

Diversified Chaetoglobosins from the marine-derived fungus *Emericellopsis* sp. SCSIO41202

Surun Shao², Xueni Wang¹, Jianglian She¹, Han Zhang², Xiaoyan Pang¹, Xiuping
Lin^{1,3}, Xuefeng Zhou^{1,3}, Yonghong Liu^{1,3*}, Yunqiu Li^{2*} and Bin Yang^{1,3*}

¹ CAS Key Laboratory of Tropical Marine Bio-resources and Ecology/Guangdong Key Laboratory of Marine Materia Medica/Innovation Academy of South China Sea Ecology and Environmental Engineering, South China Sea Institute of Oceanology, Chinese Academy of Sciences, Guangzhou 510301, P. R. China; wangxueni@scsio.ac.cn (X.-N.W.); shejianglian20@mails.ucas.ac.cn (J.L. S.); xypang@scsio.ac.cn (X.-Y.P.); xiupinglin@scsio.ac.cn (X.-P.L.); xfzhou@scsio.ac.cn (X.-F.Z.)

² Pharmacy School of Guilin Medical University, Guilin 541004, P. R. China; shaosurun@163.com (S.-R.S.); zhanghanmarc@163.com (H. Z.)

³ Southern Marine Science and Engineering Guangdong Laboratory (Guangzhou), Guangzhou 511458, China

* Correspondence: yangbin@scsio.ac.cn (B.Y.); Tel.: +86-20-89023174; leeyq88@126.com (Y.-Q. L.); yonghongliu@scsio.ac.cn (Y.-H.L.)

Contents of Supporting Information

| | |
|---|----|
| Figure S1. ^1H NMR of compound 1 (in CD_3OD) | 3 |
| Figure S2. ^{13}C NMR of compound 1 (in CD_3OD) | 3 |
| Figure S3. HSQC of compound 1 (in CD_3OD) | 4 |
| Figure S4. HMBC of compound 1 (in CD_3OD) | 4 |
| Figure S5. ^1H - ^1H COSY of compound 1 (in CD_3OD) | 5 |
| Figure S6. NOESY of compound 1 (in CD_3OD) | 5 |
| Figure S7. HRESIMS of compound 1 | 6 |
| Figure S8. UV of compound 1 | 7 |
| Figure S9. IR of compound 1 | 8 |
| Figure S10. ^1H NMR of compound 2 (in CD_3OD) | 8 |
| Figure S11. ^{13}C NMR of compound 2 (in CD_3OD) | 9 |
| Figure S12. HSQC of compound 2 (in CD_3OD) | 9 |
| Figure S13. HMBC of compound 2 (in CD_3OD) | 10 |
| Figure S14. NOESY of compound 2 (in CD_3OD) | 10 |
| Figure S15. HRESIMS of compound 2 | 11 |
| Figure S16. UV of compound 2 | 12 |
| Figure S17. IR of compound 2 | 13 |
| Figure S18. CD of compounds 1 and 2 | 13 |
| Figure S19. Molecular docking of chaetoglobosin Fex | 14 |
| Figure S20. Molecular docking of chaetoglobosin G | 14 |
| Figure S21. Molecular docking of chaetoglobosin Vb | 14 |

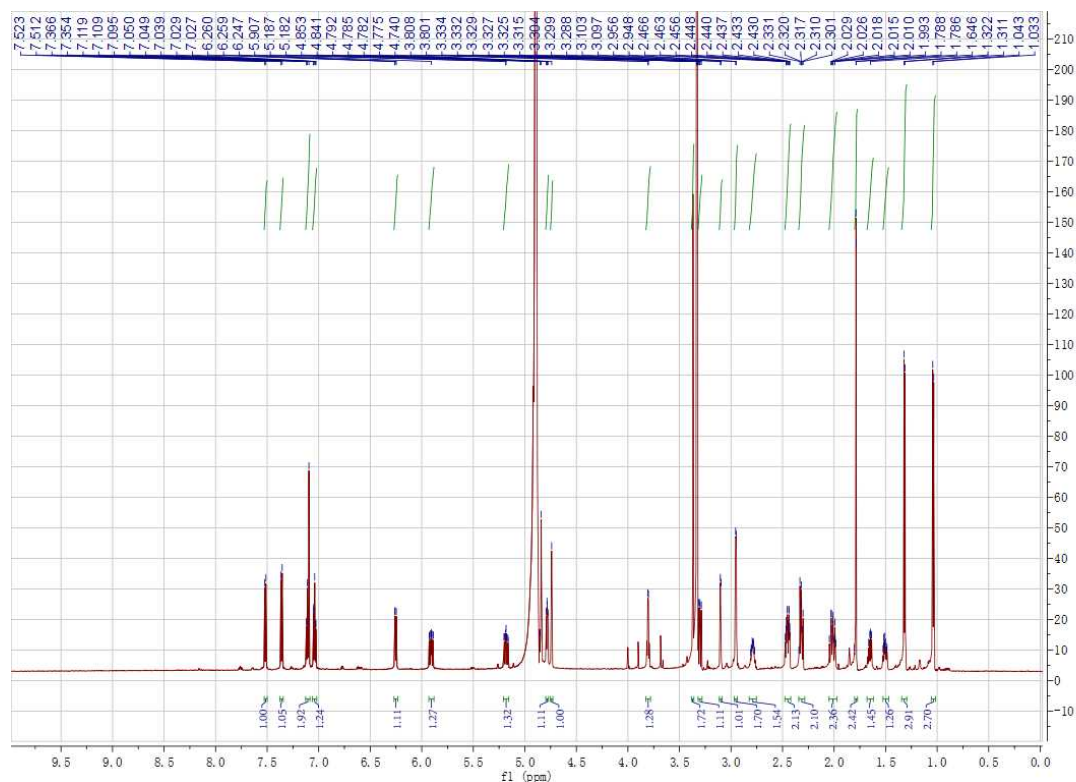


Figure S1. ¹H NMR of compound **1** (in CD₃OD)

