Supporting Information

***Rec. Nat. Prod*. 15:5 (2021) 363-367**

A New Cyclic Tetrapeptide from Endophytic Fungus *Aspergillus versicolor* E-2

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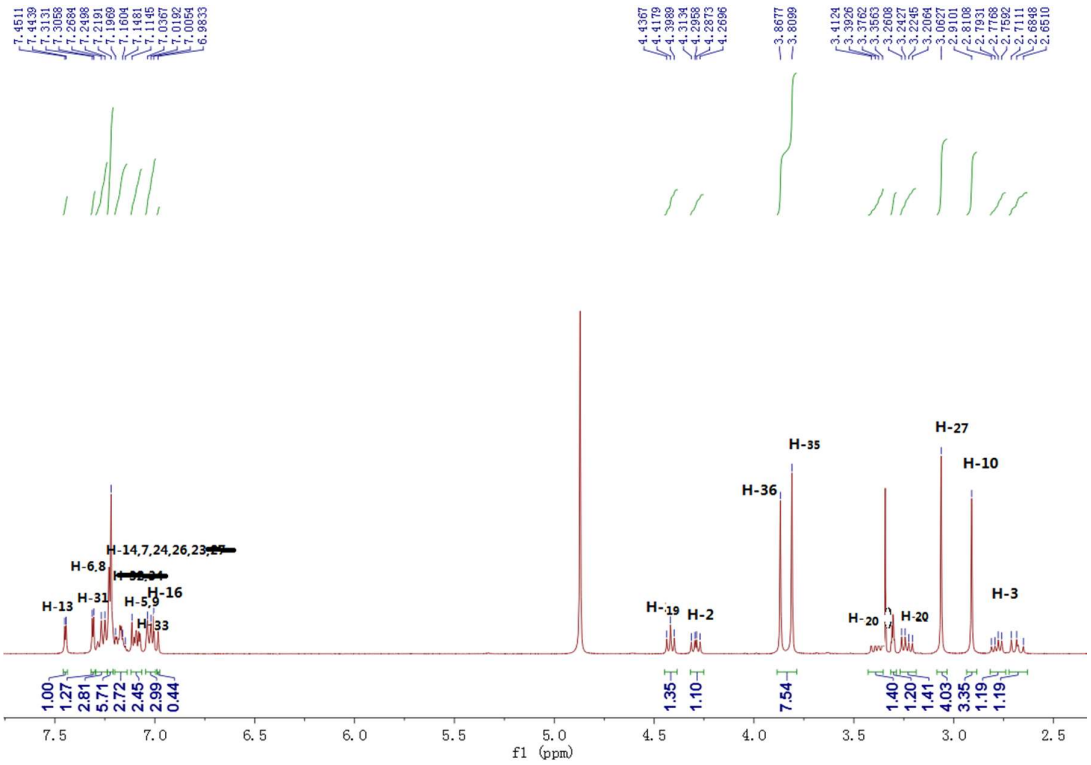


