

**Sorbicillinoid Derivatives with the Radical Scavenging Activities from the
Marine-Derived Fungus *Acremonium chrysogenum* C10**

**Chengbao Duan^{1,2,†}, Shiyuan Wang^{1,2,†}, Ruiyun Huo^{1,2,†}, Erwei Li³, Min Wang⁴,
Jinwei Ren¹, Yuanyuan Pan^{1,*}, Ling Liu^{1,2,*} and Gang Liu^{1,2,*}**

1 State Key Laboratory of Mycology, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, China; 18813111804@163.com (C.D.); wangshiyuan20@mails.ucas.ac.cn (S.W.); huory@im.ac.cn (R.H.); renjw@im.ac.cn (J.R.); panny@im.ac.cn (Y.P.); liul@im.ac.cn (L.L.); liug@im.ac.cn (G.L.)

2 University of Chinese Academy of Sciences, Beijing 100049, China

3 Institutional Center for Shared Technologies and Facilities, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, China; liew@im.ac.cn (E.L.)

4 State Key Laboratory of Microbial Resources, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, China; hualuozhisheng@126.com (M.W.)

[†]These authors contributed equally to this work.

*Correspondences:

Yuanyuan Pan, E-mail: panny@im.ac.cn; Tel.: +86-10-64806113

Ling Liu, E-mail: liul@im.ac.cn; Tel.: +86-10-64807043

Gang Liu, E-mail: liug@im.ac.cn; Tel.: +86-10-64806017

| No. | Contents | Pages |
|-----|---|-------|
| 1. | Figure S1. ^1H NMR spectrum of acresorbicillinol A (1 ; 500 MHz, CD_3OD) | 3 |
| 2. | Figure S2. ^{13}C NMR spectrum of acresorbicillinol A (1 ; 125 MHz, CD_3OD) | 4 |
| 3. | Figure S3. ^1H - ^1H COSY spectrum of acresorbicillinol A (1 , CD_3OD) | 5 |
| 4. | Figure S4. HSQC spectrum of acresorbicillinol A (1 , CD_3OD) | 6 |
| 5. | Figure S5. HMBC spectrum of acresorbicillinol A (1 , CD_3OD) | 7 |
| 6. | Figure S6. NOESY spectrum of acresorbicillinol A (1 , CD_3OD) | 8 |
| 7. | Figure S7. ^1H NMR spectrum of acresorbicillinol B (2 ; 500 MHz, CD_3OD) | 9 |
| 8. | Figure S8. ^{13}C NMR spectrum of acresorbicillinol B (2 ; 125 MHz, CD_3OD) | 10 |
| 9. | Figure S9. ^1H - ^1H COSY spectrum of acresorbicillinol B (2 , CD_3OD) | 11 |
| 10. | Figure S10. HSQC spectrum of acresorbicillinol B (2 , CD_3OD) | 12 |
| 11. | Figure S11. HMBC spectrum of acresorbicillinol B (2 , CD_3OD) | 13 |
| 12. | Figure S12. NOESY spectrum of acresorbicillinol B (2 , CD_3OD) | 14 |
| 13. | Figure S13. ^1H NMR spectrum of acresorbicillinol C (3 ; 500 MHz, $\text{DMSO}:\text{CDCl}_3 = 3:1$) | 15 |
| 14. | Figure S14. ^{13}C NMR spectrum of acresorbicillinol C (3 ; 125 MHz, $\text{DMSO}:\text{CDCl}_3 = 3:1$) | 16 |
| 15. | Figure S15. ^1H - ^1H COSY spectrum of acresorbicillinol C (3 , $\text{DMSO}:\text{CDCl}_3 = 3:1$) | 17 |
| 16. | Figure S16. HSQC spectrum of acresorbicillinol C (3 , $\text{DMSO}:\text{CDCl}_3 = 3:1$) | 18 |
| 17. | Figure S17. HMBC spectrum of acresorbicillinol C (3 , $\text{DMSO}:\text{CDCl}_3 = 3:1$) | 19 |
| 18. | Figure S18. NOESY spectrum of acresorbicillinol C (3 , $\text{DMSO}:\text{CDCl}_3 = 3:1$) | 20 |
| 19. | Figure S19. ECD conformers of acresorbicillinols A–C (1–3) | 21 |
| 20. | Figure S20. HPLC profiles of the extracts from the rice solid medium of <i>A. chrysogenum</i> after 7 days fermentation | 25 |
| 21. | Tale S1: Primers used in this study | 26 |

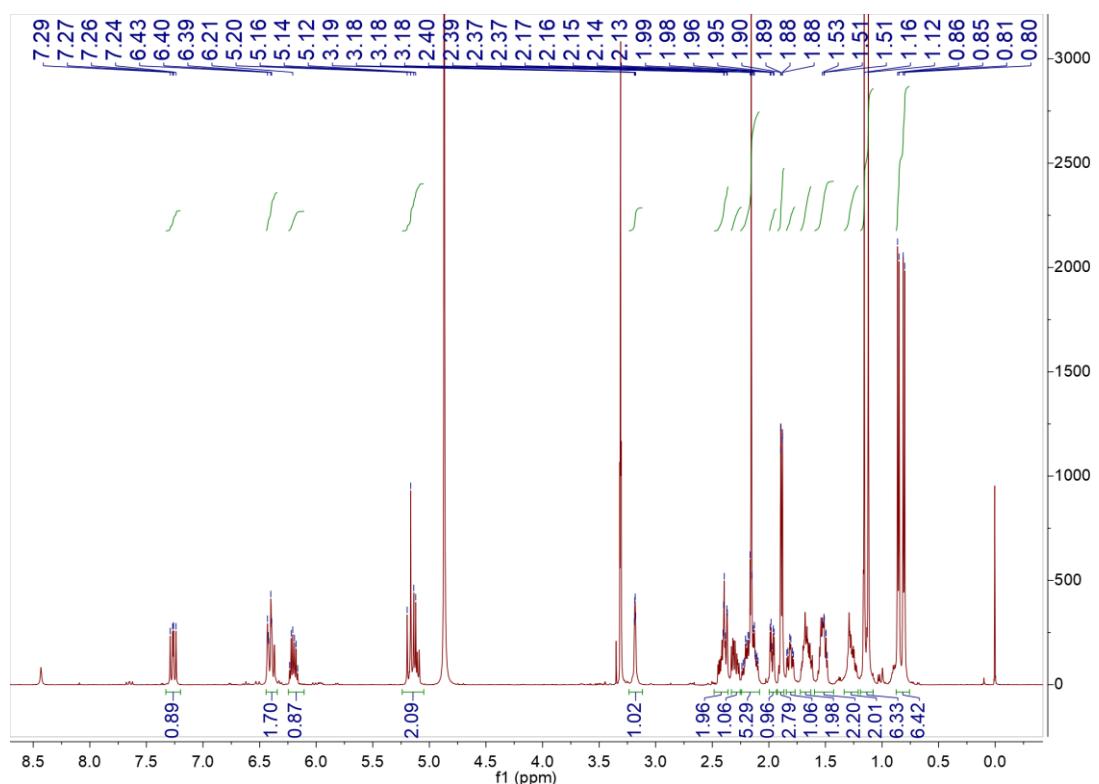


Figure S1. ^1H NMR spectrum of acresorbicillinol A (**1**; 500 MHz, CD_3OD)