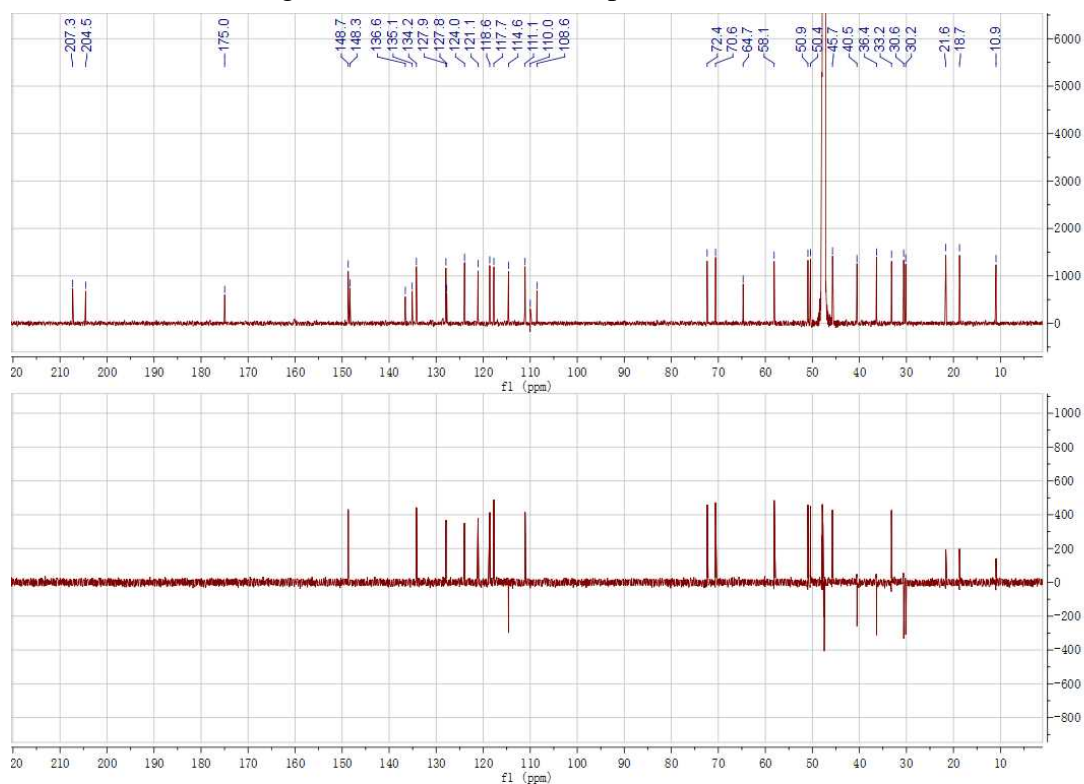


Figure S2. ¹³C NMR of compound **1** (in CD₃OD)

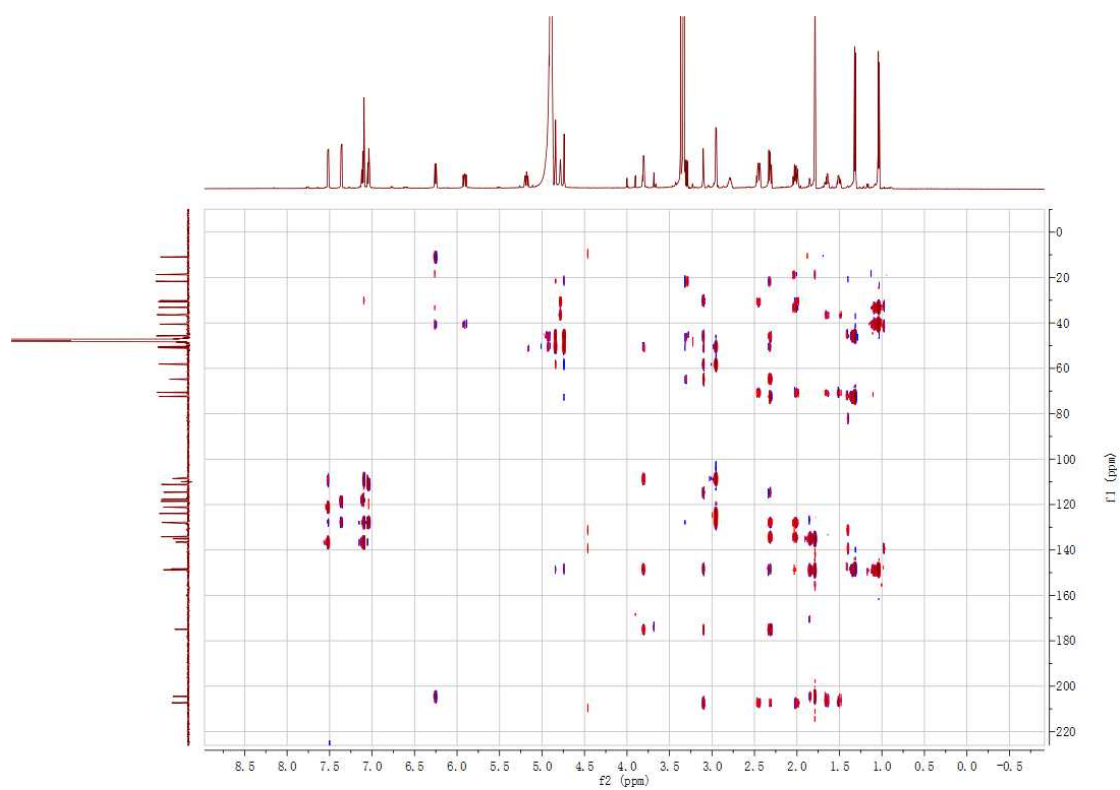


Figure S3. HSQC of compound **1** (in CD₃OD)

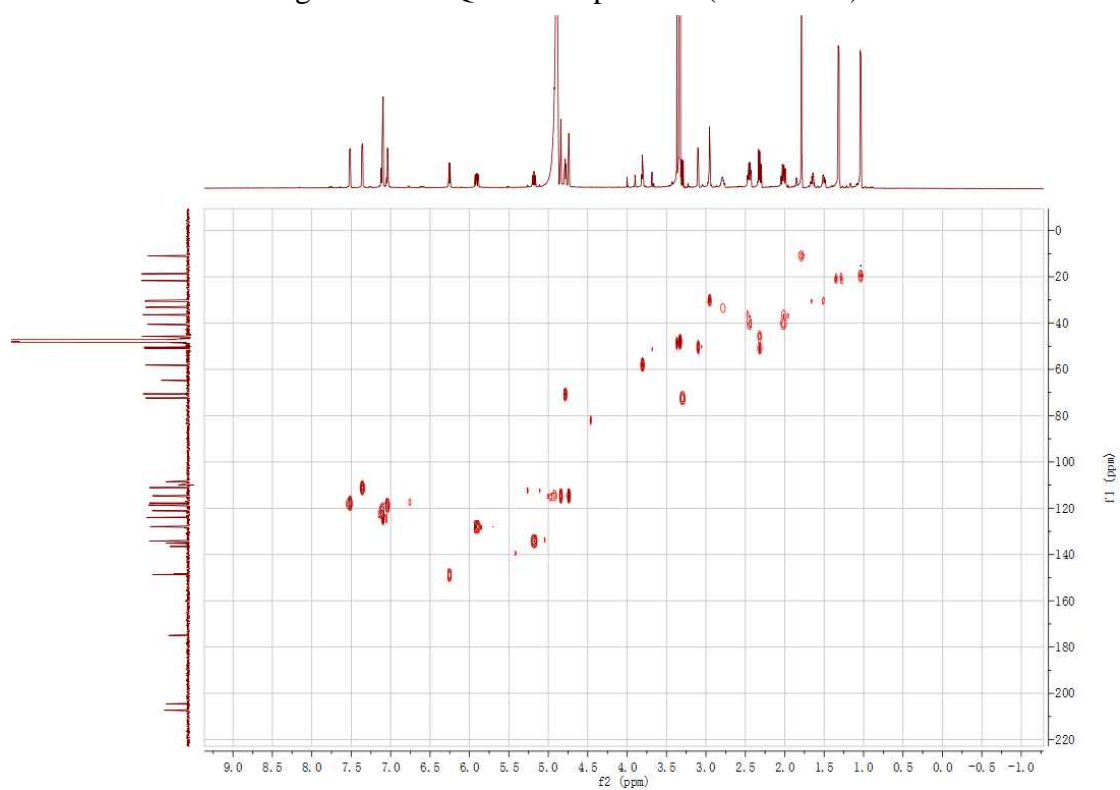


Figure S4. HMBC of compound **1** (in CD₃OD)

