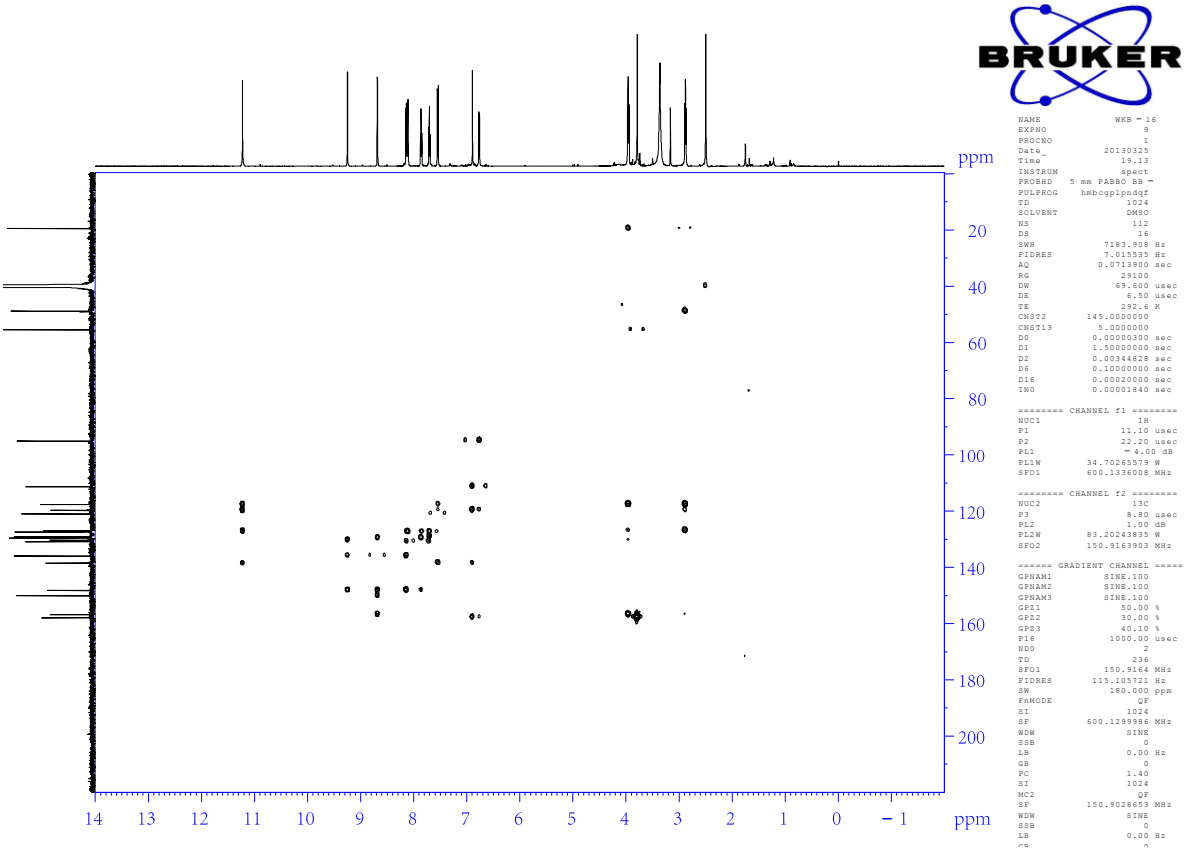


Figure S39 The HRESIMS spectrum of pegaharmine G (**6**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

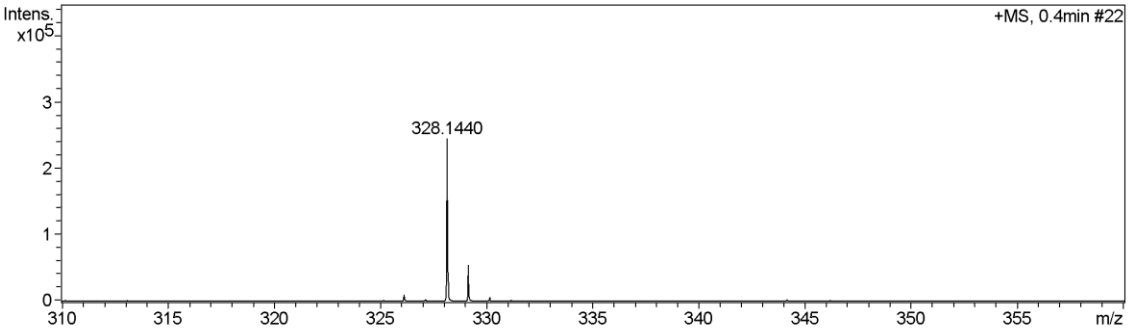
Analysis Name	D:\Data\20130328\WKB-16.d	Acquisition Date	3/28/2013 3:31:37 PM
Method	LIU 250-550POS.m	Operator	Bruker Customer
Sample Name	WKB-16	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C21H18N3O1						
Formula, max.							
Measured m/z	328.144	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 21 H 18 N 3 O 1	0.014	328.1444	1.32	1.69	0.43	14.50	ok	even

Figure S40 The ^{1}H NMR spectrum of pegaharmine H (**7**) in DMSO-d_6 (600 MHz)

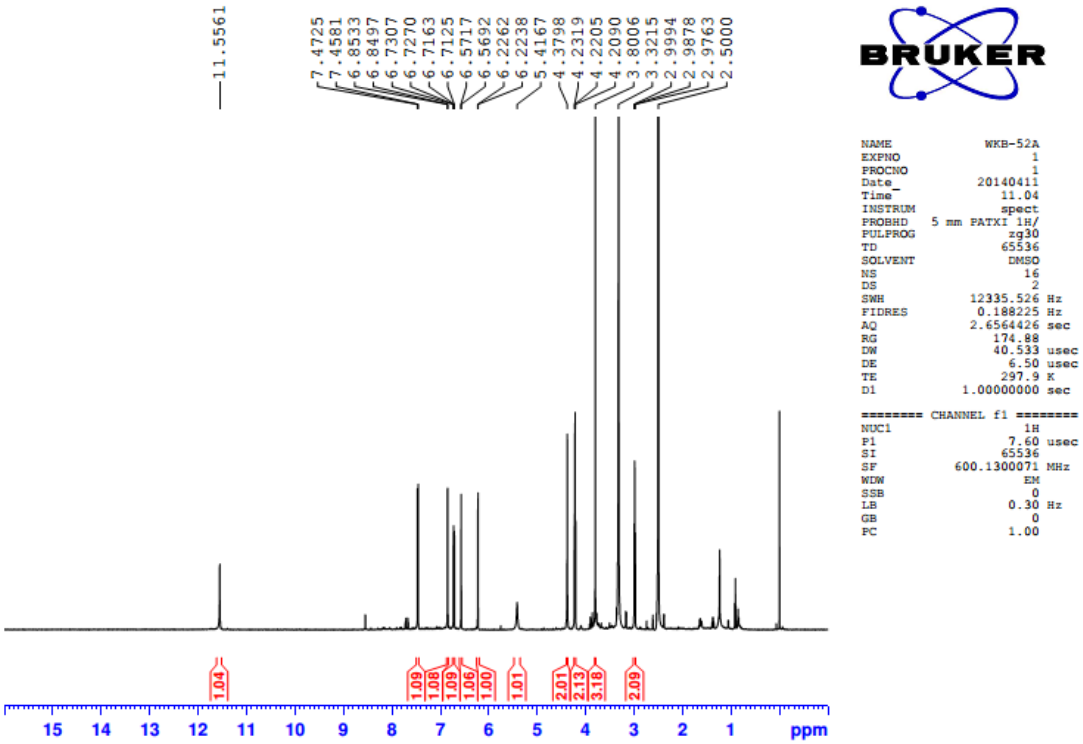


Figure S41 The ^{13}C NMR spectrum of pegaharmine H (**7**) in DMSO-d_6 (150 MHz)