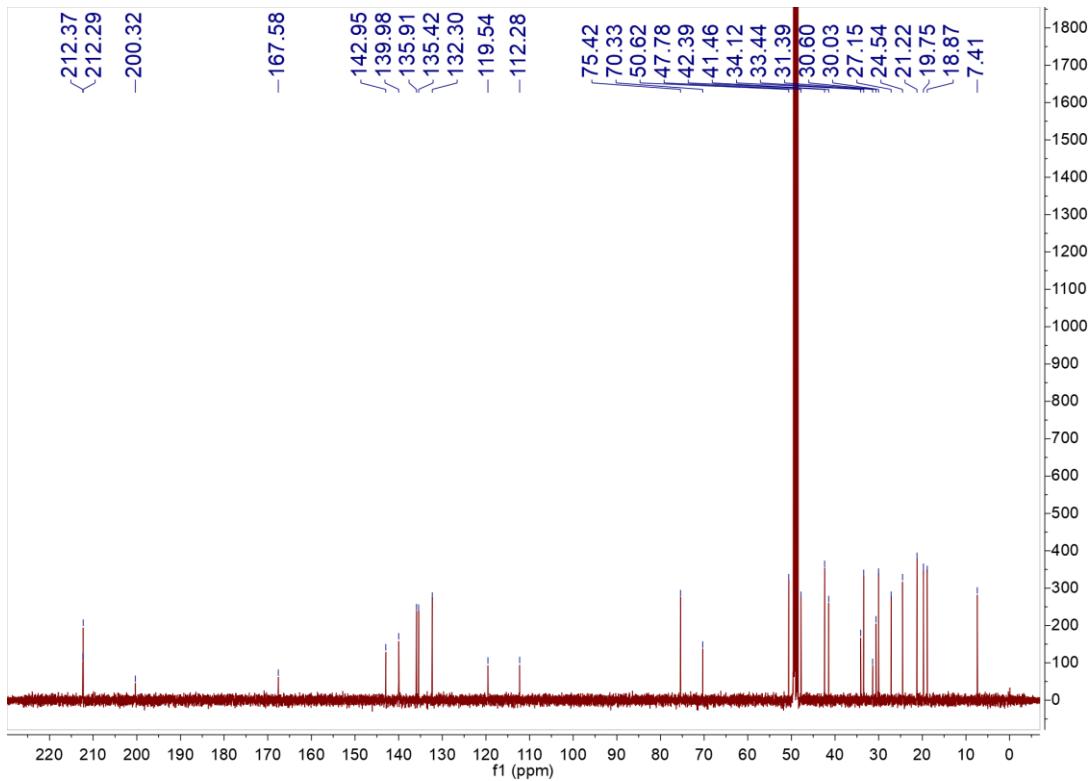


Figure S2. ¹³C NMR spectrum of acresorbicillinol A (**1**; 125 MHz, CD₃OD)

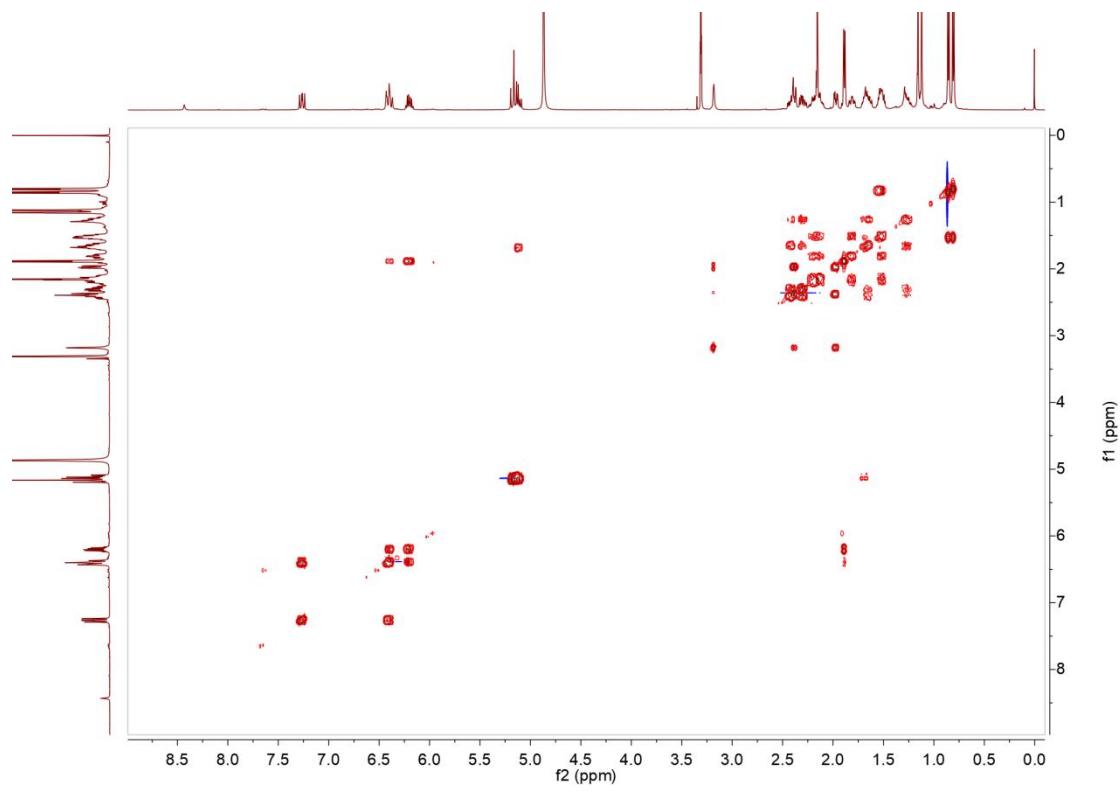


Figure S3. ^1H - ^1H COSY spectrum of acresorbicillinol A (**1**, CD_3OD)

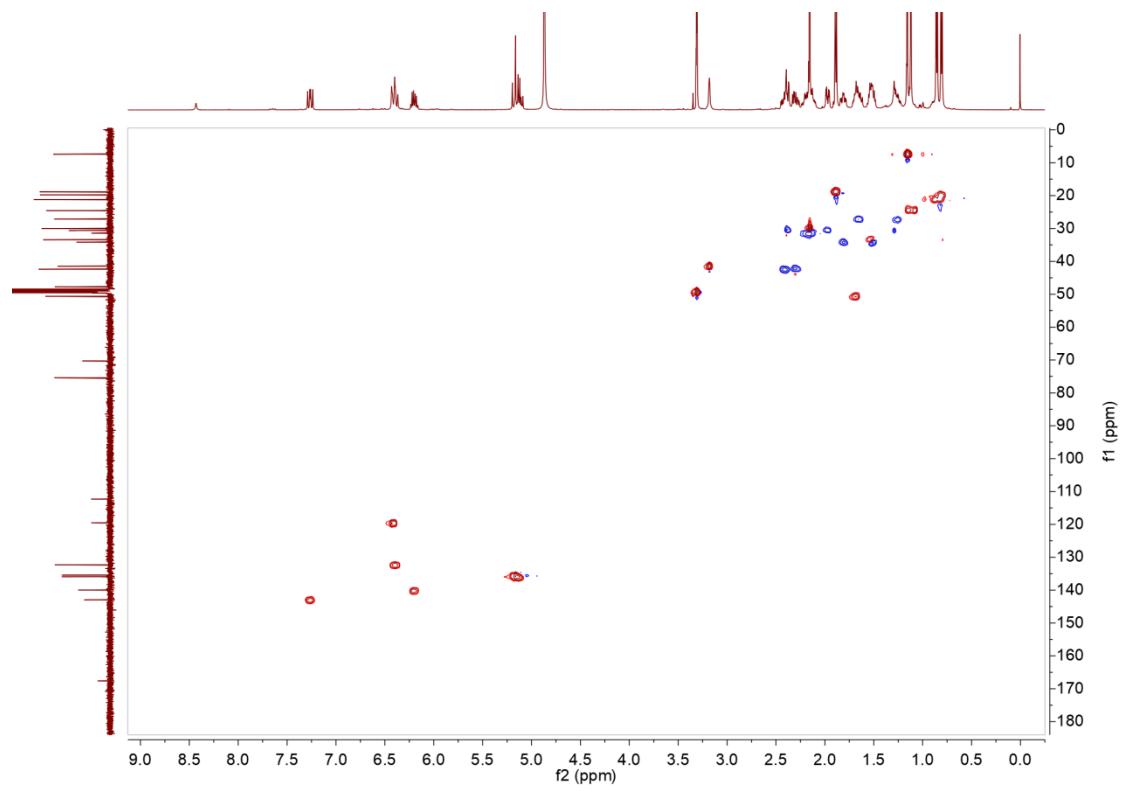


Figure S4. HSQC spectrum of acresorbicillinol A (**1**, ^{CD}₃OD)