Figure S1: ^{1}H NMR spectrum of aspergilpeptide A (**1**) in CD_3OD

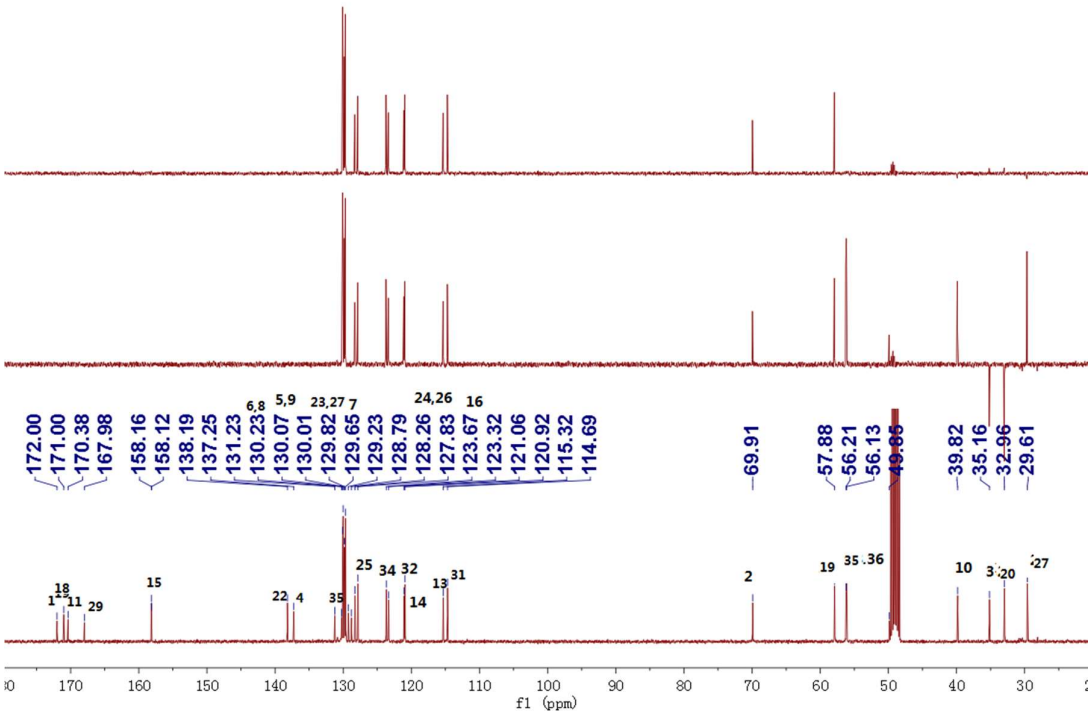


Figure S2: ^{13}C NMR spectrum of aspergilpeptide A (**1**) in CD_3OD