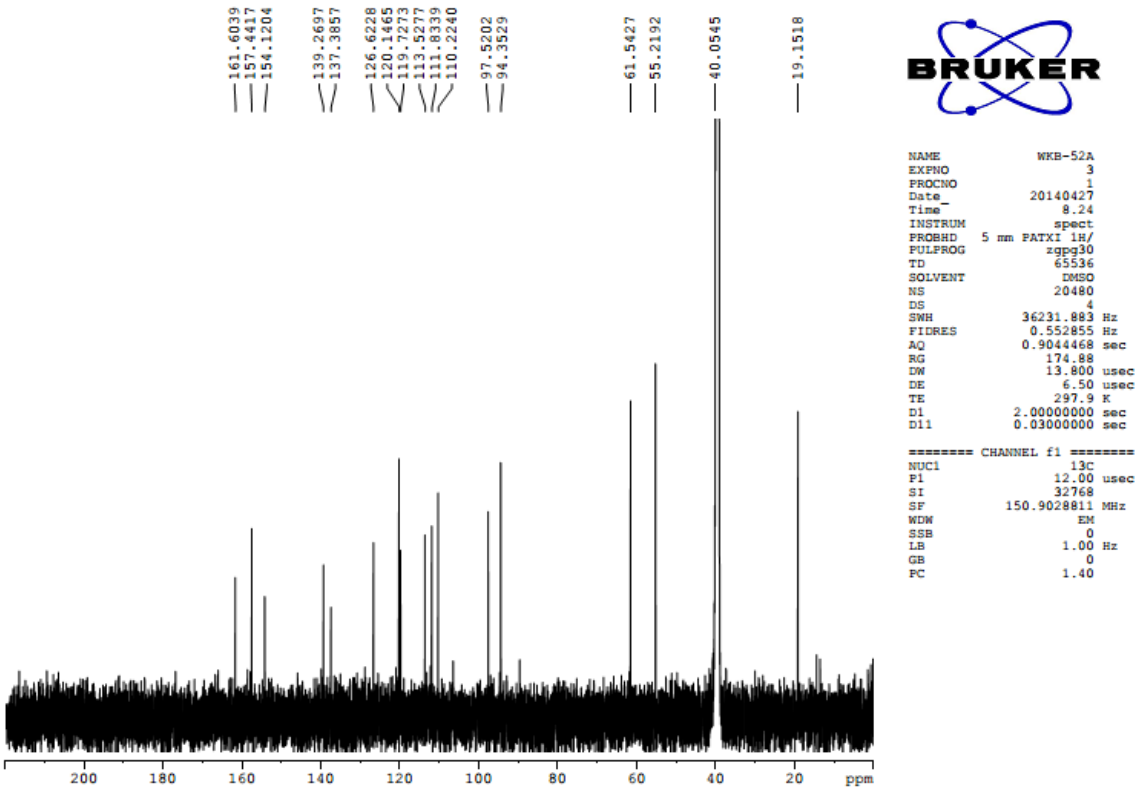


Figure S42 The HSQC spectrum of pegaharmine H (**7**) in DMSO-d_6 (600 MHz)

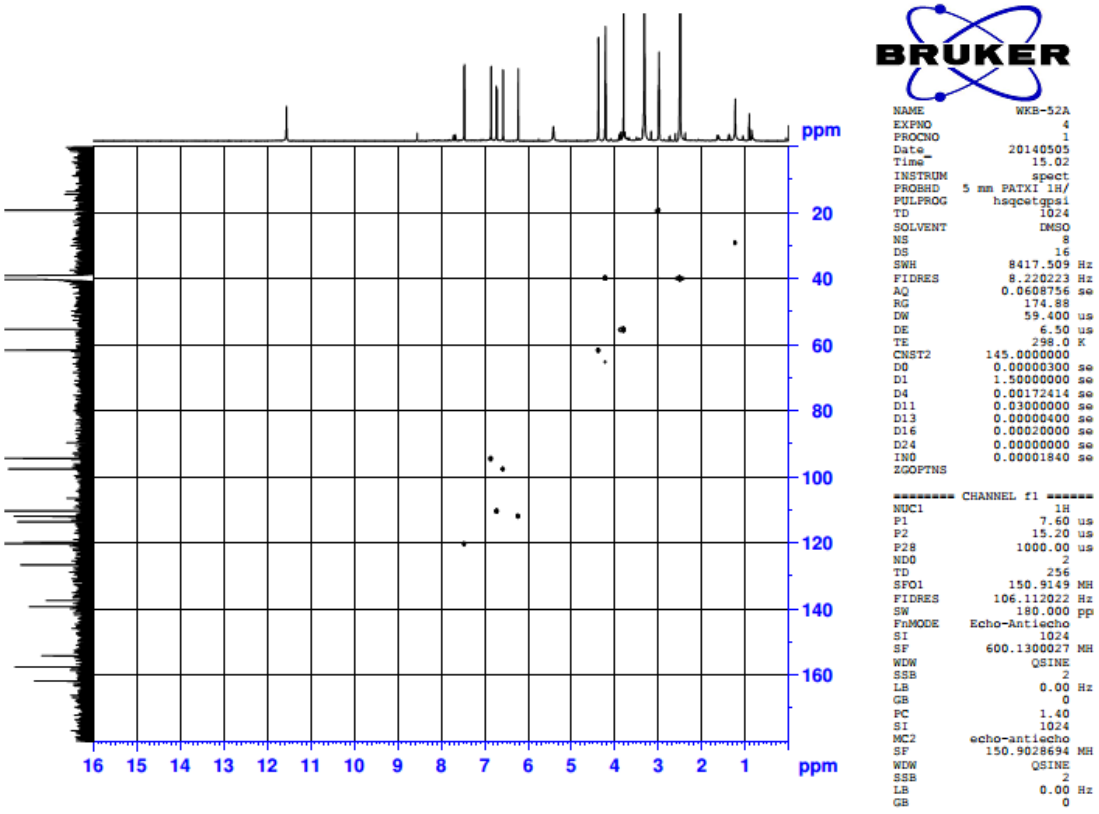


Figure S43 The HMBC spectrum of pegaharmine H (**7**) in DMSO-d_6 (600 MHz)

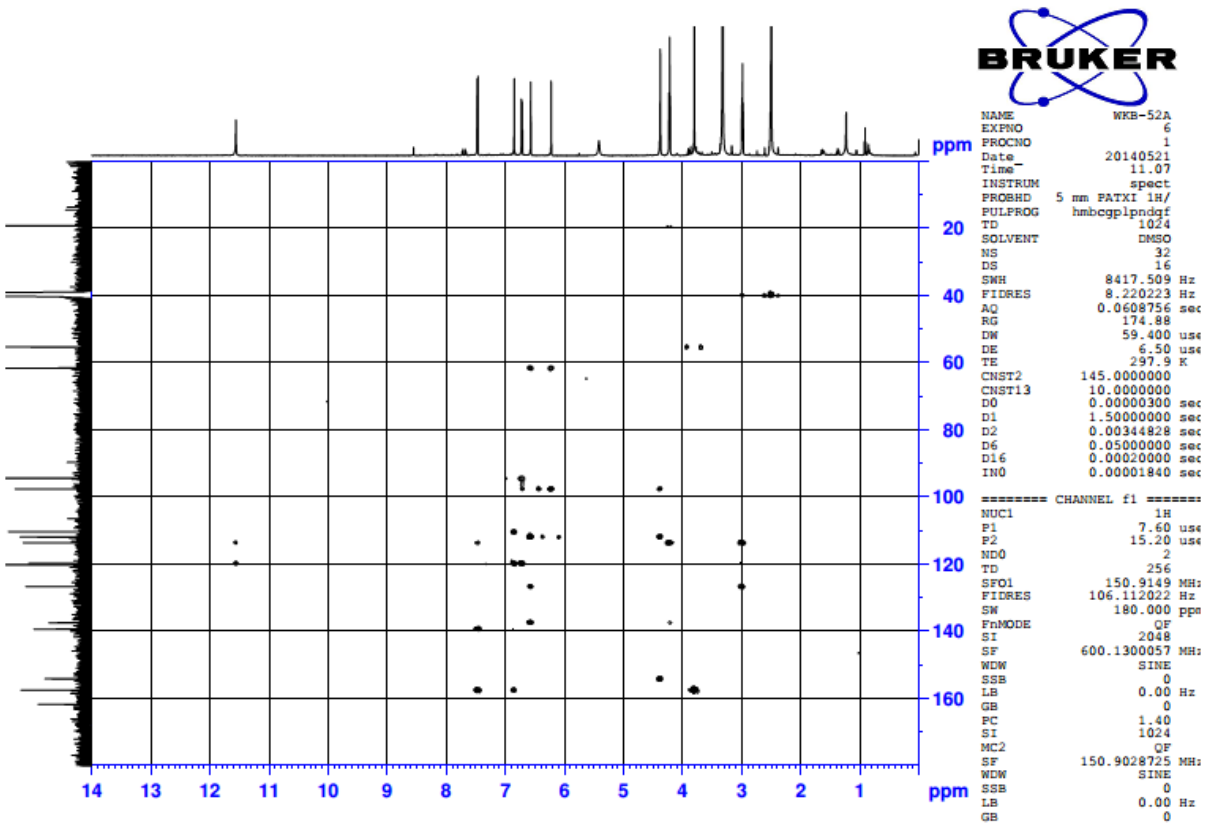


Figure S44 The HRESIMS spectrum of pegaharmine H (**7**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