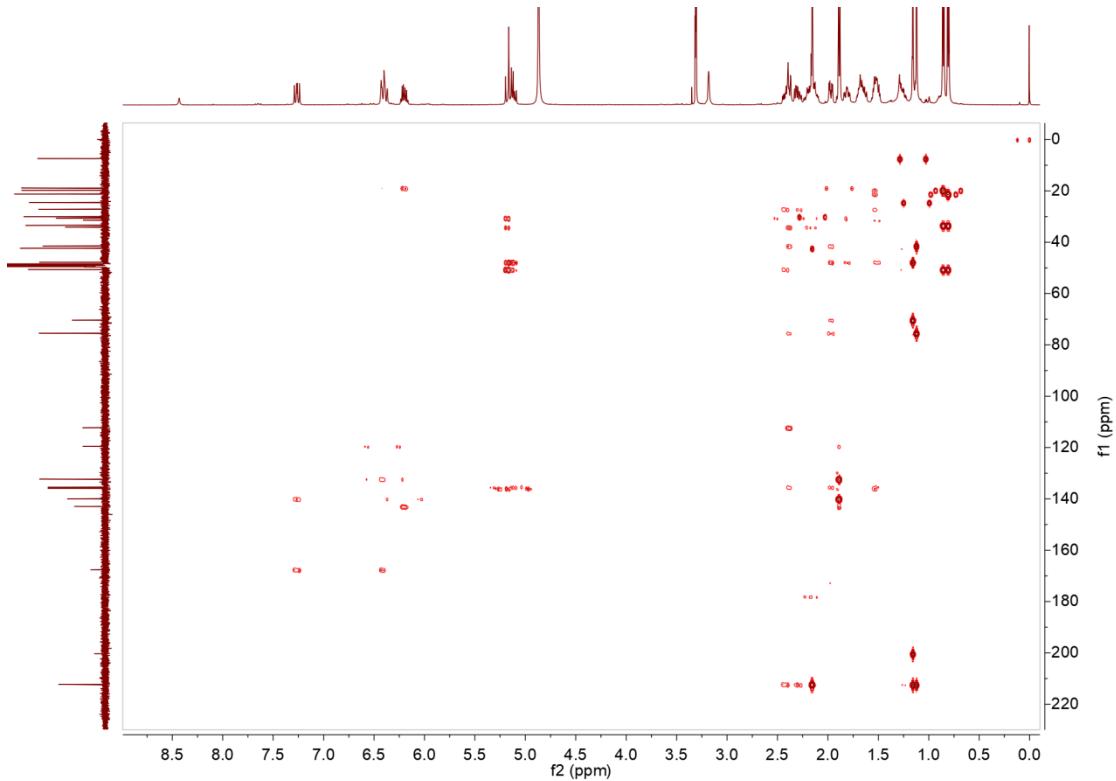


Figure S5. HMBC spectrum of acresorbicillinol A (**1**, CD₃OD)

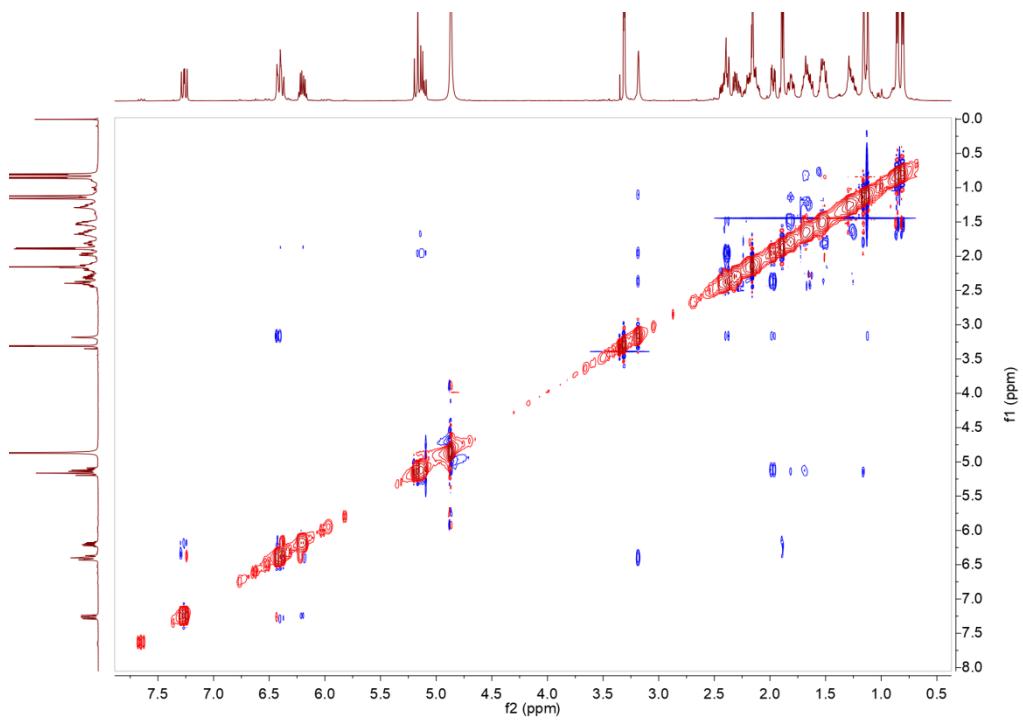


Figure S6. NOESY spectrum of acresorbicillinol A (**1**, CD_3OD)

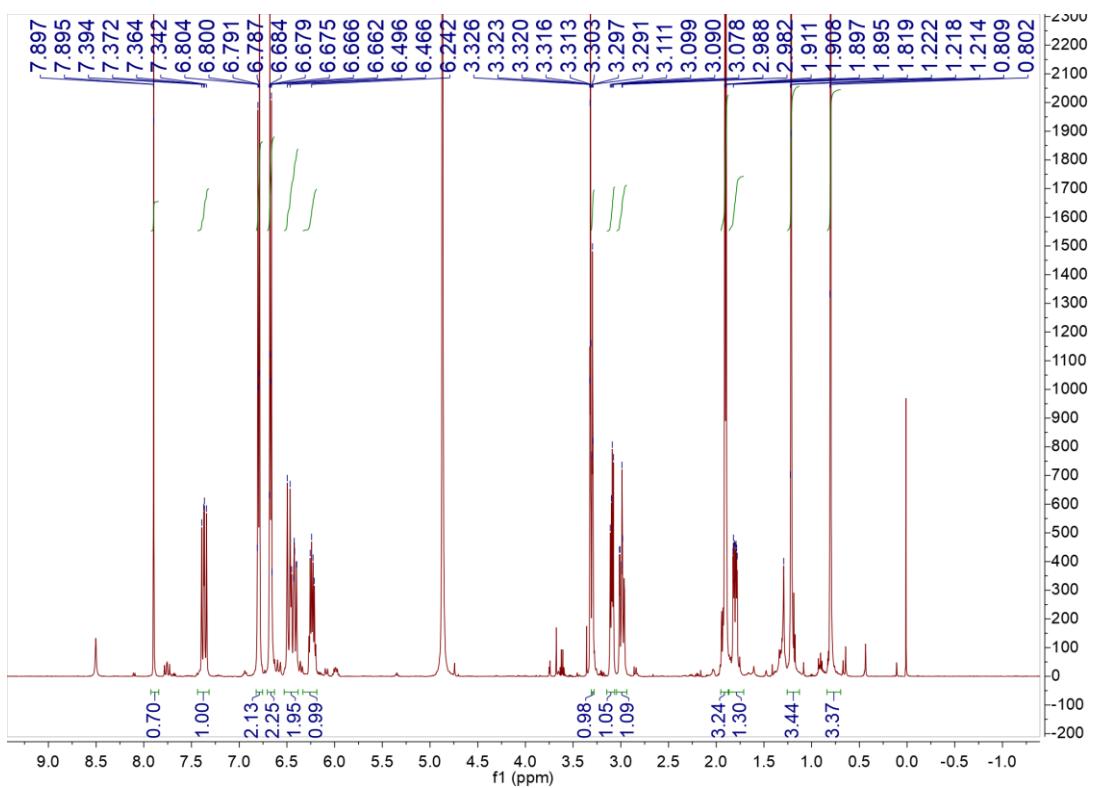


Figure S7. ^1H NMR spectrum of acresorbicillinol B (**2**; 500 MHz, CD_3OD)