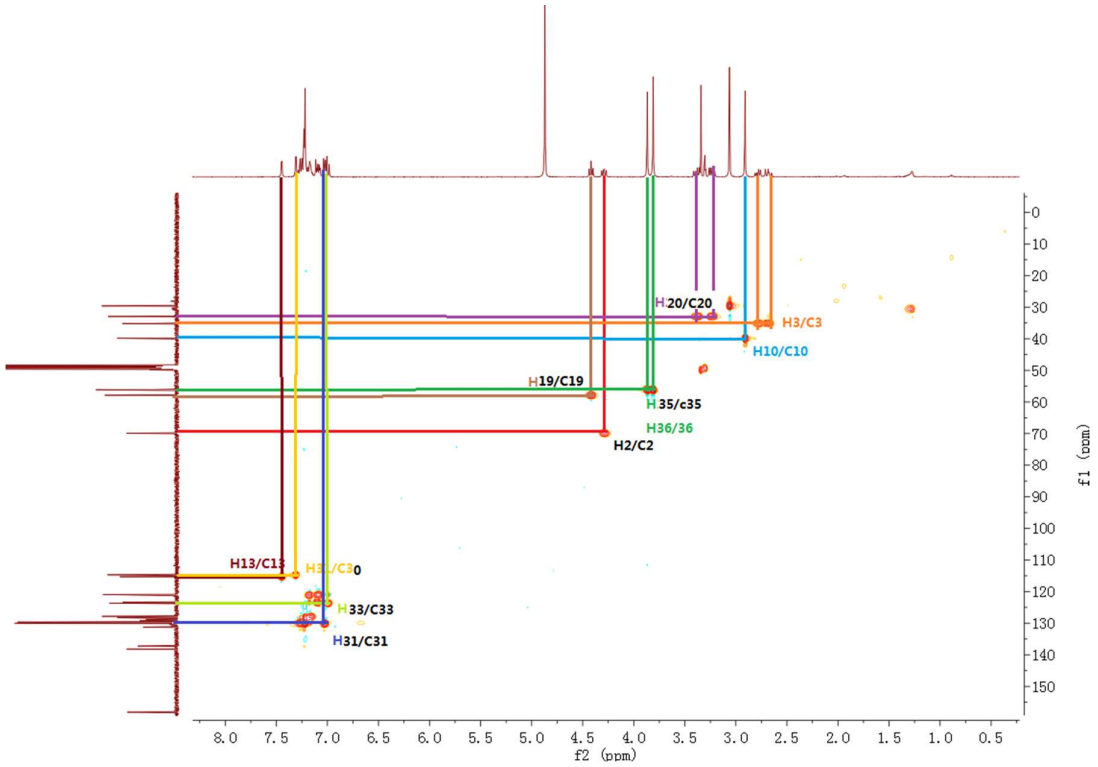


Figure S3: HSQC spectrum of aspergilpeptide A (**1**) in CD_3OD

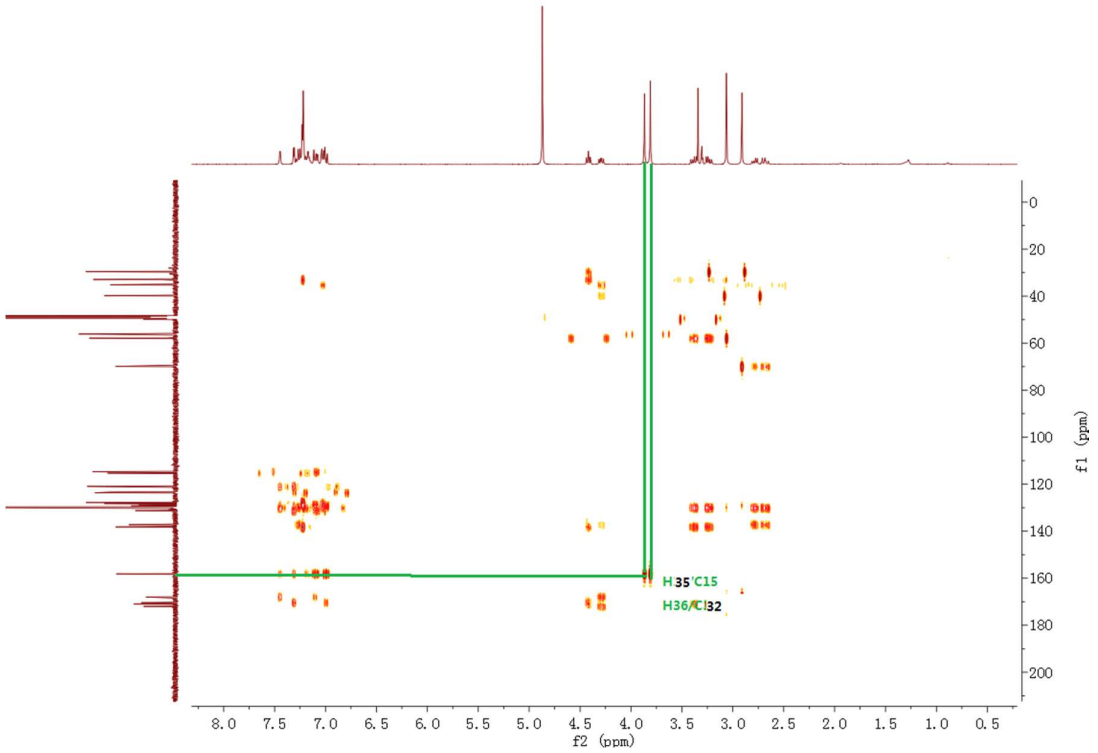