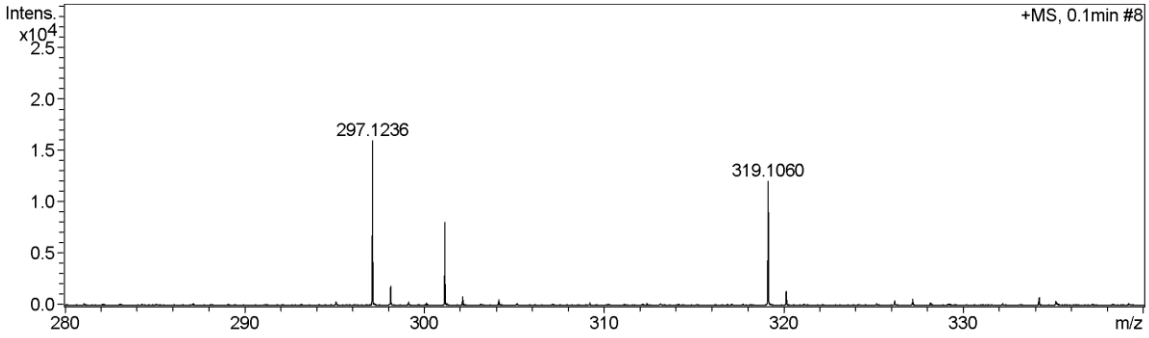
Analysis Name	D:\Data\20140516CEYANG\WKB-52A.d	Acquisition Date	5/16/2014 7:34:28 PM
Method	Liu_low_20131025.m	Operator	Bruker Customer
Sample Name	WKB-52A	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C17H16N2O3H						
Formula, max.							
Measured m/z	297.124	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 17 H 17 N 2 O 3	0.046	297.1234	-0.93	-2.04	-0.28	10.50	ok	even

Figure S45 The ^{1}H NMR spectrum of pegaharmine I (**8**) in DMSO-d_6 (400 MHz)

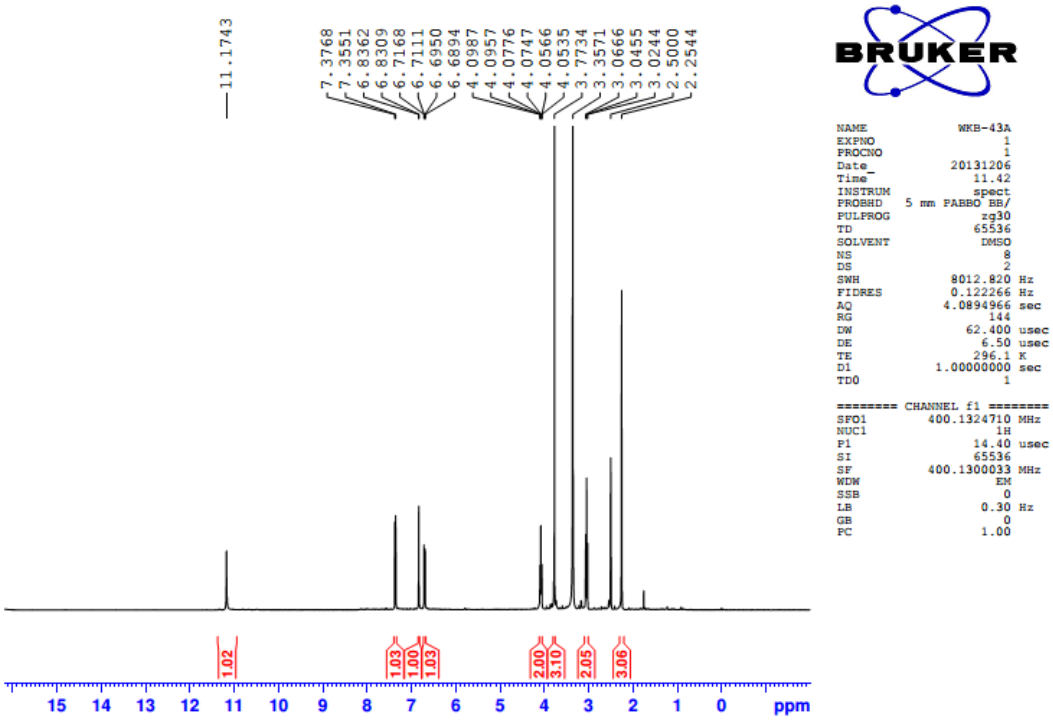


Figure S46 The ^{13}C NMR spectrum of pegaharmine I (**8**) in DMSO-d_6 (100 MHz)

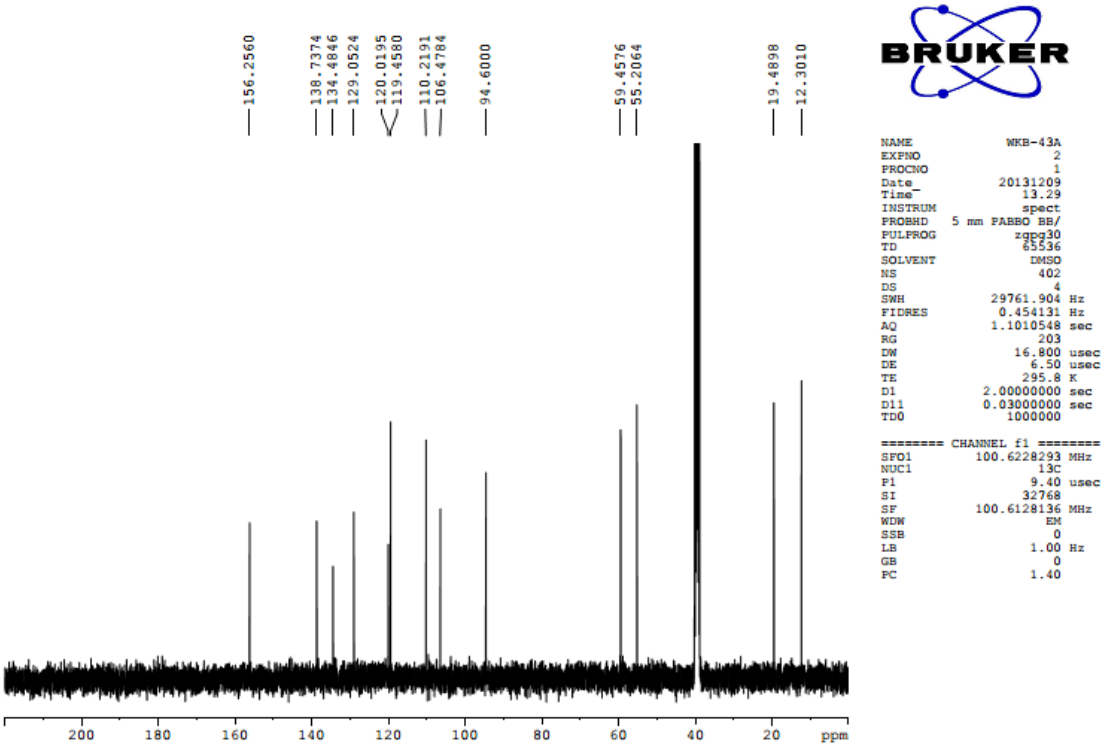


Figure S47 The HSQC spectrum of pegaharmine I (**8**) in DMSO-d_6 (600 MHz)