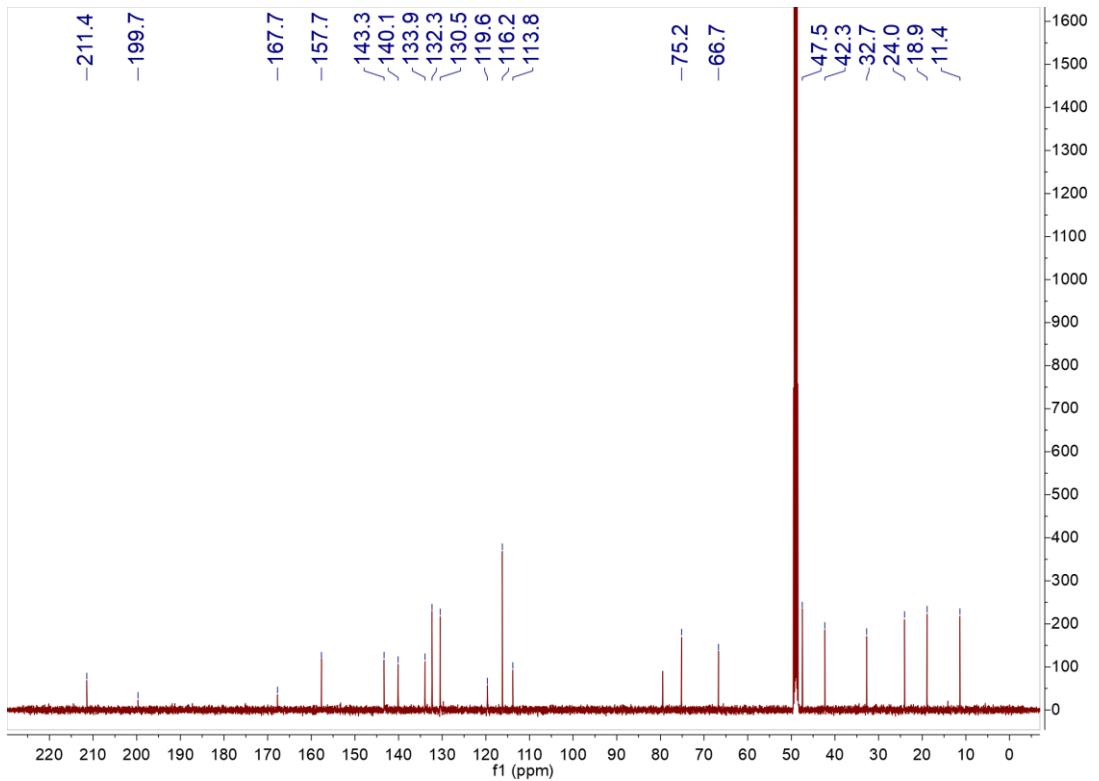


Figure S8. ¹³C NMR spectrum of acresorbicillinol B (2; 125 MHz, CD₃OD)

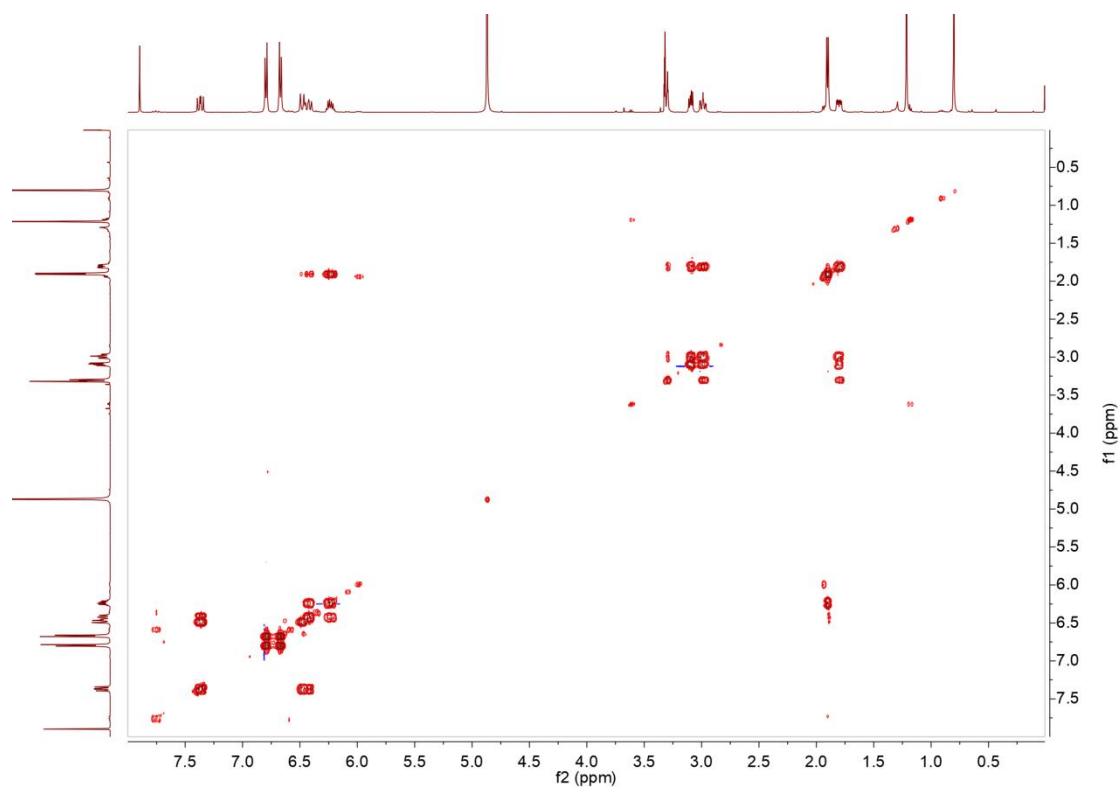


Figure S9. ¹H-¹H COSY spectrum of acresorbicillinol B (**2**, CD₃OD)

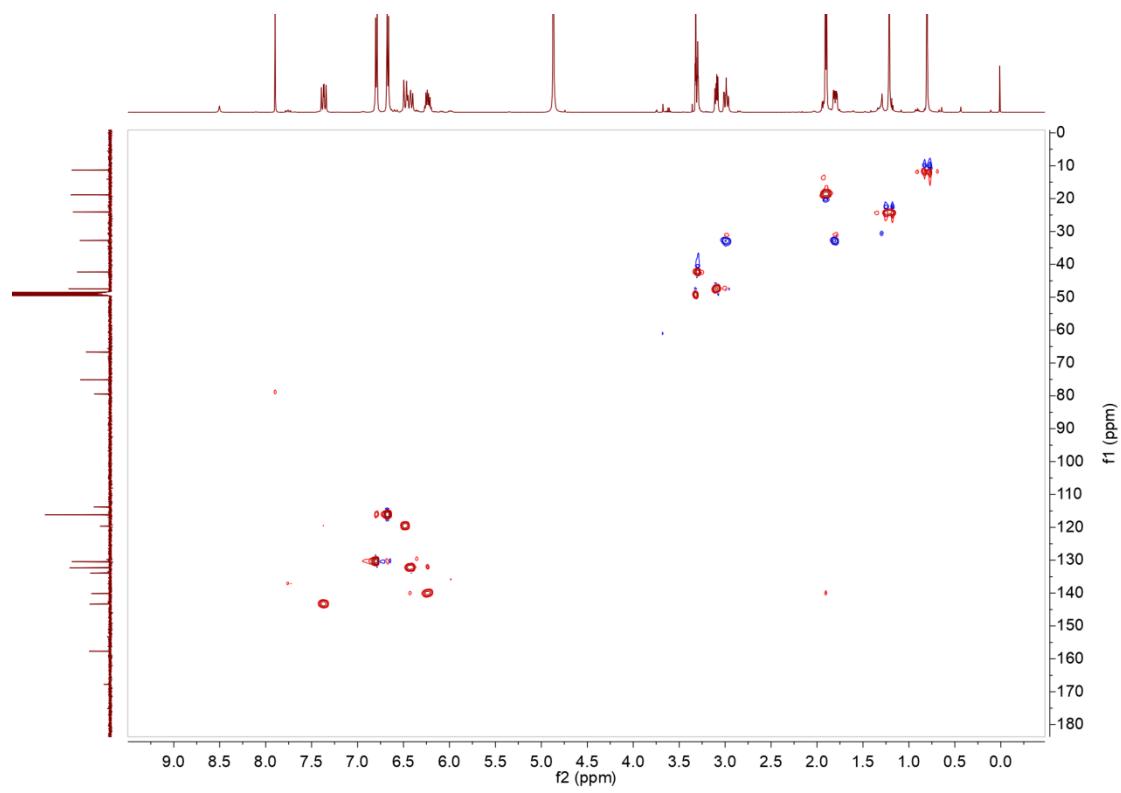


Figure S10. HSQC spectrum of acresorbicillinol B (**2**, CD_3OD)