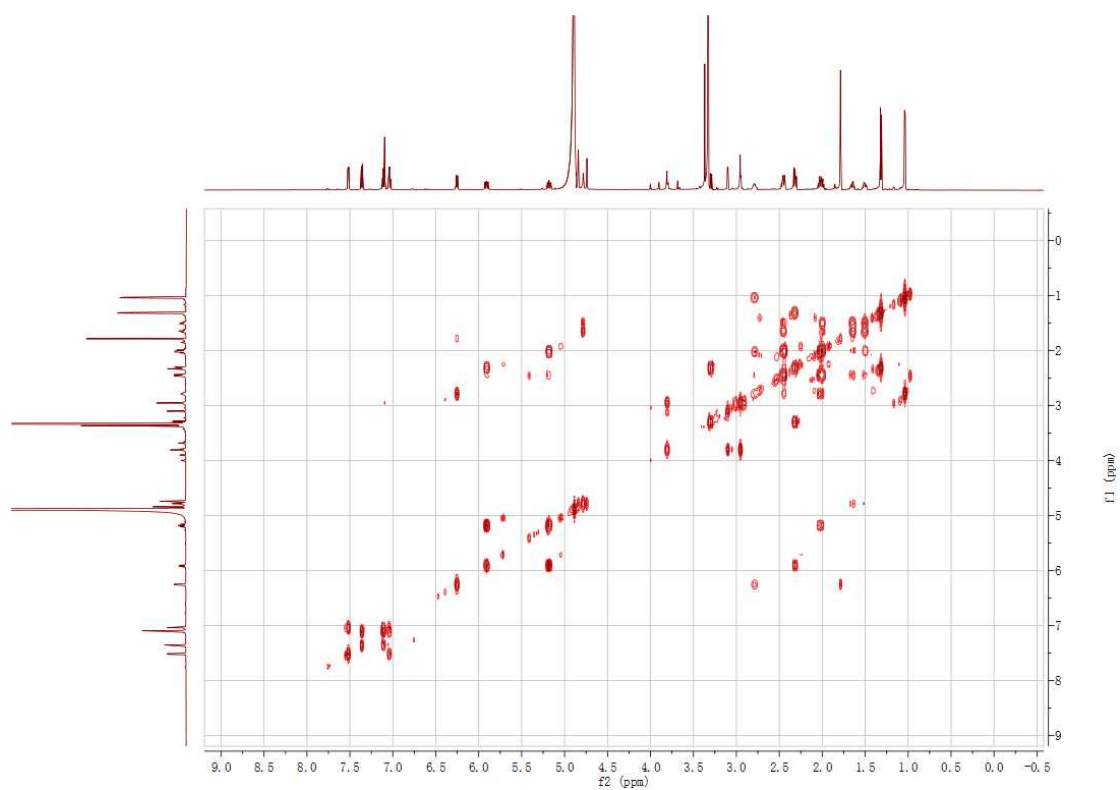


Figure S5. ^1H - ^1H COSY of compound **1** (in CD_3OD)

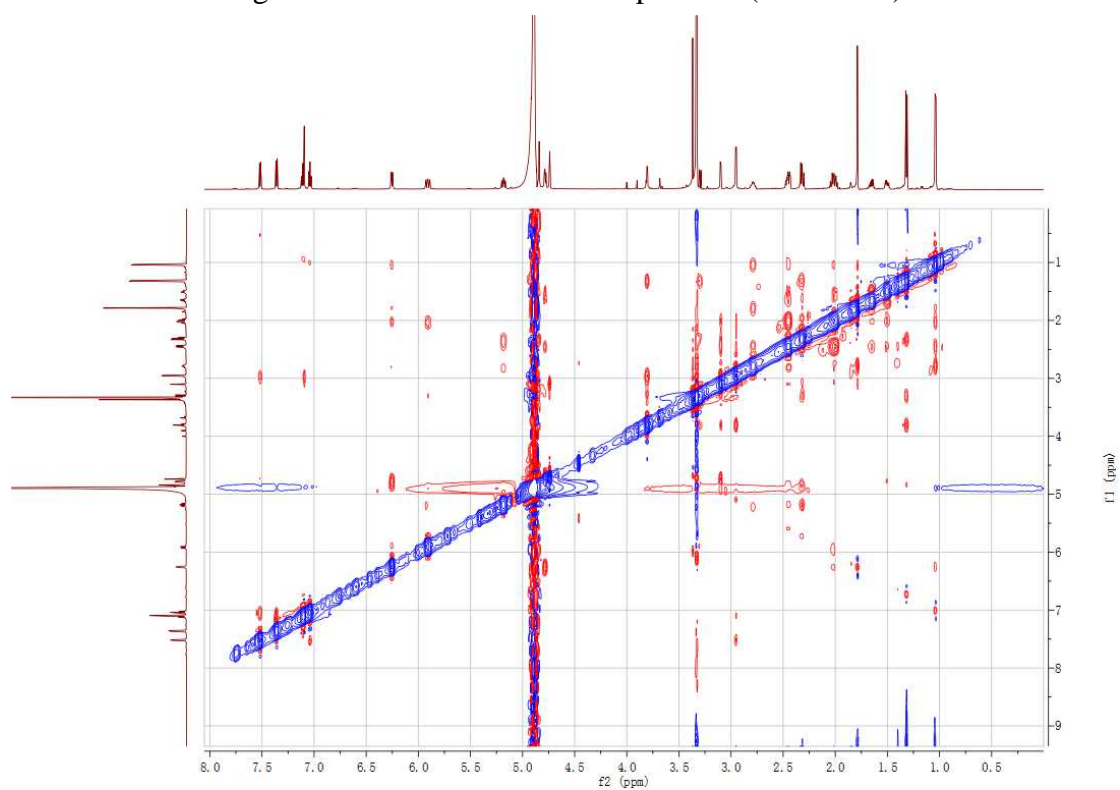


Figure S6. NOESY of compound **1** (in CD_3OD)