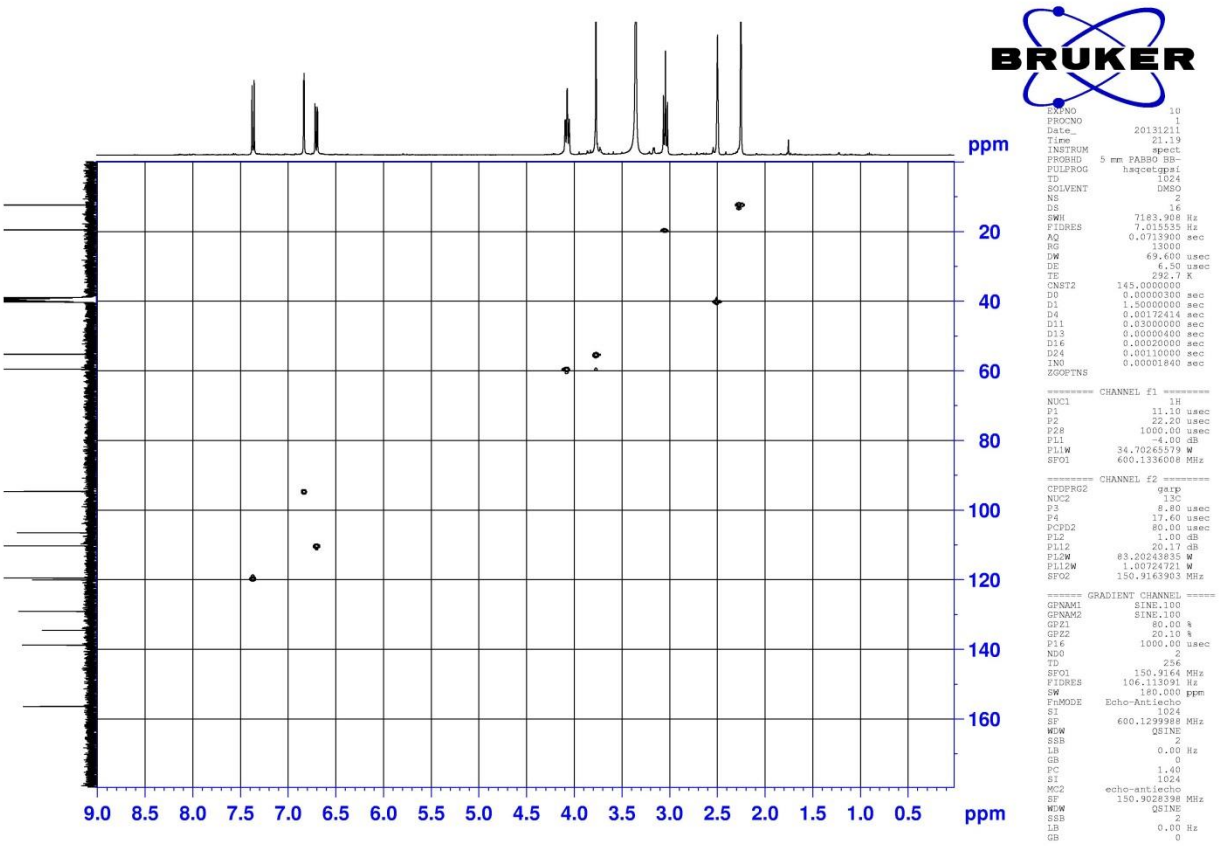


Figure S48 The HMBC spectrum of pegaharmine I (**8**) in DMSO-d_6 (600 MHz)

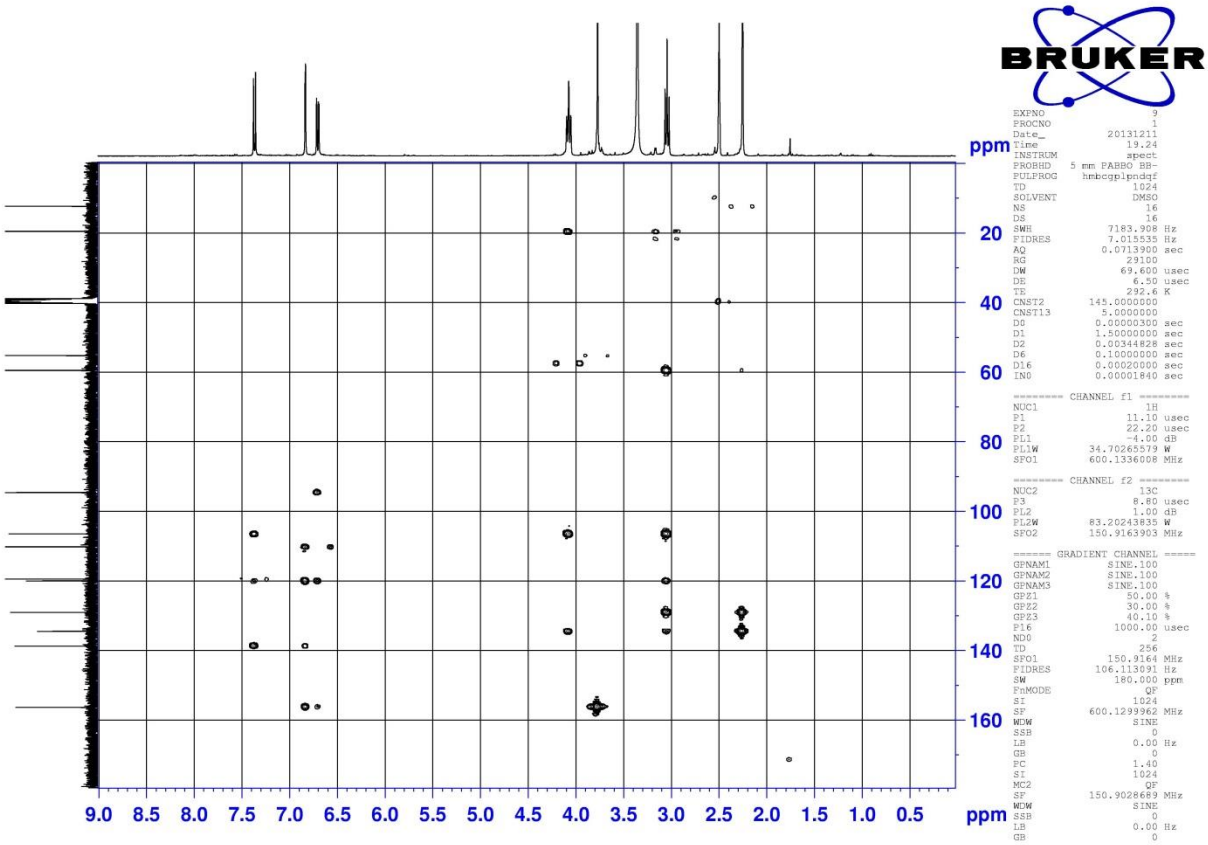


Figure S49 The HRESIMS spectrum of pegaharmine I (**8**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

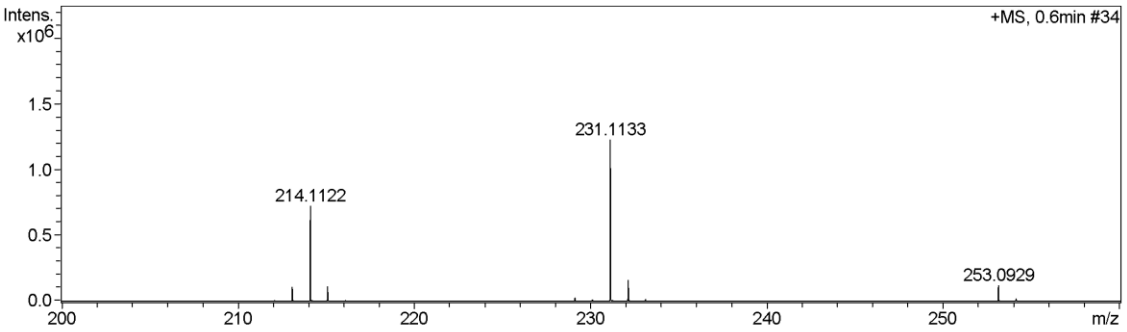
Analysis Name	D:\Data\20131218-CEYANG\WKB-43A_1-b,2_01_2475.d	Acquisition Date	12/18/2013 2:10:20 PM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	WKB-43A	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C13H14N2O2H						
Formula, max.							
Measured m/z	231.113	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	yes	Electron Configuration	both				
Filter H/C Ratio	yes	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 13 H 15 N 2 O 2	0.014	231.1128	-2.19	-1.23	-0.51	7.50	ok	even

Figure S50 The ^{1}H NMR spectrum of pegaharmine J (**9**) in DMSO-d_6 (400 MHz)