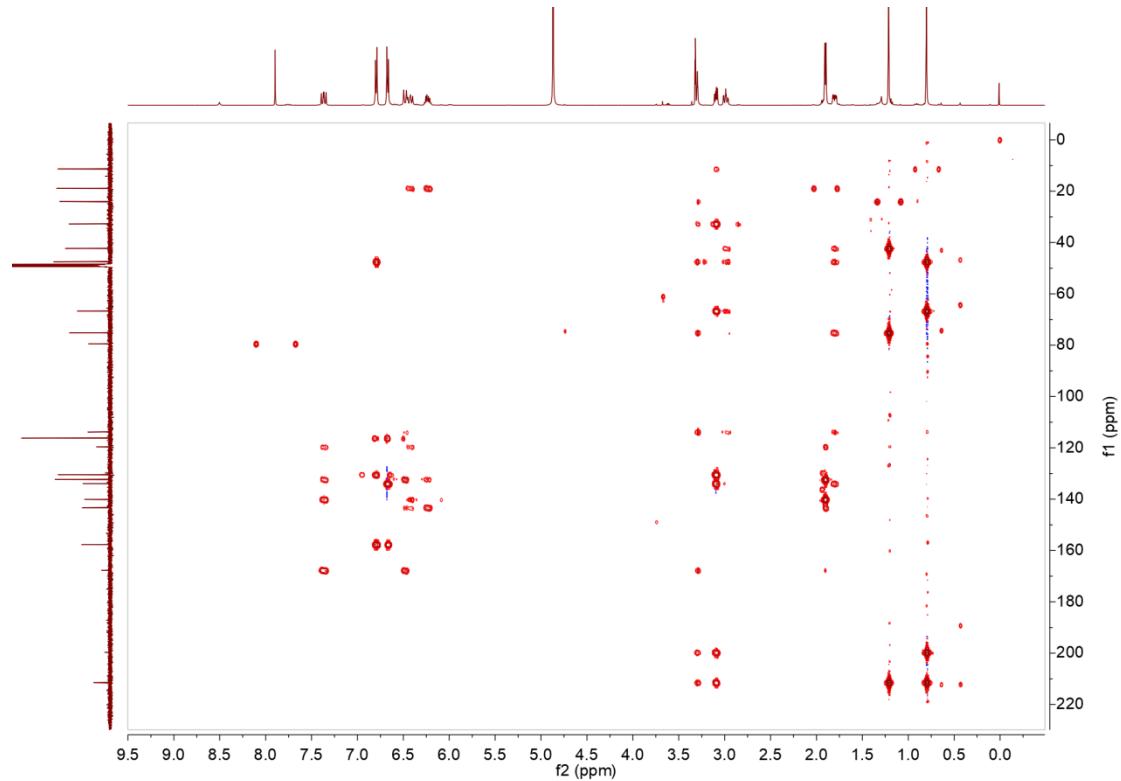


Figure S11. HMBC spectrum of acresorbicillinol B (**2**, CD₃OD)

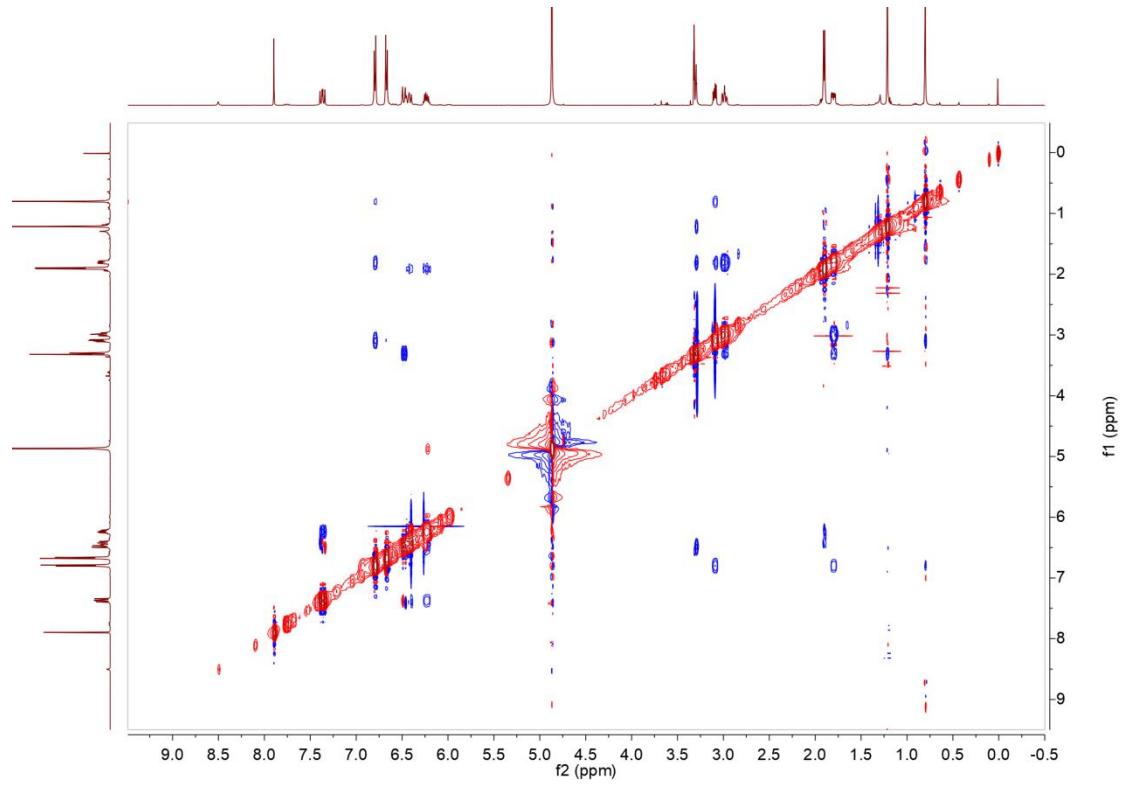


Figure S12. NOESY spectrum of acresorbicillinol B (**2**, CD₃OD)

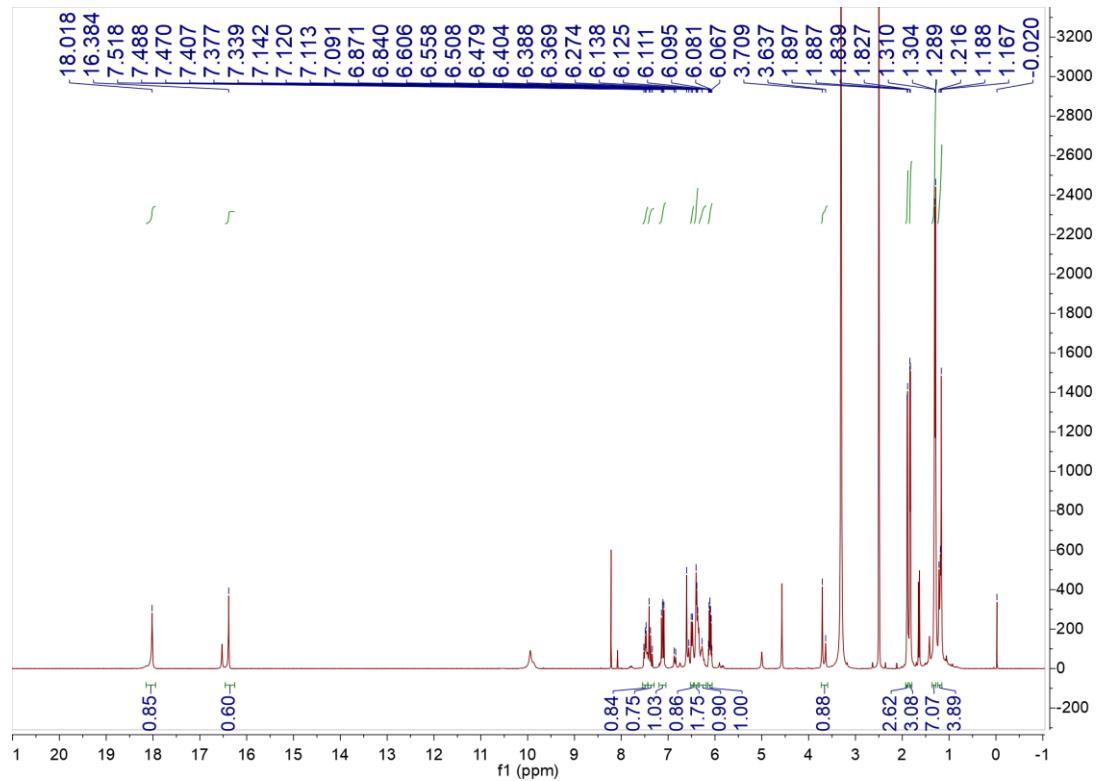


Figure S13. ¹H NMR spectrum of acresorbicillinol C (**3**; 500 MHz, DMSO:CDCl₃ = 3:1)