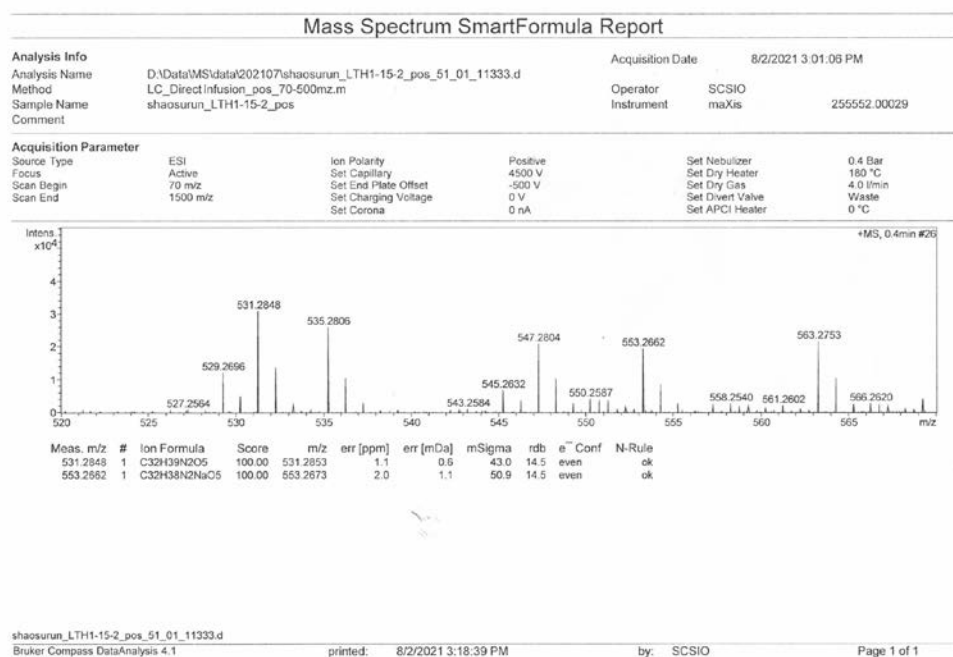
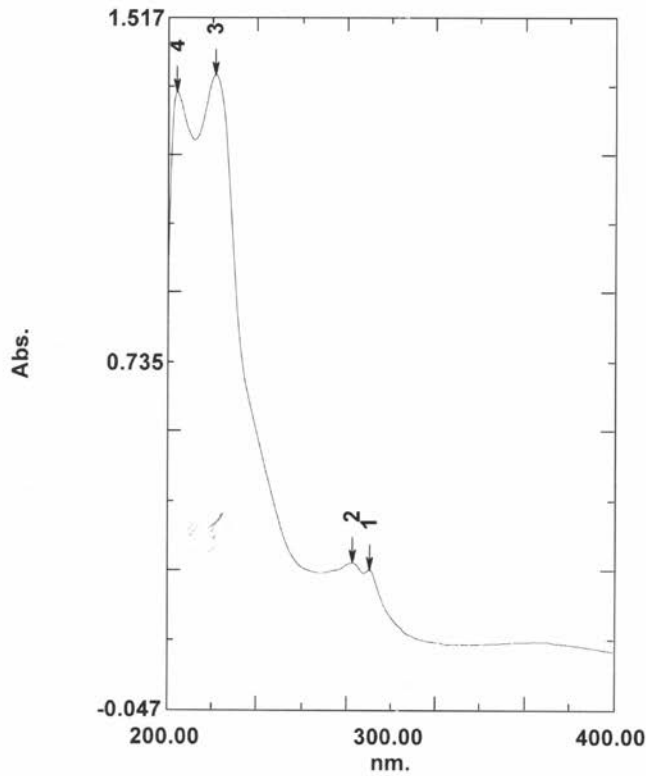


Figure S7. HRESIMS of compound **1**

光谱峰值检测报告

2021/07/02 16:43:10

数据集: LTH1-15-2 - RawData



[测定属性]
波长范围(nm): 200.00 到 400.00
扫描速度: 中速
采样间隔: 0.2
自动采样间隔: 启用
扫描模式: 单个

[仪器属性]
仪器类型: UV-2600 系列
测定方式: 吸收值
狭缝宽: 2.0
积分时间: 0.1 秒
光源转换波长: 323.0 nm
检测器单元: 直接
S/R 转换: 标准
阶梯校正: OFF

[附件属性]
附件: 无

[数据处理参数]
阈值: 0.0010000
点: 4
内插: 停用
平均: 停用

[样品准备属性]
重量:
体积:
稀释:
光程长:
附加信息:

| No. | P/V | 波长(nm) | Abs. | 描述 |
|-----|-----|--------|-------|----|
| 1 | ⊕ | 290.20 | 0.267 | |
| 2 | ⊕ | 282.60 | 0.282 | |
| 3 | ⊕ | 221.20 | 1.386 | |
| 4 | ⊕ | 204.00 | 1.346 | |