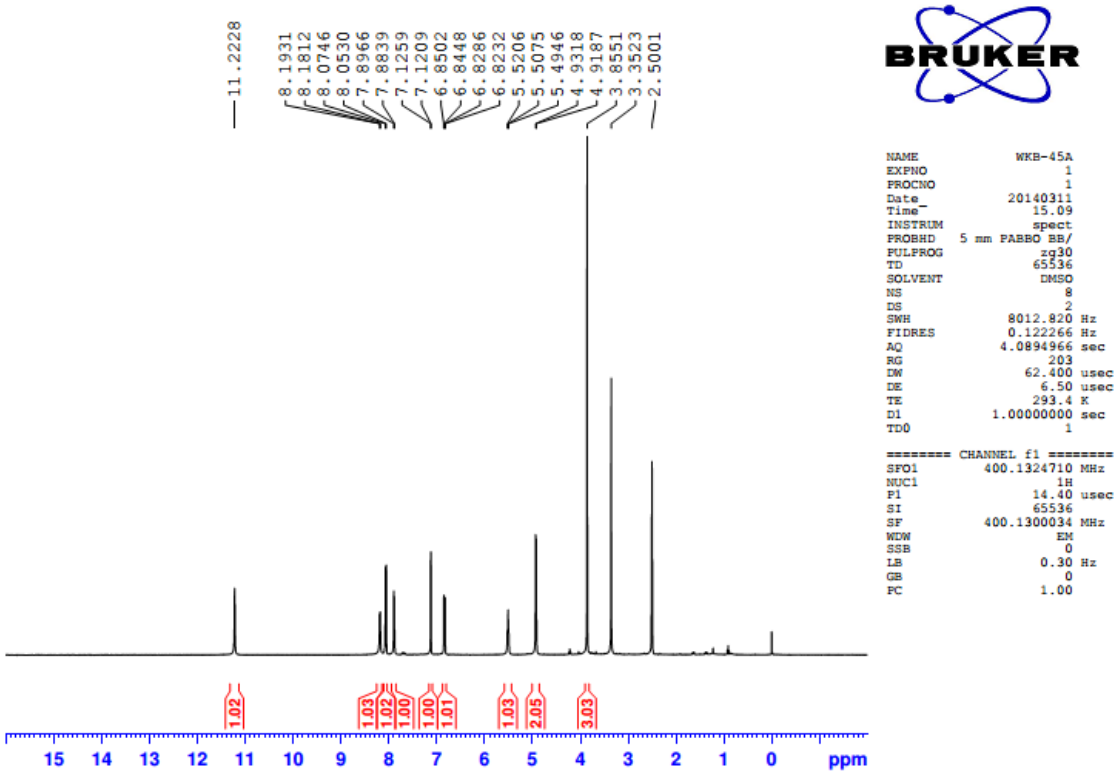


Figure S51 The ^{13}C NMR spectrum of pegaharmine J (**9**) in DMSO-d_6 (100 MHz)

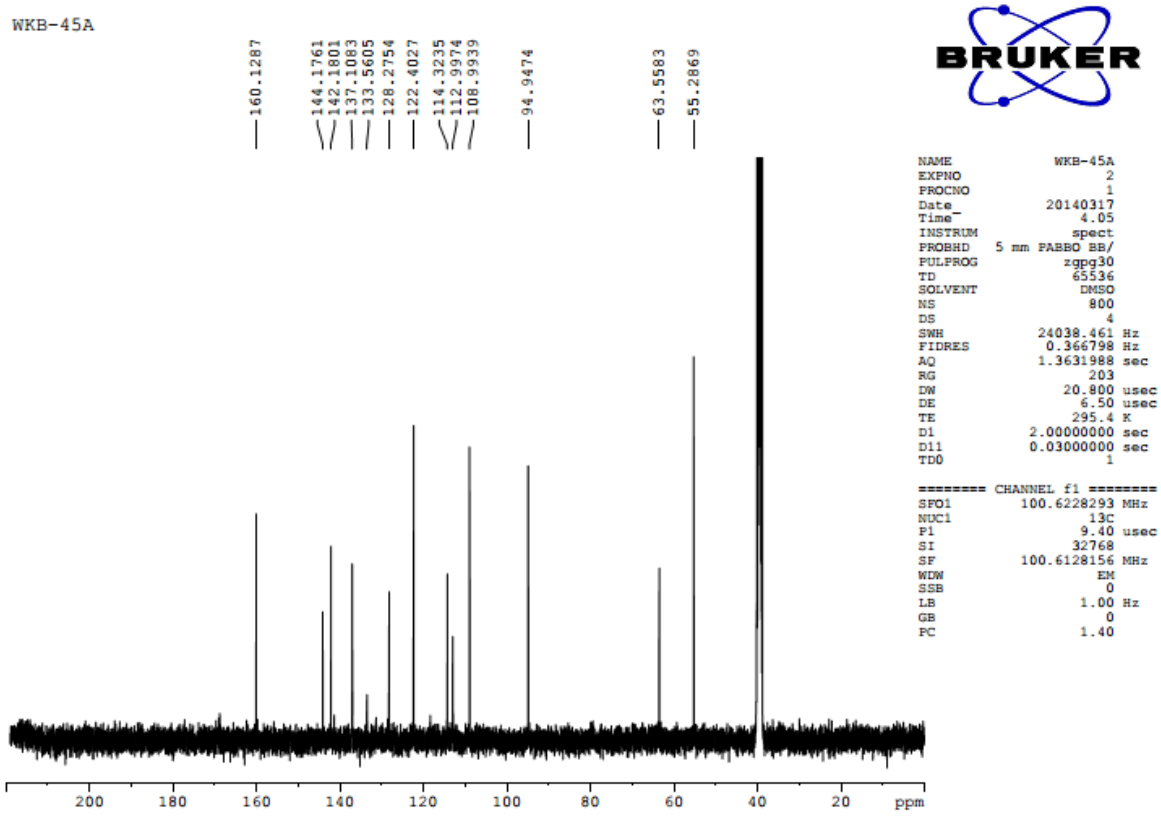


Figure S52 The HSQC spectrum of pegaharmine J (**9**) in DMSO-d_6 (600 MHz)