Figure S4: HMBC spectrum of aspergilpeptide A (**1**) in CD_3OD

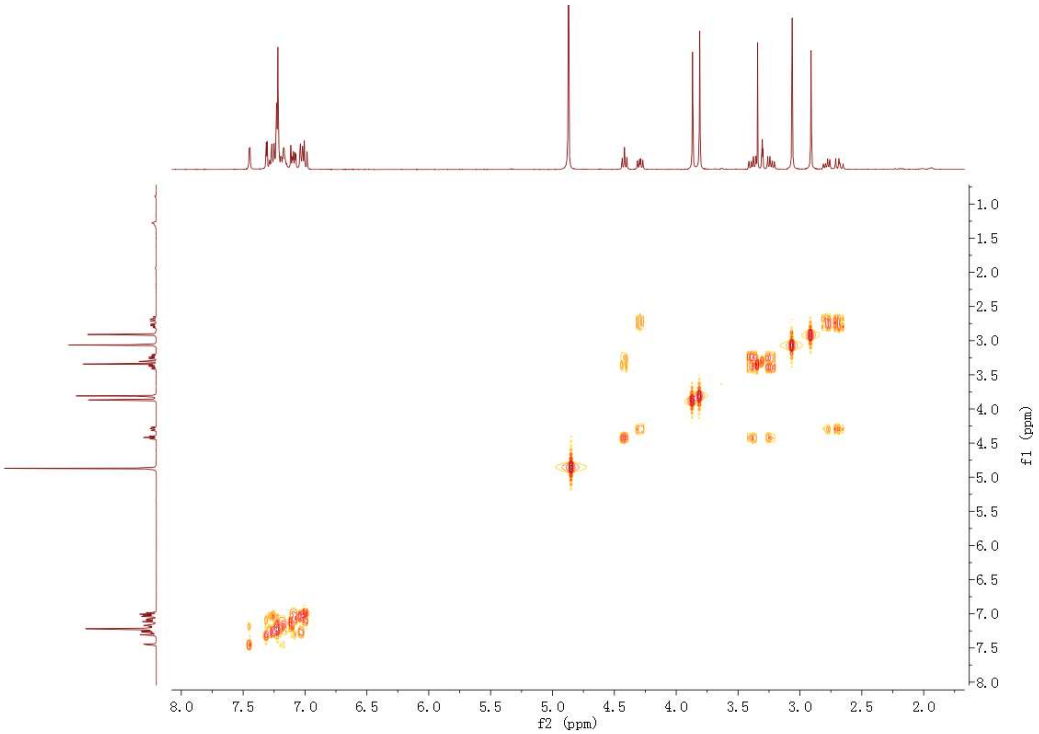
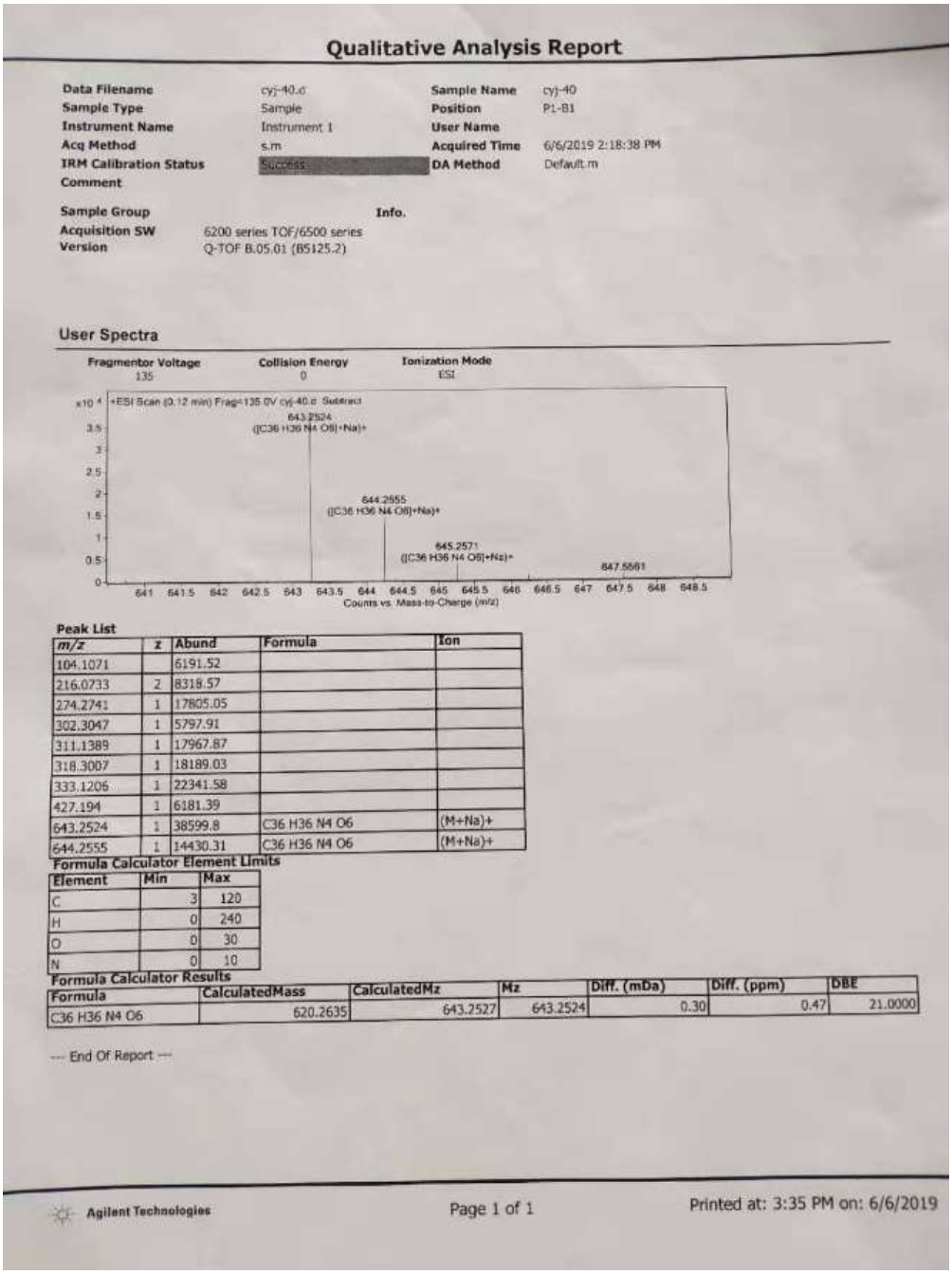