Figure S8. UV of compound 1

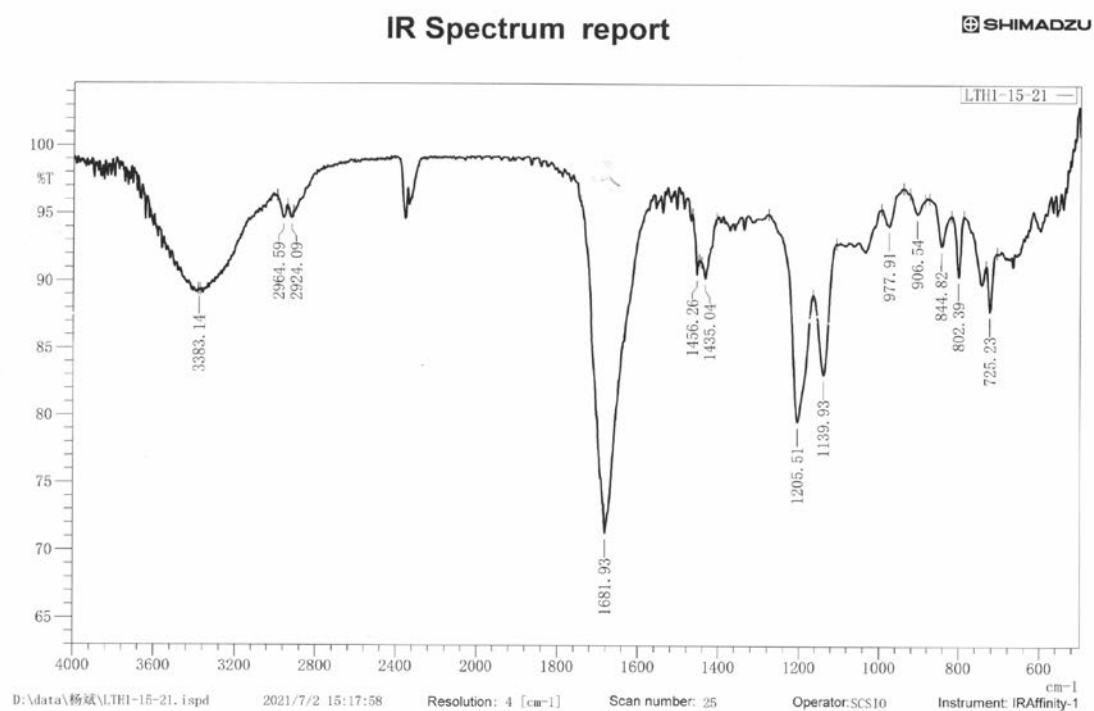


Figure S9. IR of compound **1**

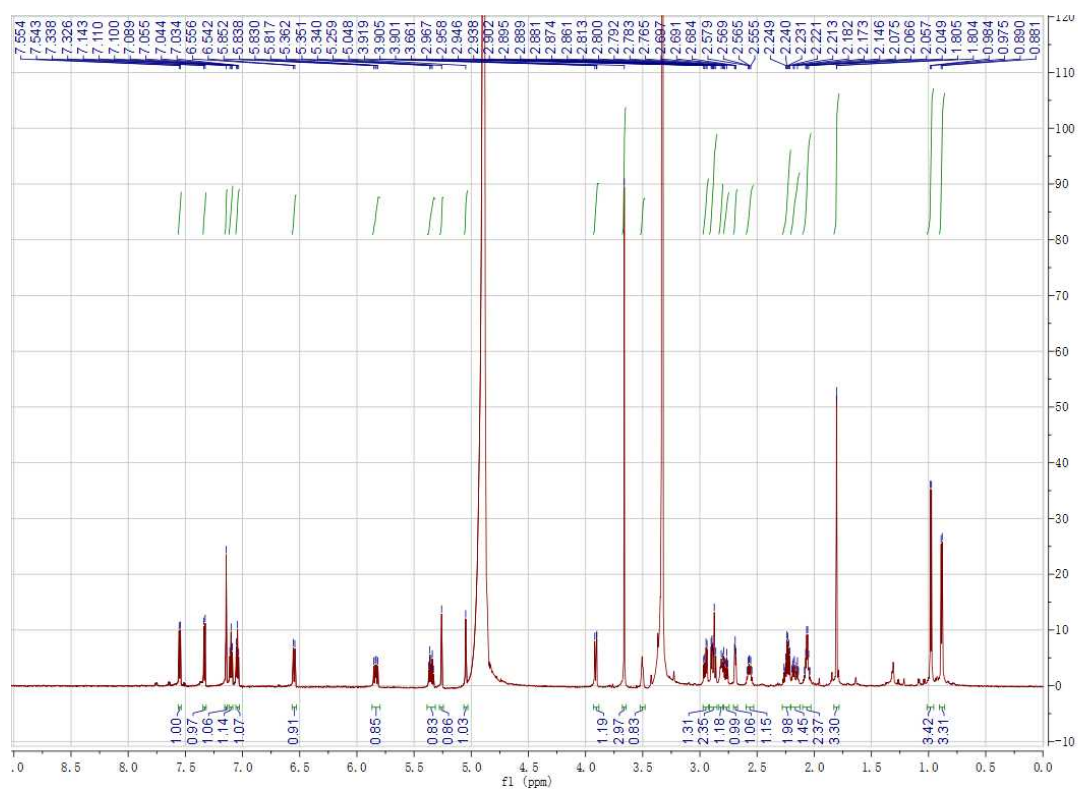


Figure S10. ¹H NMR of compound **2** (in CD₃OD)

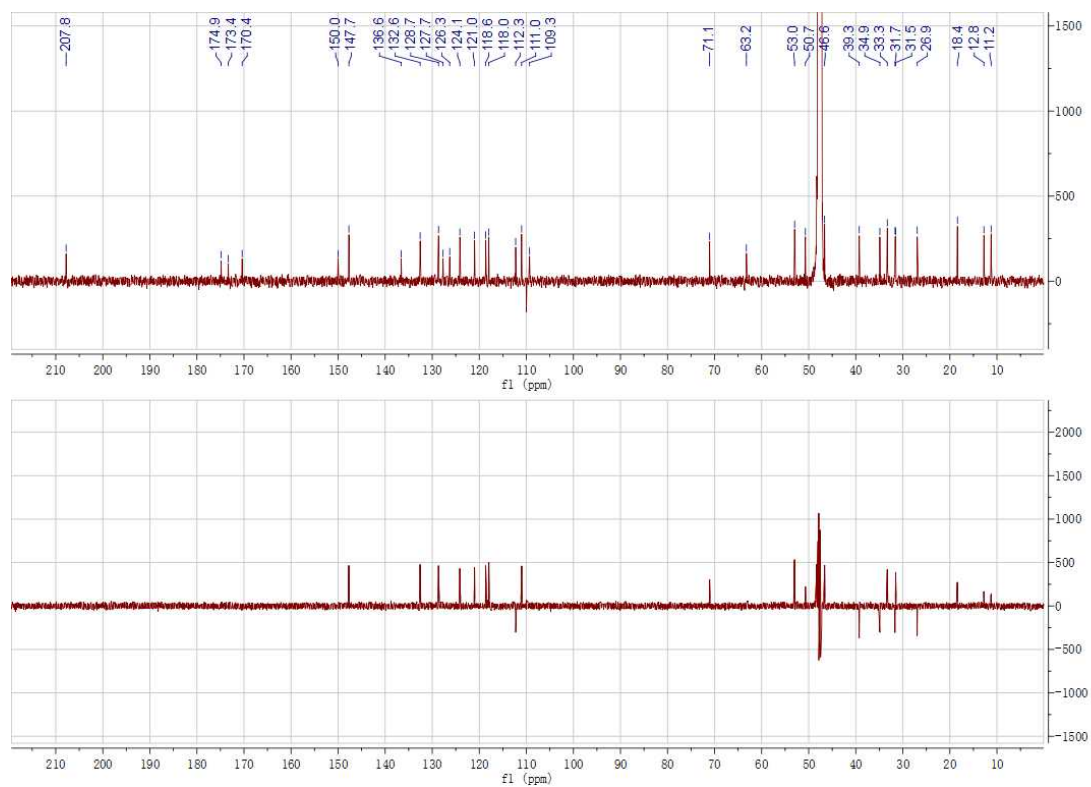


Figure S11. ^{13}C NMR of compound **2** (in CD_3OD)