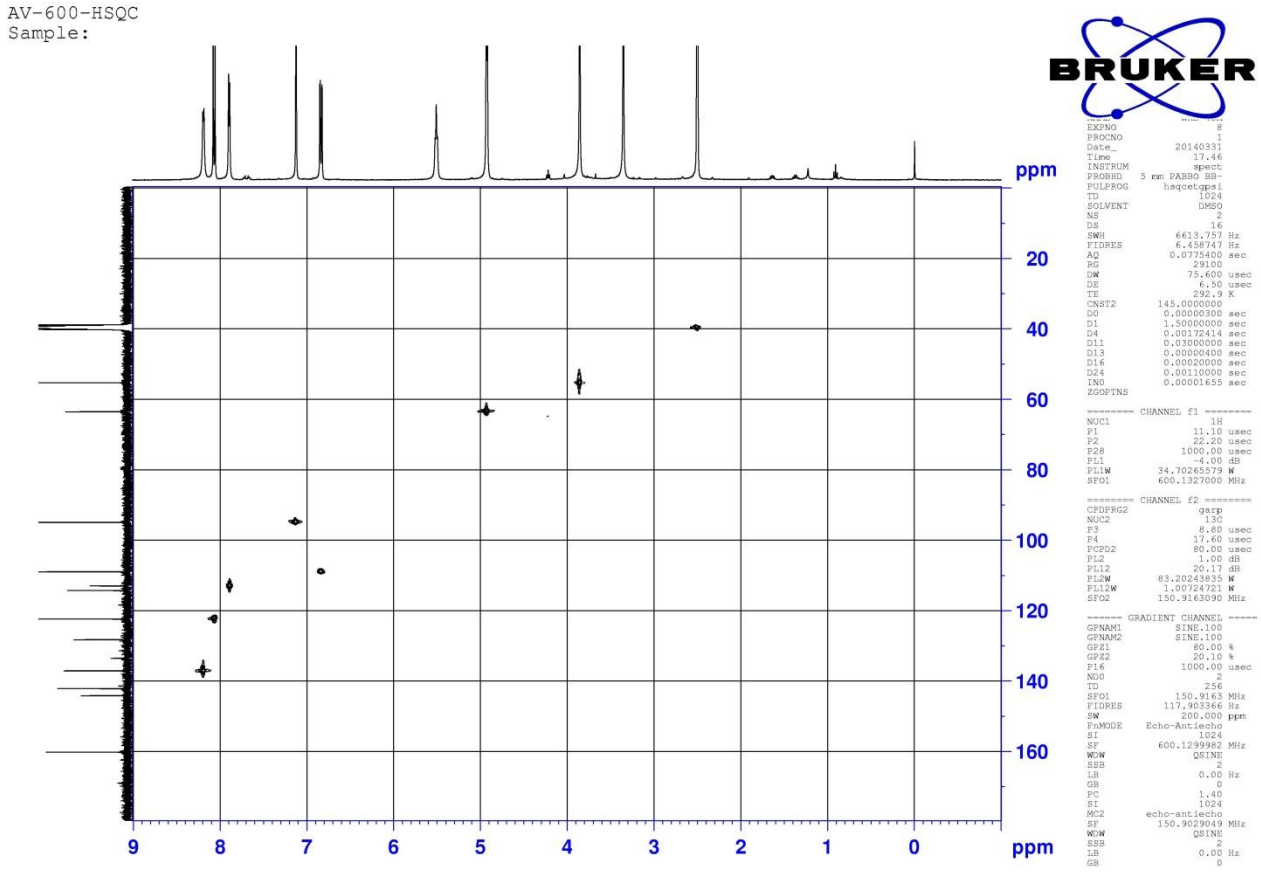


Figure S53 The HMBC spectrum of pegaharmine J (**9**) in DMSO-d_6 (600 MHz)

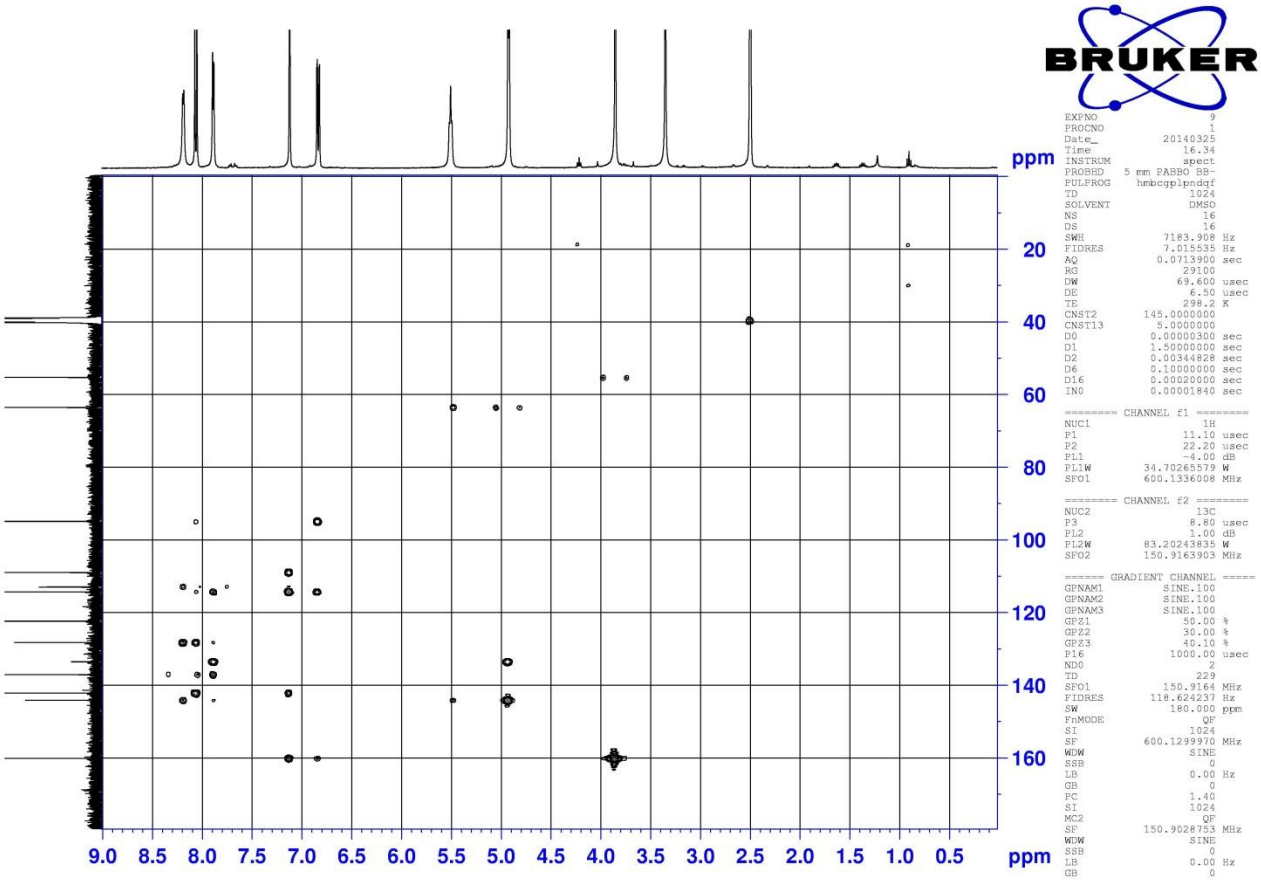


Figure S54 The HRESIMS spectrum of pegaharmine J (**9**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

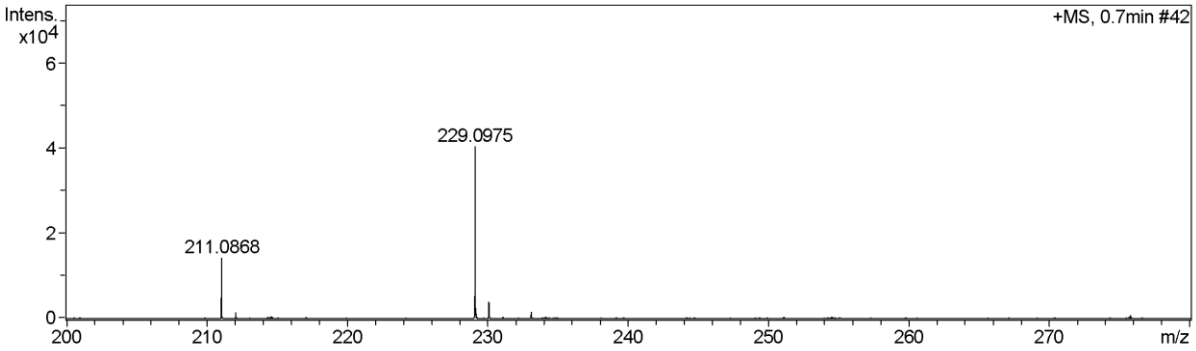
Analysis Name	D:\Data\20140327CEYANG\WKB-45A_2-a,6_01_3010.d	Acquisition Date	3/27/2014 6:24:31 PM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	WKB-45A	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C13H12N2O2H						
Formula, max.							
Measured m/z	229.098	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 13 H 13 N 2 O 2	0.032	229.0972	-1.53	-2.32	-0.35	8.50	ok	even

Figure S55 The ^{1}H NMR spectrum of pegaharmine K (**10**) in DMSO-d_6 (600 MHz)