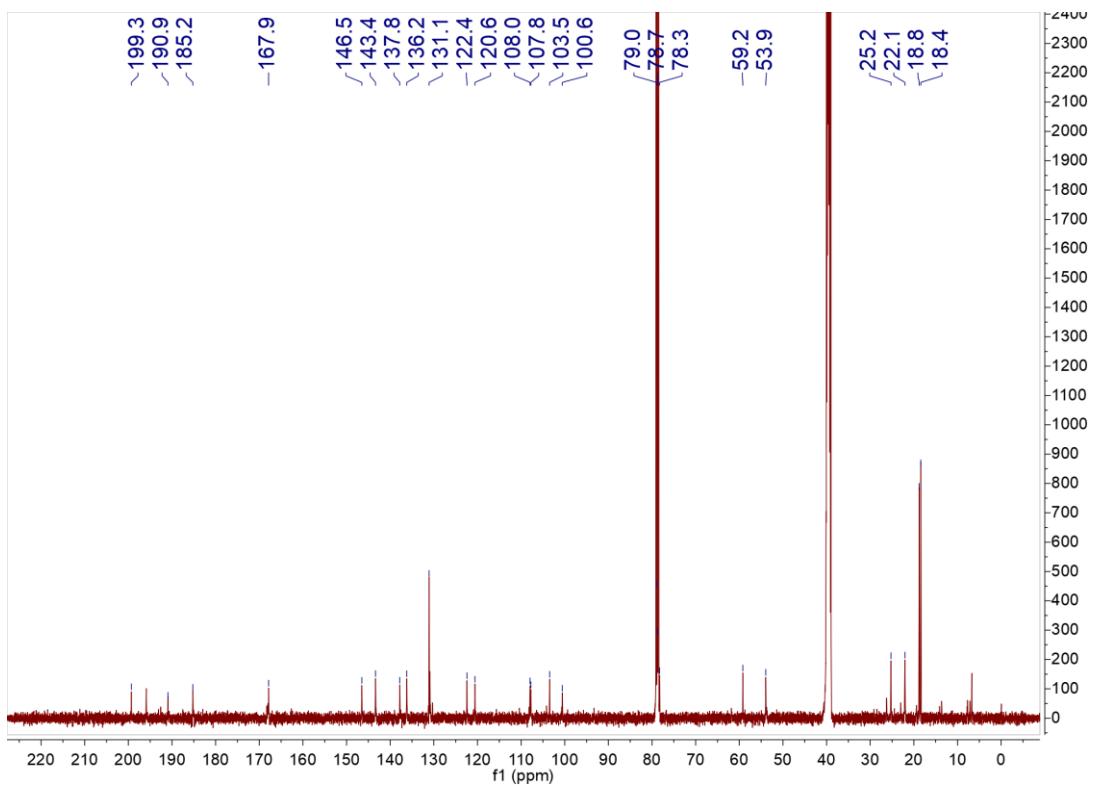


Figure S14. ¹³C NMR spectrum of acresorbicillinol C (**3**; 125 MHz, DMSO:CDCl₃ = 3:1)

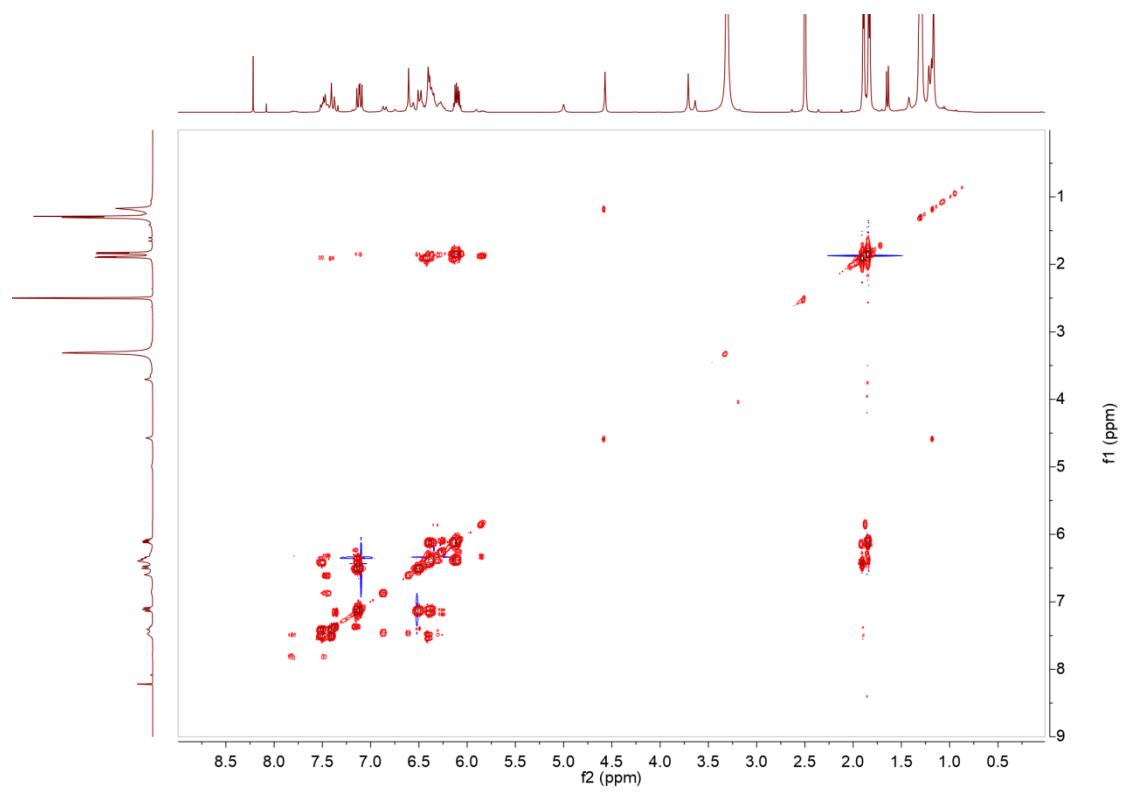


Figure S15. ¹H-¹H COSY spectrum of acresorbicillinol C (3, DMSO:CDCl₃ = 3:1)

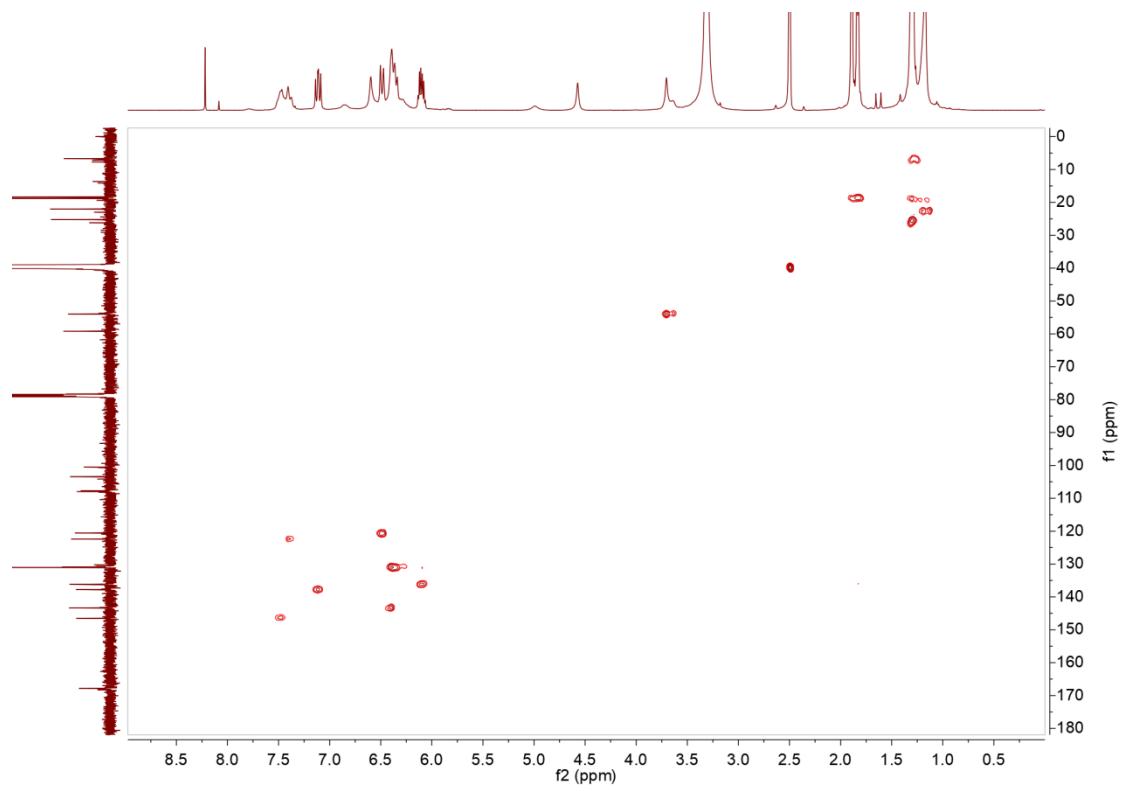


Figure S16. HSQC spectrum of acresorbicillinol C (**3**, DMSO:CDCl₃ = 3:1)