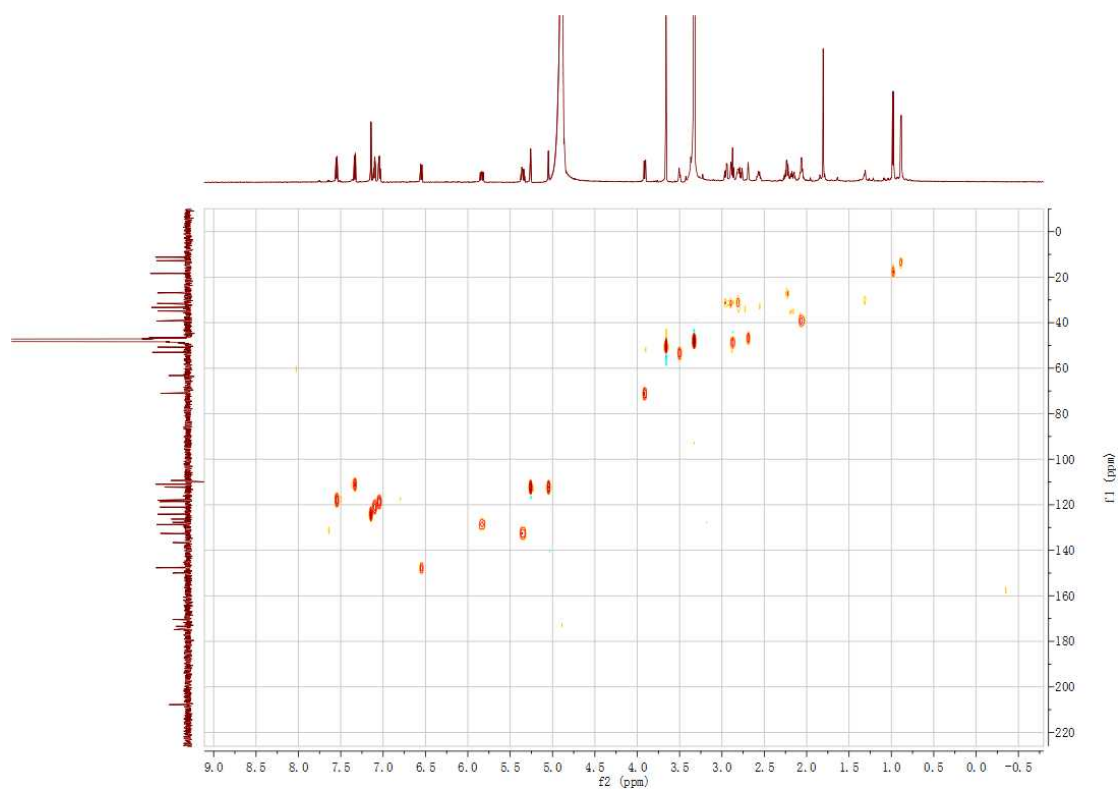


Figure S12. HSQC of compound **2** (in CD_3OD)

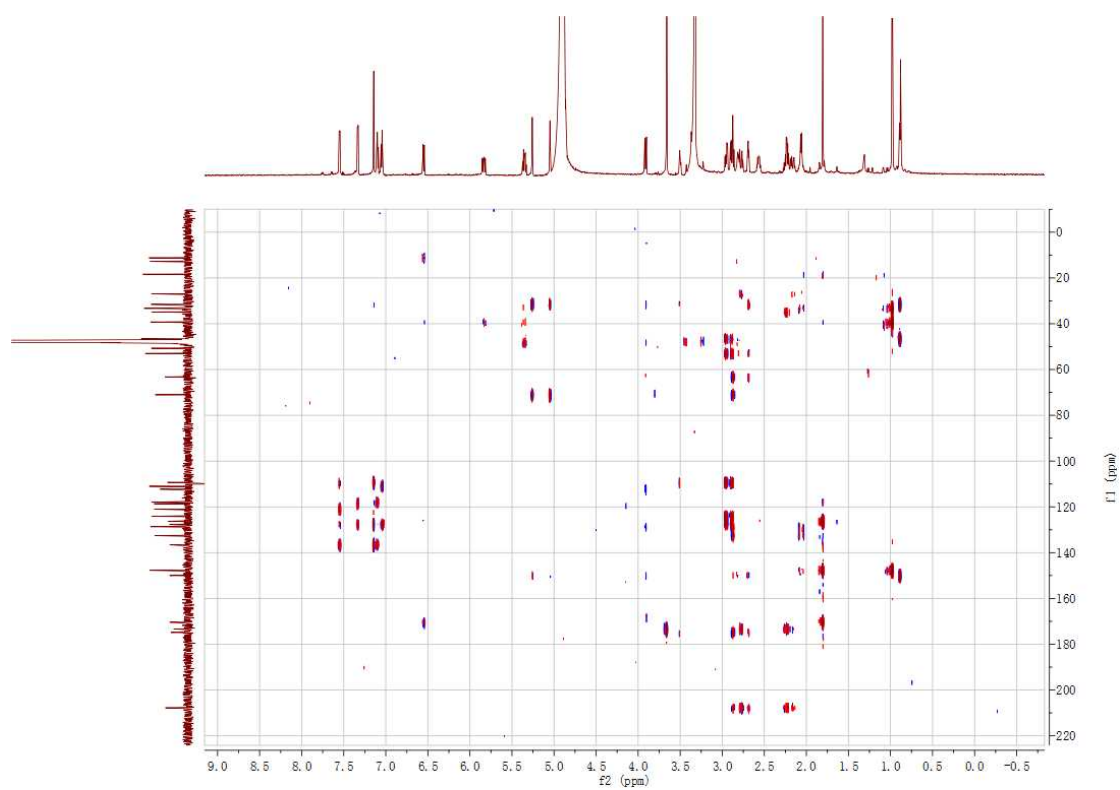


Figure S13. HMBC of compound **2** (in CD₃OD)

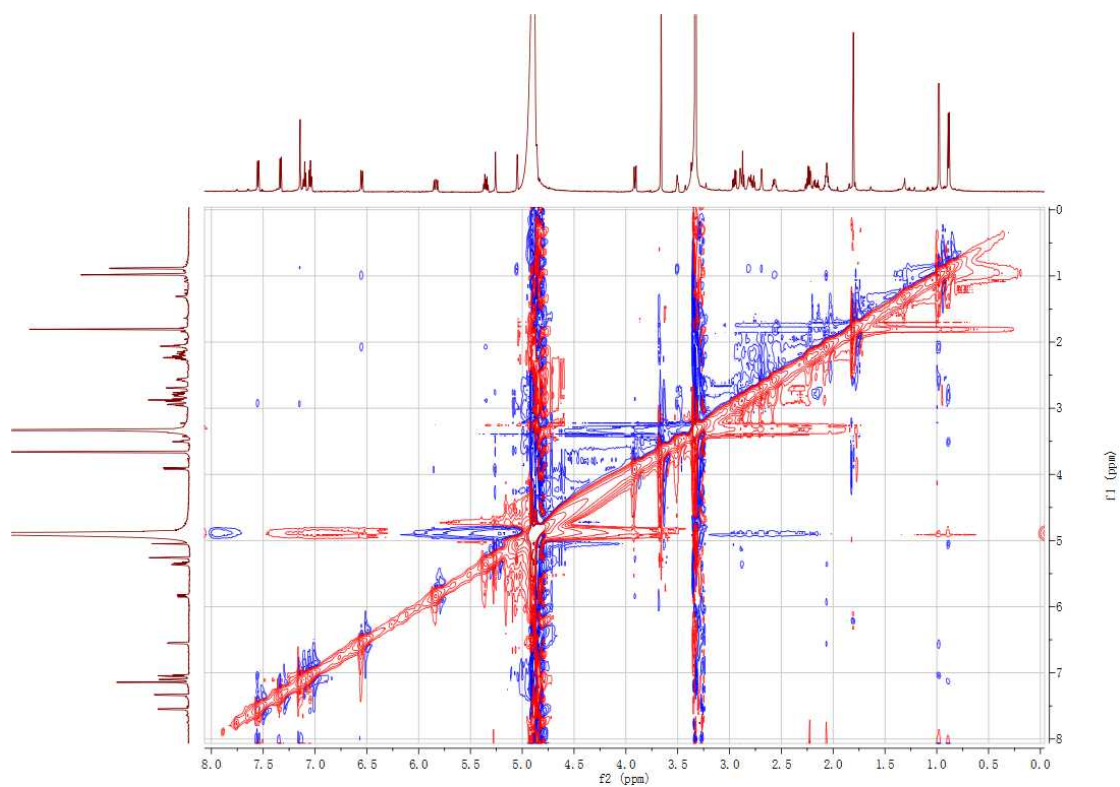
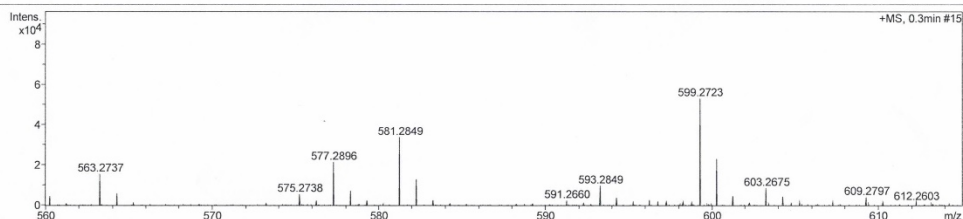