Figure S5: ^{1}H-^{1}H COSY spectrum of aspergilpeptide A (**1**) in CD_3OD



Qualitative Analysis Report

Data Filename	cyj-40.d	**Sample Name**	cyj-40
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	s.m	**Acquired Time**	6/6/2019 2:18:38 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

Peak List

m/z	z	Abund	Formula	Ion
104.1071		6191.52		
216.0733	2	8318.57		
274.2741	1	17805.05		
302.3047	1	5797.91		
311.1389	1	17967.87		
318.3007	1	18189.03		
333.1206	1	22341.58		
427.194	1	6181.39		
643.2524	1	38599.8	C36 H36 N4 O6	(M+Na)+
644.2555	1	14430.31	C36 H36 N4 O6	(M+Na)+

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30
N	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C36 H36 N4 O6	620.2635	643.2527	643.2524	0.30	0.47	21.0000

--- End Of Report ---

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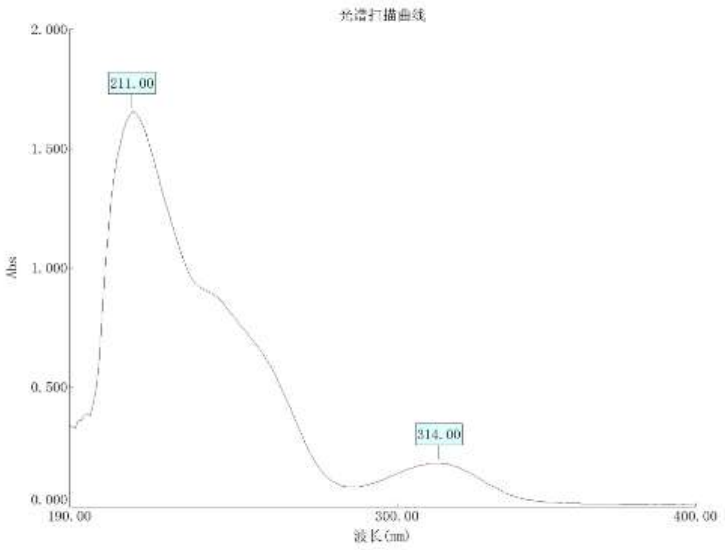
Figure S6: HRESIMS spectrum of aspergilpeptide A (**1**)



●仪器性能
仪器型号 ： TU-1901
序号 ： 18-1901-01-0476
光谱带宽 ： 2.00 nm
●光谱扫描参数设置
扫描范围 ： 190.00 至 400.00 nm
光度模式 ： Abs
扫描间隔 ： 1.00 nm
扫描速度 ： 快
数据文件 ： D:\紫外分光光度计\UVWinb紫外软件\Data\30.spc
创建时间 ： 2019年6月5日 18:47:11
数据类型 ： 原始数据
参数文件 ：

●序号	峰/谷	波长(nm)	Abs	注释
1	峰	314.00	0.183	
2	峰	211.00	1.655	

Figure S7: The UV spectrum of aspergilpeptide A (**1**)

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Sunday, 09-JUN-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-62.01	0.16	-0.25	-61.83	-62.24

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	cyj-40	11:13:07 AM	-61.90	SR	-0.2600	589	100.00	0.420	27.2
2	cyj-40	11:13:16 AM	-62.00	SR	-0.2604	589	100.00	0.420	27.2
3	cyj-40	11:13:23 AM	-61.83	SR	-0.2597	589	100.00	0.420	27.3
4	cyj-40	11:13:32 AM	-62.24	SR	-0.2614	589	100.00	0.420	27.3
5	cyj-40	11:13:40 AM	-62.07	SR	-0.2607	589	100.00	0.420	27.3