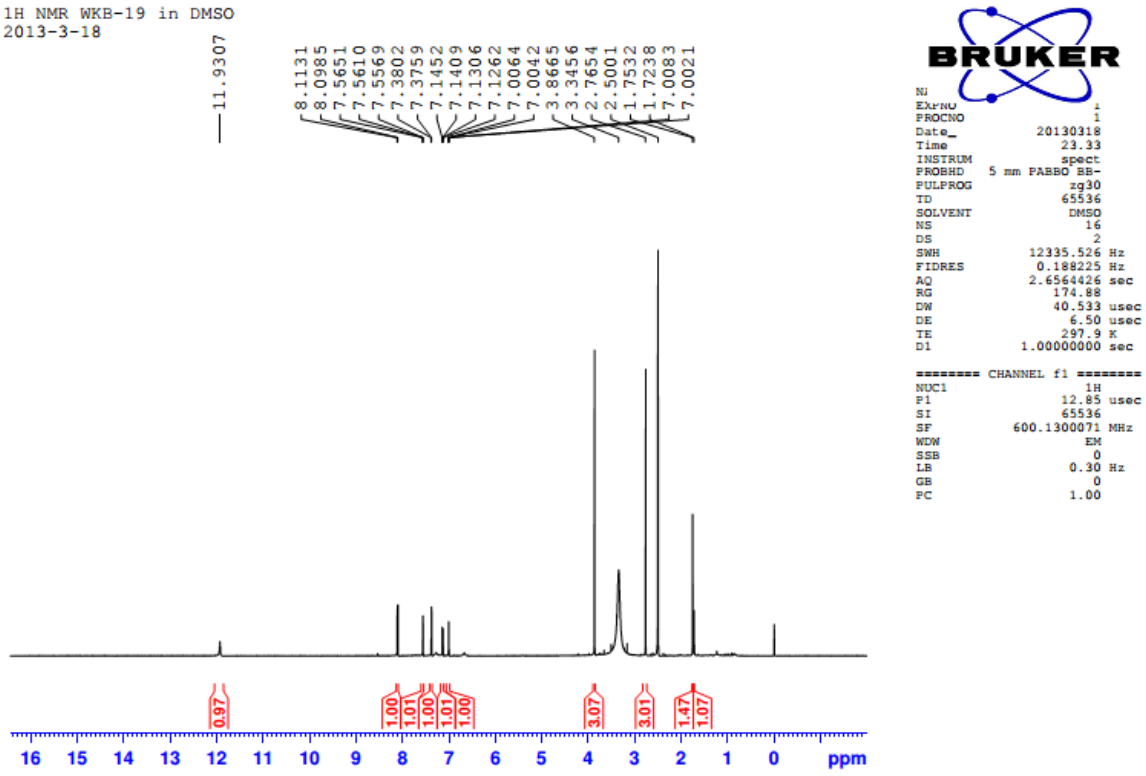


Figure S56 The ^{13}C NMR spectrum of pegaharmine K (**10**) in DMSO-d_6 (150 MHz)

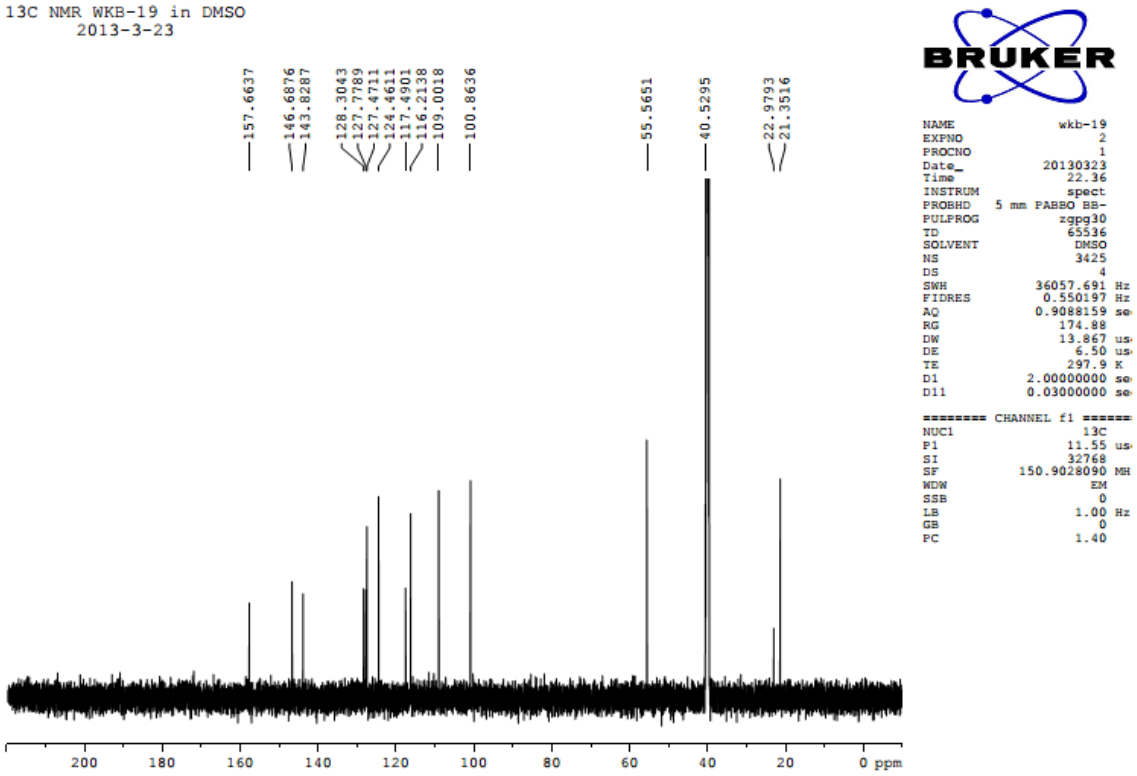


Figure S57 The ^{1}H-^{1}H COSY spectrum of pegaharmine K (**10**) in DMSO-d_6 (600 MHz)

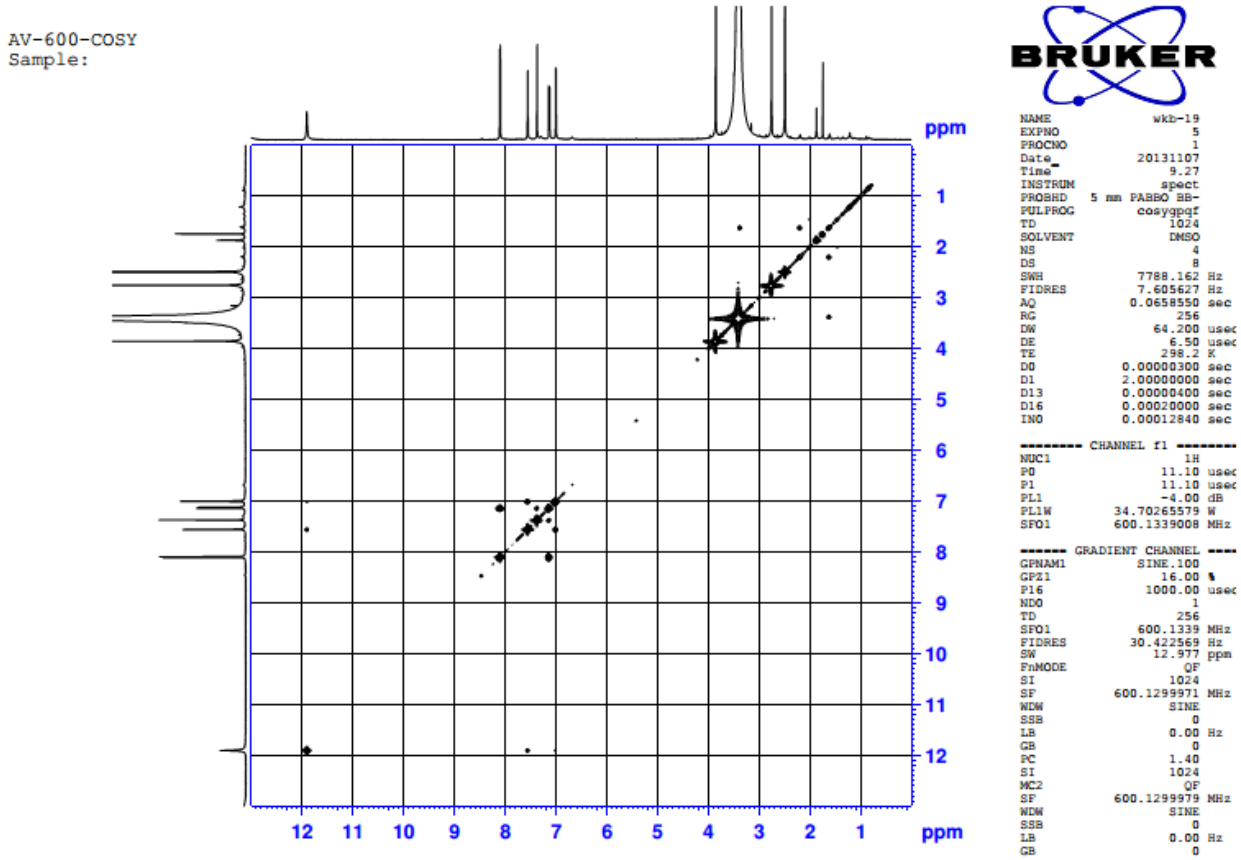


Figure S58 The HMBC spectrum of pegaharmine K (**10**) in DMSO-d_6 (600 MHz)