Figure S14. NOESY of compound **2** (in CD₃OD)

Mass Spectrum SmartFormula Report

Analysis Info
 Analysis Name D:\Data\MS\data\202107\shaosurun_LTH1-15-3_pos_52_01_11334.d
 Method LC_Direct Infusion_pos_70-500mz.m
 Sample Name shaosurun_LTH1-15-3_pos
 Comment
 Acquisition Date 8/2/2021 3:04:33 PM
 Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter
 Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar
 Focus Active Set Capillary 4500 V Set Dry Heater 180 °C
 Scan Begin 70 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min
 Scan End 1500 m/z Set Charging Voltage 0 V Set Divert Valve Waste
 Set Corona 0 nA Set APCI Heater 0 °C



| Meas. m/z | # | Ion Formula | Score | m/z | err [ppm] | err [mDa] | mSigma | rdB | e ⁻ Conf | N-Rule |
|-----------|---|---------------|--------|-----------|-----------|-----------|--------|------|---------------------|--------|
| 577.2896 | 1 | C33H41N2O7 | 100.00 | 577.2908 | -2.1 | -1.2 | 24.0 | 14.5 | even | ok |
| 599.2723 | 1 | C33H40N2NaO7 | 100.00 | 599.2728 | 0.8 | 0.5 | 32.4 | 14.5 | even | ok |
| 1153.5709 | 1 | C66H81N4O14 | 100.00 | 1153.5744 | 3.0 | 3.5 | 558.7 | 28.5 | even | ok |
| 1175.5542 | 1 | C66H80N4NaO14 | 100.00 | 1175.5563 | 1.8 | 2.2 | 217.1 | 28.5 | even | ok |

shaosurun_LTH1-15-3_pos_52_01_11334.d
 Bruker Compass DataAnalysis 4.1

printed: 8/2/2021 3:14:45 PM

by: SCSIO

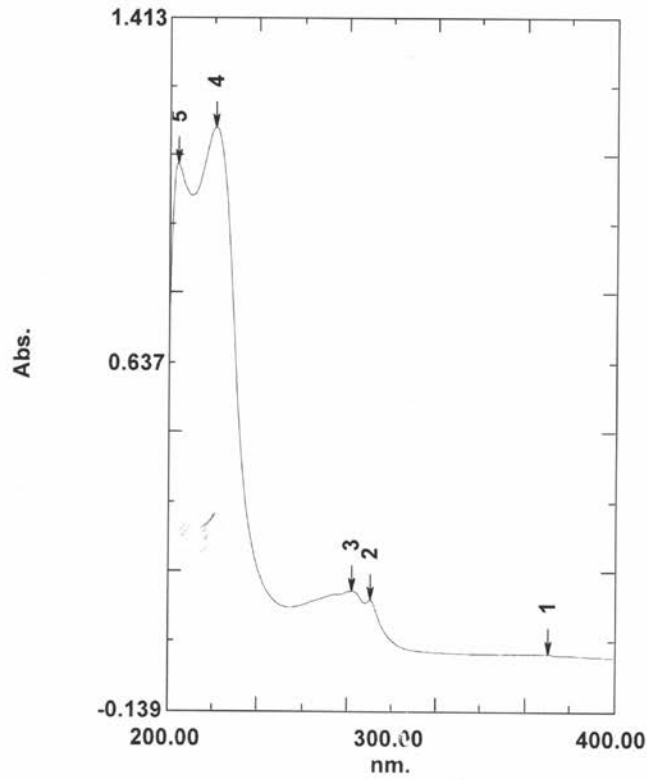
Page 1 of 1

Figure S15. HRESIMS of compound 2

光谱峰值检测报告

2021/07/02 16:51:27

数据集: LTH1-15-3 - RawData



[测定属性]
 波长范围(nm): 200.00 到 400.00
 扫描速度: 中速
 采样间隔: 0.2
 自动采样间隔: 启用
 扫描模式: 单个

[仪器属性]
 仪器类型: UV-2600 系列
 测定方式: 吸收值
 狭缝宽: 2.0
 积分时间: 0.1 秒
 光源转换波长: 323.0 nm
 检测器单元: 直接
 S/R 转换: 标准
 阶梯校正: OFF

[附件属性]
 附件: 无

[数据处理参数]
 阈值: 0.0010000
 点: 4
 内插: 停用
 平均: 停用

[样品准备属性]
 重量:
 体积:
 稀释:
 光程长:
 附加信息:

| No. | P/V | 波长(nm) | Abs. | 描述 |
|-----|-----|--------|--------|----|
| 1 | ☉ | 370.80 | -0.013 | |
| 2 | ☉ | 290.20 | 0.106 | |
| 3 | ☉ | 282.20 | 0.126 | |
| 4 | ☉ | 220.60 | 1.164 | |
| 5 | ☉ | 203.60 | 1.082 | |