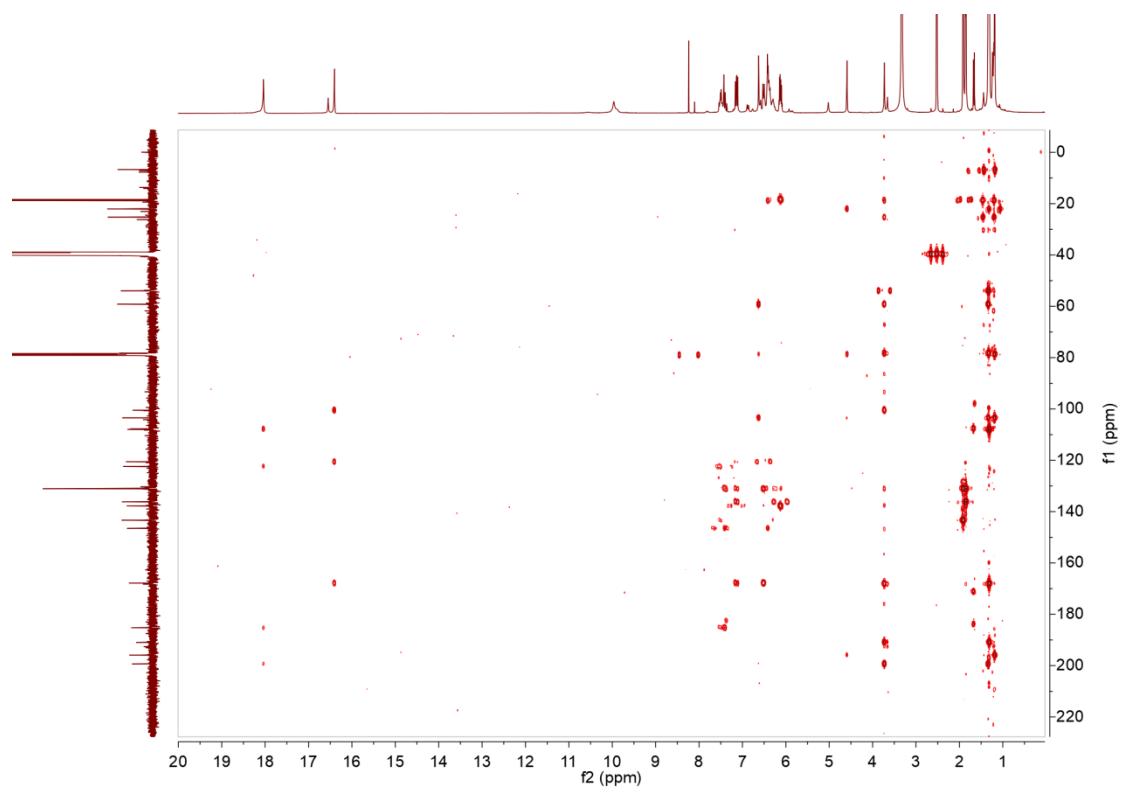


Figure S17. HMBC spectrum of acresorbicillinol C (**3**, DMSO:CDCl₃ = 3:1)

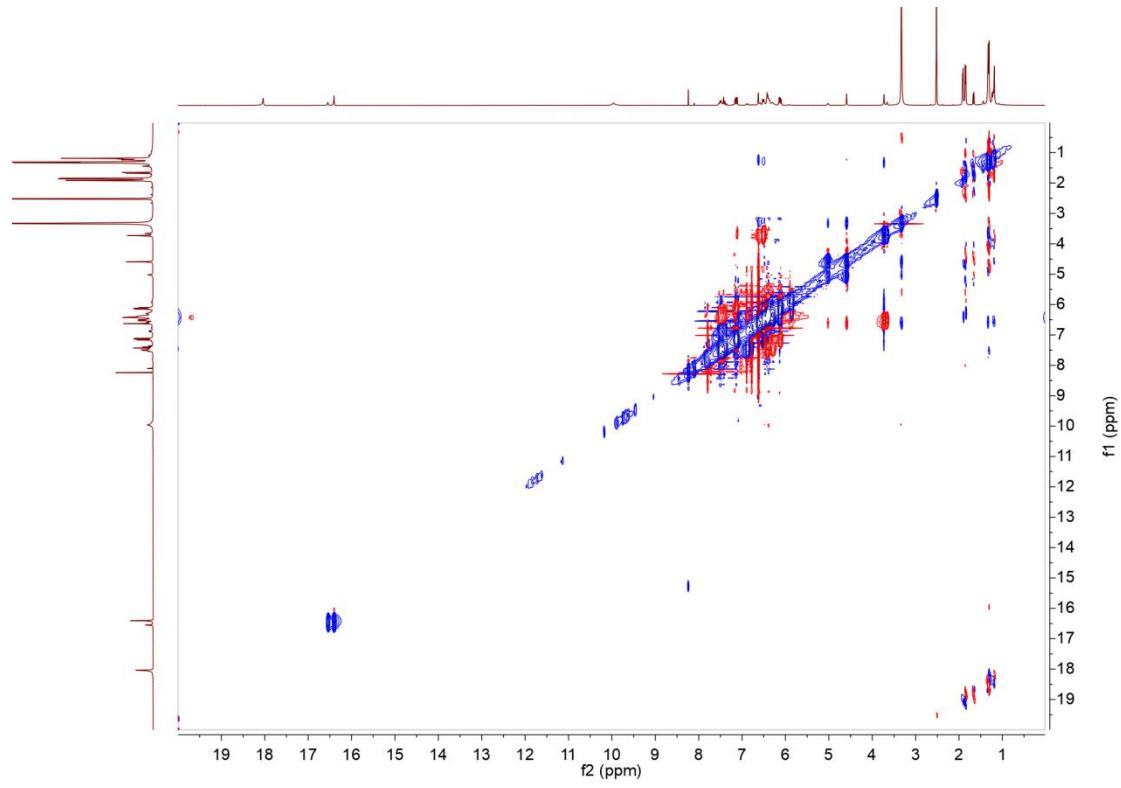
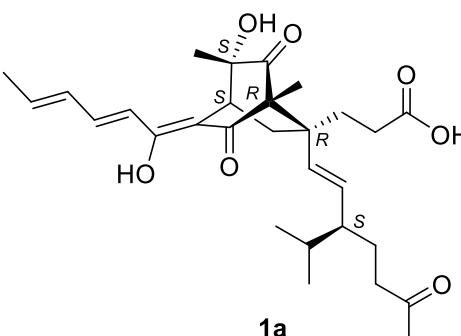
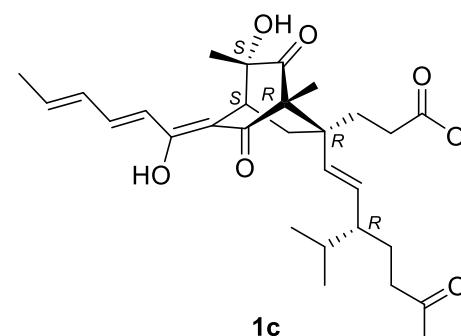
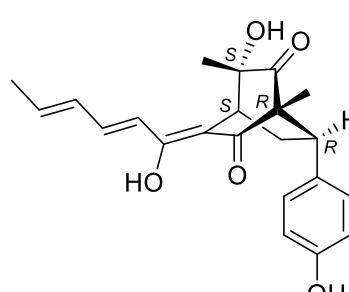
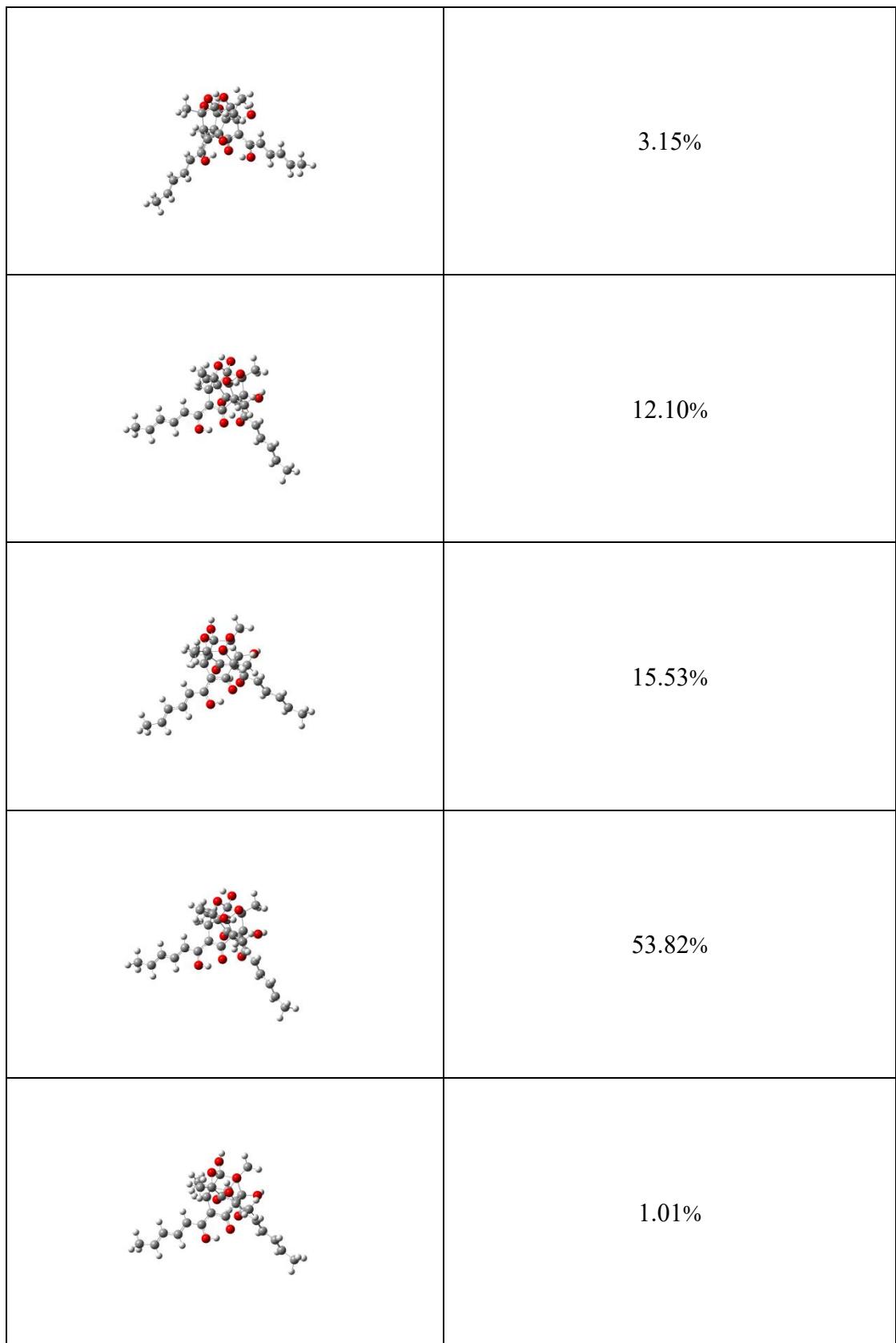