Figure S8: The optical rotation spectrum of aspergilpeptide A (**1**)

>qmj_ITS1_Y90709001_E11

TTTTTAATGGCGGGCTGCTCGGGCGCCAACCTCCCACCCGTGACTACCTAACACTGTTGCTTCGGCGGGGAGCCCTCTCGGGGGCGA

GCCGCCGGGGACTACTGAACTTCATGCCTGAGAGTGATGCAGTCTGAGTCTGAATATAAAATCAGTCAAAACTTTCAACAATGGATCT

CTTGGTTCCGGCATCGATGAAGAACGCAGCGAACTGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGC

ACATTGCGCCCCCTGGCATTCCGGGGGGGCATGCCTGTCCGAGCGTCATTGCTGCCCATCAAGCCCGGCTTGTGTGTTGGGTCGTCGTC

CCCCCCGGGGGACGGGCCCGAAAGGCAGCGGCGGCACCGTGTCCGGTCCTCGAGCGTATGGGGCTTTGTCACCCGCTCGATTTAGGG

CCGGCCGGGCGCCAGCCGACGTCCAACCATTTTTCTTCAGGTTGACCTCGGATCAGGTAGGGATACCCGCTGAACTTAAGCATATCAA

TAAGCGGAGGA>qmj_ITS4_Y90709002_E12 (Reverse + Complement)

Aspergillus versicolor strain MF22122 small subunit ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and large subunit ribosomal RNA gene, partial sequence

Sequence ID: **MH911364.1** Length: 570 Number of Matches: 1

Range 1: 1 to 569

Score	Expect	Identities	Gaps	Strand	Frame
1051 bits(569)	0.0()	569/569(100%)	0/569(0%)	Plus/Plus	

Features:

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Query  1    CTTCCGTAGGTGAACCTGCGGAAGGATCATTACTGAGTGCGGGCTGCCTCCGGGCGCCCA  60
Sbjct  1    CTTCCGTAGGTGAACCTGCGGAAGGATCATTACTGAGTGCGGGCTGCCTCCGGGCGCCCA  60
Query  61   ACCTCCCACCCGTGACTACCTAACACTGTTGCTTCGGCGGGGAGCCCTCTCGGGGGCGAG  120
Sbjct  61   ACCTCCCACCCGTGACTACCTAACACTGTTGCTTCGGCGGGGAGCCCTCTCGGGGGCGAG  120
Query  121  CCGCCGGGGACTACTGAACTTCATGCCTGAGAGTGATGCAGTCTGAGTCTGAATATAAAA  180
Sbjct  121  CCGCCGGGGACTACTGAACTTCATGCCTGAGAGTGATGCAGTCTGAGTCTGAATATAAAA  180
Query  181  TCAGTCAAAACTTTCAACAATGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAA  240
Sbjct  181  TCAGTCAAAACTTTCAACAATGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAA  240
Query  241  CTGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCACATT  300
Sbjct  241  CTGCGATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCACATT  300
Query  301  GCGCCCCCTGGCATTCCGGGGGGGCATGCCTGTCCGAGCGTCATTGCTGCCCATCAAGCCC  360
Sbjct  301  GCGCCCCCTGGCATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTGCCCATCAAGCCC  360
Query  361  GGCTTGTGTGTTGGGTCGTCGTccccccGGGGGACGGGCCCGAAAGGCAGCGGCGGCAC  420
Sbjct  361  GGCTTGTGTGTTGGGTCGTCGTCCCCCCCGGGGGACGGGCCCGAAAGGCAGCGGCGGCAC  420
Query  421  CGTGTCCGGTCCTCGAGCGTATGGGGCTTTGTCACCCGCTCGATTTAGGGCCGGCCGGGC  480
Sbjct  421  CGTGTCCGGTCCTCGAGCGTATGGGGCTTTGTCACCCGCTCGATTTAGGGCCGGCCGGGC  480
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Query  541  TGAACTTAAGCATATCAATAAGCGGAGGA  569
Sbjct  541  TGAACTTAAGCATATCAATAAGCGGAGGA  569
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GTTGCTTCGGCGGGGAGCCCTCTCGGGGGCGAGCCGCCGGGGACTACTGAACTTCATGCCTGAGAGTGATGCAGTCTGAGTCTGAAT