Figure S16. UV of compound 2

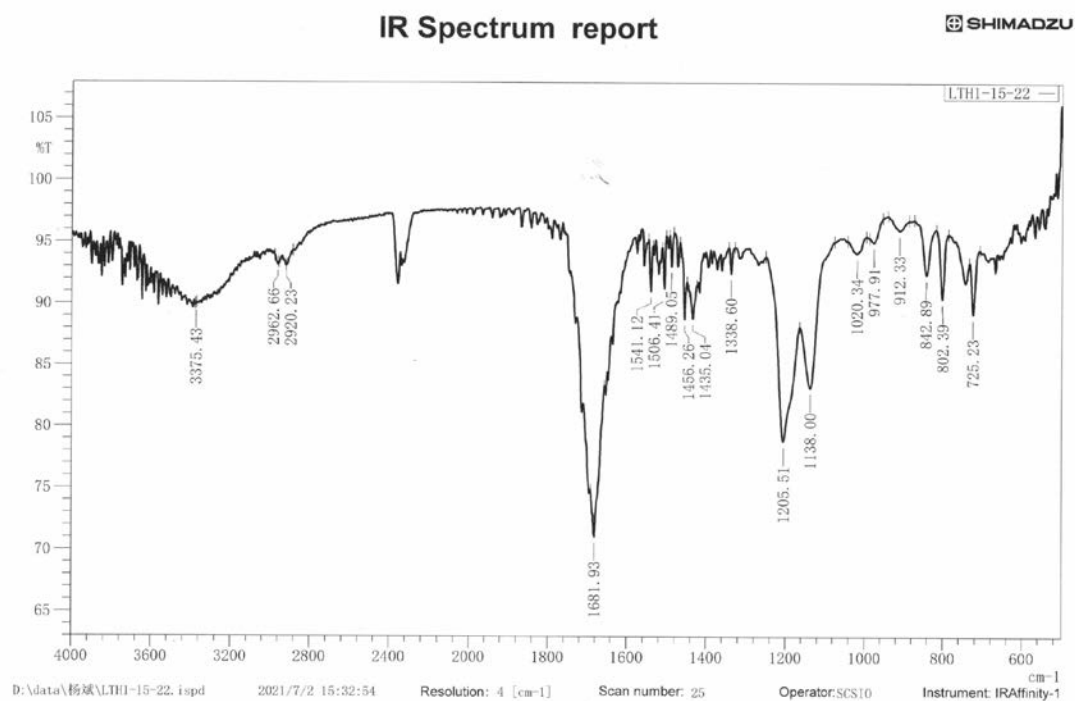


Figure S17. IR of compound **2**

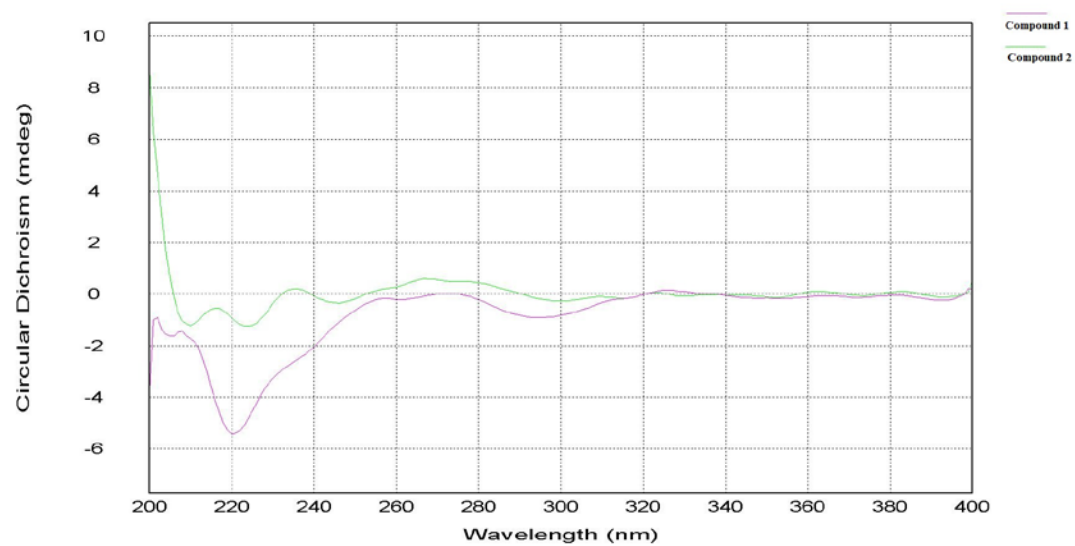


Figure S18. CD of compounds **1** and **2**

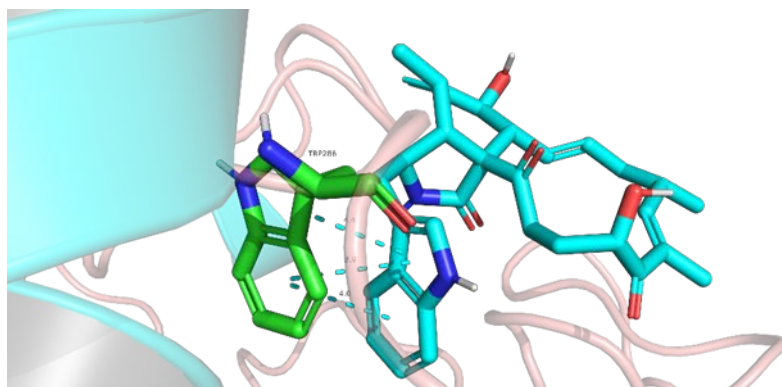


Figure S19. Molecular docking of chaetoglobosin Fex

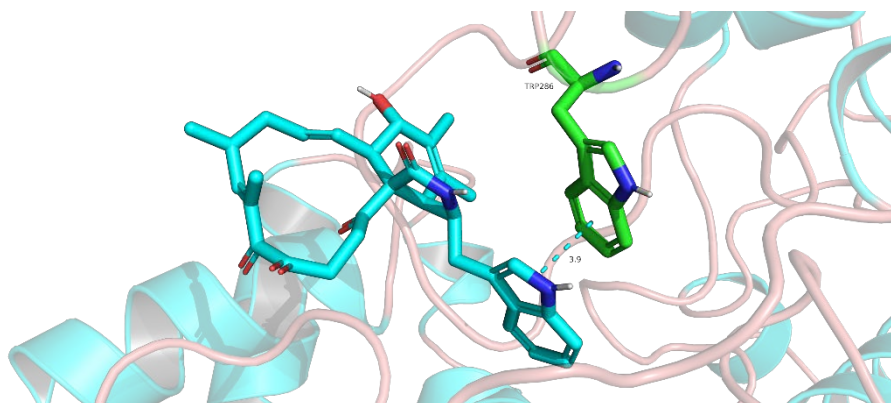


Figure S20. Molecular docking of chaetoglobosin G

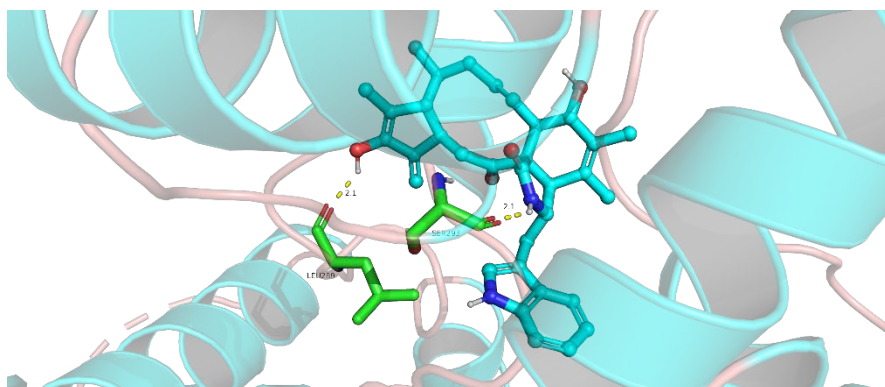


Figure S21. Molecular docking of chaetoglobosin Vb