Figure S18. NOESY spectrum of acresorbicillinol C (**3**, DMSO:CDCl₃ = 3:1)

|  <p>1a</p> | |  <p>1c</p> | |
|--|-------------|---|-------------|
| Conformers | Populations | Conformers | Populations |
|  | 25.49% |  | 68.26% |
|  | 53.89% |  | 31.74% |
|  | 20.62% | | |
|  <p>2a</p> | | | |

| Conformers | Populations |
|------------|-------------|
| | 51.44% |
| | 48.56% |
| | 3a |
| Conformers | Populations |
| | 1.97% |
| | 8.24% |



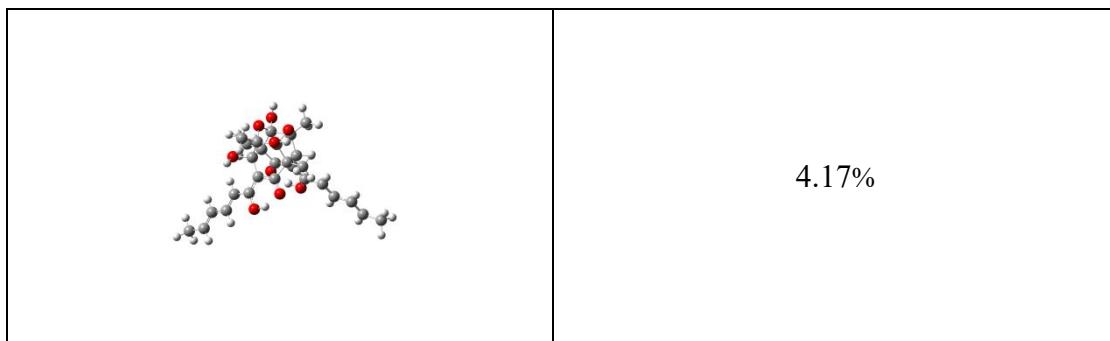


Figure S19. ECD conformers of acresorbicillinols A–C (**1–3**)

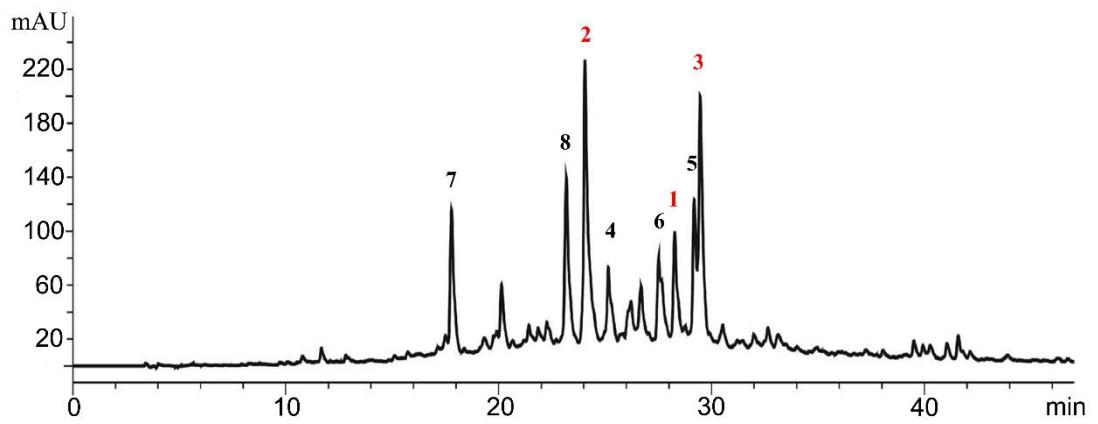


Figure S20. HPLC profiles of the extracts from the rice solid medium of *A. chrysogenum* after 7 days fermentation

Table S1. Primers used in this study

| Primer | Sequence |
|---------------|-----------------------|
| actin-F(RT) | AGTCCAAGCGTGATCC |
| actin-R(RT) | TAGAAGGCAGGGCGTTG |
| AcsorA-F(RT) | CGCACTTCTTGACCTCCG |
| AcsorA-R(RT) | TTGGCACCGCCCACGAT |
| AcsorB-F(RT) | GCCATCCTGGGACCACT |
| AcsorB-R(RT) | TGAACACGCCGAGACAAC |
| AcsorC-F(RT) | TCGGGAAAGGGTACAAGGC |
| AcsorC-R(RT) | CTCGACGGACCGCAAGTT |
| AcsorD-F(RT) | TGATGGCAATTCCGTCTGG |
| AcsorD-R(RT) | GACTCGTTGAGGGCGTTCC |
| AcsorE-F(RT) | GGGCTCGTCCGTCTCGTCT |
| AcsorE-R(RT) | CCTCGGGCTGGGATTGAT |
| AcsorT-F(RT) | GTATTCTCGCGTCGTCTTC |
| AcsorT-R(RT) | TTCTTCTGCCCTGGTTCTT |
| AcsorR1-F(RT) | CGATGTGGACGACTTGAGG |
| AcsorR1-R(RT) | TCATACTGCGAGTCCTGTTAG |
| AcsorR2-F(RT) | GCTGACCAGTACCGCATCG |
| AcsorR2-R(RT) | GCCCCCCTAACGTCTAT |
| orf1-F(RT) | CGGGATTGTTCCAAGTCG |
| orf1-R(RT) | TCCACCAGGGTTGTGCC |
| orf2-F(RT) | CGGAGATAACAGGAAGGC |
| orf2-R(RT) | CCGCTAAGGCTAGGGTC |