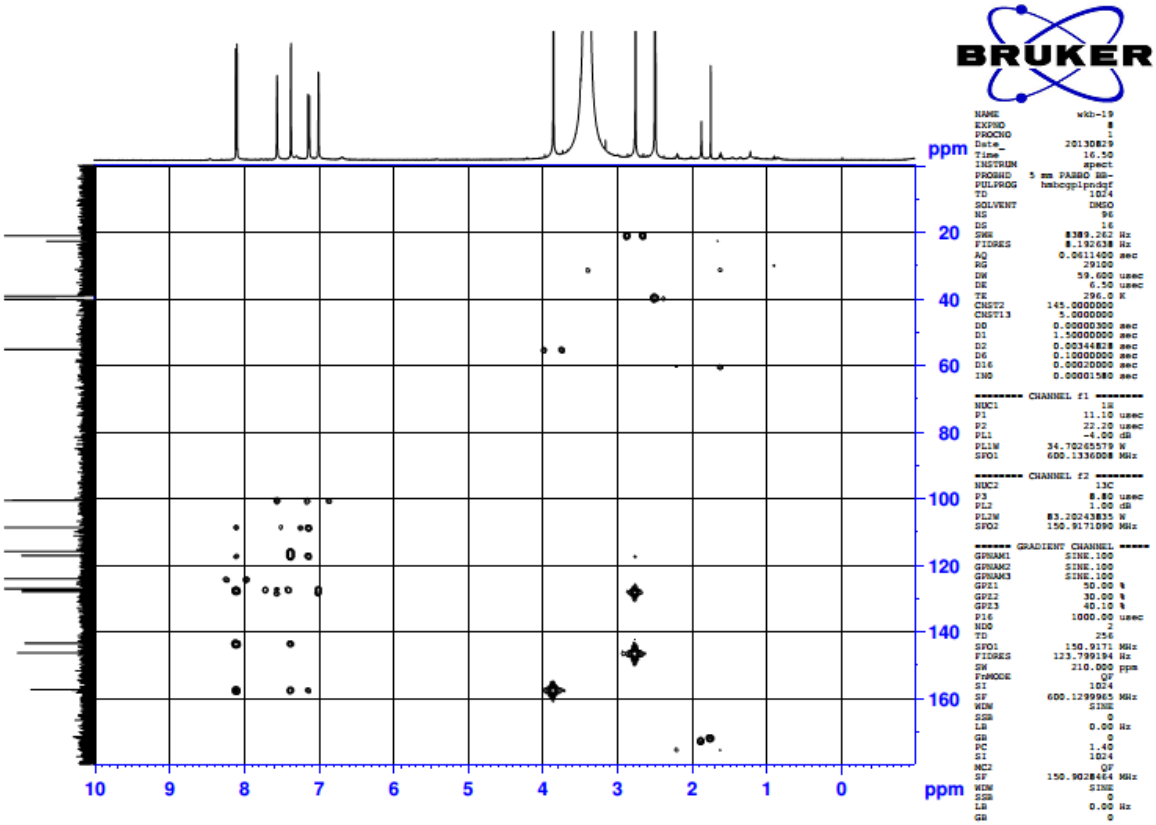


Figure S59 The NOESY spectrum of pegaharmine K (**10**) in DMSO-d_6 (600 MHz)

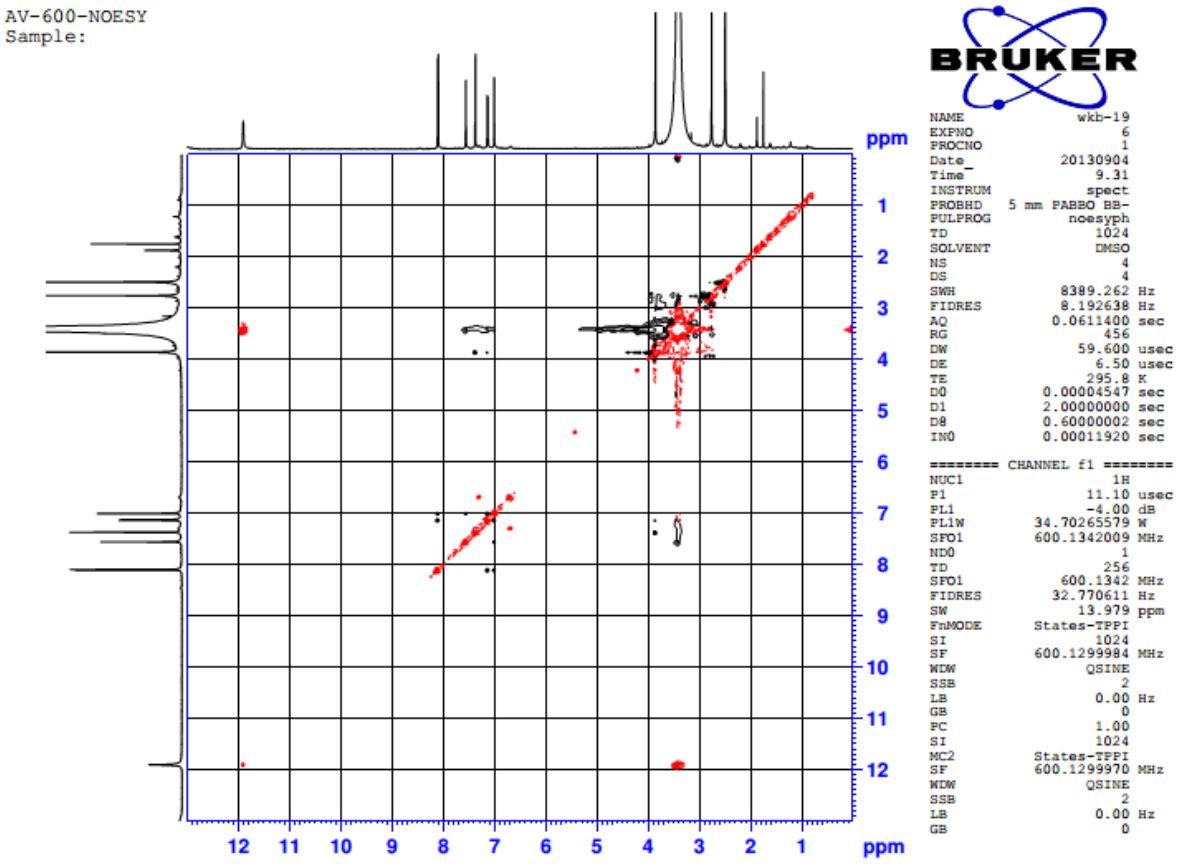


Figure S60 The HRESIMS spectrum of pegaharmine K (**10**) in MeOH

Mass Spectrum Molecular Formula Report

Analysis Info

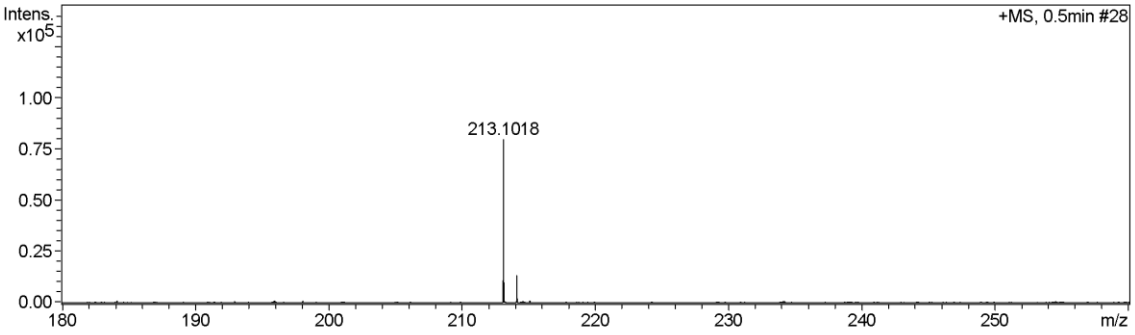
Analysis Name	D:\Data\20131031-CEYANG\WKB-19_1-a,1_01_1959.d	Acquisition Date	10/31/2013 1:52:49 PM
Method	ldj_bga_jh.m	Operator	Bruker Customer
Sample Name	WKB-19	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C13H13N2O1				
Formula, max.					
Measured m/z	213.102	Tolerance	10 mDa	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 13 H 13 N 2 O 1	0.011	213.1022	1.95	4.76	0.42	8.50	ok	even