ATAAAATCAGTCAAAACTTTCAACAATGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAACTGCGATAAGTAATGTGAATTG

CAGAATTCAGTGAATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGCATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTGCC

CATCAAGCCCGGCTTGTGTGTTGGGTCGTCGTCCCCCCCGGGGGACGGGCCCGAAAGGCAGCGGCGGCACCGTGTCCGGTCCTCGA

GCGTATGGGGCTTTGTCACCCGCTCGATTTAGGGCCGGCCGGGCGCCAGCCGACGTCCAACCATTTTCTTCAGGTTGACCTCGGAGCA

GGTAGGT 拼接结果：

>qmjCTTCCGTAGGTGAACCTGCGGAAGGATCATTACTGAGTGCGGGCTGCCTCCGGGCGCCCAACCTCCCACCCGTGACTACCTAAC

ACTGTTGCTTCGGCGGGGAGCCCTCTCGGGGGCGAGCCGCCGGGGACTACTGAACTTCATGCCTGAGAGTGATGCAGTCTGAGTCTG

AATATAAAATCAGTCAAAACTTTCAACAATGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAACTGCGATAAGTAATGTGAA

TTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGCATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCT

GCCCATCAAGCCCGGCTTGTGTGTTGGGTCGTCGTCCCCCCCGGGGGACGGGCCCGAAAGGCAGCGGCGGCACCGTGTCCGGTCCT

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ATCAGGTAGGGATACCCGCTGAACTTAAGCATATCAATAAGCGGAGGA

Figure S9: The BLAST results of the endophytic fungus *A. versicolor* E-2

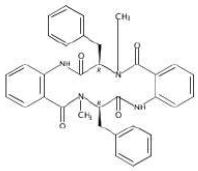
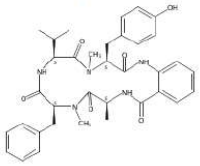
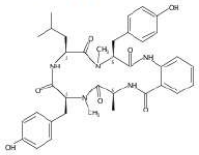
Score: 92 1. **2211978-03-7**  Absolute stereochemistry. $C_{34}H_{32}N_4O_4$ INDEX NAME NOT YET ASSIGNED **Key Physical Properties:** **Molecular Weight** 560.64 **Boiling Point (Predicted)** Value: 832.3±65.0 °C | Condition: Press: 760 Torr **Density (Predicted)** Value: 1.206±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr **pKa (Predicted)** Value: 12.73±0.60 | Condition: Most Acidic Temp: 25 °C **Related Info:** ~ 1 References	*Score: 85* 2. **691363-62-9**  Absolute stereochemistry. $C_{35}H_{41}N_5O_6$ Cyclo(L-alanyl-*N*-methyl-L-phenylalanyl-L-valyl-*N*-methyl-L-tyrosyl-2-aminobenzoyl) **Protein Sequence** Sequence Length: 5 **Key Physical Properties:** **Molecular Weight** 627.73 **Melting Point (Experimental)** Value: 186-189 °C **Boiling Point (Predicted)** Value: 968.7±65.0 °C | Condition: Press: 760 Torr **Density (Predicted)** Value: 1.176±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr **pKa (Predicted)** Value: 9.89±0.15 | Condition: Most Acidic Temp: 25 °C **Related Info:** ~ 3 References ~ 6 Commercial Sources Spectra Experimental Properties	*Score: 85* 3. **1174132-24-1**  Rotation (-)., Absolute stereochemistry. $C_{36}H_{43}N_5O_7$ Cyclo(L-alanyl-*N*-methyl-L-tyrosyl-L-leucyl-*N*-methyl-L-tyrosyl-2-aminobenzoyl) **Protein Sequence** Sequence Length: 5 **Key Physical Properties:** **Molecular Weight** 657.76 **Boiling Point (Predicted)** Value: 1012.6±65.0 °C | Condition: Press: 760 Torr **Density (Predicted)** Value: 1.194±0.06 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr **pKa (Predicted)** Value: 9.89±0.15 | Condition: Most Acidic Temp: 25 °C **Related Info:** ~ 2 References

Figure S10: The Scifinder similarity search for the compound **1**