

Supporting Information

Butenolides from the Coral-Derived Fungus *Aspergillus terreus* SCSIO41404

Qingyun Peng^{1,2,†}, Weihao Chen^{1,3,†}, Xiuping Lin³, Jiao Xiao⁴, Yonghong Liu,^{1,3,4} and Xuefeng Zhou^{1,3,*}

¹ Southern Marine Science and Engineering Guangdong Laboratory (Guangzhou), Guangzhou 511458, China; pengqingyun18@mails.ucas.ac.cn (Q.P.); chenweihao17@mails.ucas.ac.cn (W.C.); yonghongliu@scsio.ac.cn (Y.L.)

² Research Center for Deepsea Bioresources, Sanya, Hainan 572025, China;

³ CAS Key Laboratory of Tropical Marine Bio-resources and Ecology/Guangdong Key Laboratory of Marine Materia Medica, South China Sea Institute of Oceanology, Chinese Academy of Sciences, Guangzhou 510301, China; xiupinglin@hotmail.com (X.L.)

⁴ Wuya College of Innovation, Shenyang Pharmaceutical University, Shenyang 110016, China; xj110121@126.com (J.X.)

* Correspondence: xfzhou@scsio.ac.cn (X.Z.)

† These authors contributed equally to this work.

Contents

ITS sequence of the strain <i>Aspergillus terreus</i> SCSIO41404.....	3
Physicochemical data of 4–13.	3
Table S1. X-ray Crystallographic Data of 1.	7
Table S2. The primer sequences for the genes.	8
Figure S1. Experimental ECD spectrum of 3.	8
Figure S2. ¹ H NMR spectrum of 1 (CD ₃ OD, 700 MHz).	9
Figure S3. ¹³ C NMR spectrum of 1 (CD ₃ OD, 175 MHz).	9
Figure S4. DEPT spectrum of 1 (CD ₃ OD).	10
Figure S5. COSY spectrum of 1 (CD ₃ OD).	10
Figure S6. HSQC spectrum of 1 (CD ₃ OD).	11
Figure S7. HMBC spectrum of 1 (CD ₃ OD).	11
Figure S8. HRESIMS spectrum of 1.	12
Figure S9. UV spectrum of 1.	12
Figure S10. ¹ H NMR spectrum of 2 (CD ₃ OD, 700 MHz).	13
Figure S11. ¹³ C NMR spectrum of 2 (CD ₃ OD, 175 MHz).	13
Figure S12. DEPT spectrum of 2 (CD ₃ OD).	14
Figure S13. COSY spectrum of 2 (CD ₃ OD).	14

Figure S14. HSQC spectrum of 2 (CD ₃ OD).	15
Figure S15. HMBC spectrum of 2 (CD ₃ OD).	15
Figure S16. HRESIMS spectrum of 2	16
Figure S17. UV spectrum of 2	16
Figure S18. ¹ H NMR spectrum of 3 (CD ₃ OD, 700 MHz).	17
Figure S19. ¹³ C NMR spectrum of 3 (CD ₃ OD, 175 MHz).	17
Figure S20. DEPT spectrum of 3 (CD ₃ OD).	18
Figure S21. COSY spectrum of 3 (CD ₃ OD).	18
Figure S22. HSQC spectrum of 3 (CD ₃ OD).	19
Figure S23. HMBC spectrum of 3 (CD ₃ OD).	19
Figure S24. HRESIMS spectrum of 3	20
Figure S25. UV spectrum of 3	20
Figure S26. ¹ H NMR spectrum of 4 (DMSO- <i>d</i> ₆ , 700 MHz).	21
Figure S27. ¹ H NMR spectrum of 5 (CD ₃ OD, 700 MHz).	21
Figure S28. ¹ H NMR spectrum of 6 (CD ₃ OD, 700 MHz).	22
Figure S29. ¹ H NMR spectrum of 7 (CD ₃ OD, 700 MHz).	22
Figure S30. ¹ H NMR spectrum of 8 (CD ₃ OD, 700 MHz).	23
Figure S31. ¹ H NMR spectrum of 9 (CD ₃ OD, 700 MHz).	23
Figure S32. ¹ H NMR spectrum of 10 (CDCl ₃ , 700 MHz).	24
Figure S33. ¹ H NMR spectrum of 11 (CD ₃ OD, 700 MHz).	24
Figure S34. ¹ H NMR spectrum of 12 (CD ₃ OD, 700 MHz).	25
Figure S35. ¹ H NMR spectrum of 13 (CD ₃ OD, 700 MHz).	25
Figure S36. ¹ H NMR spectrum of 14 (CD ₃ OD, 700 MHz).	26
Figure S37. ¹³ C NMR spectrum of 14 (CD ₃ OD, 175 MHz).	26
Figure S38. DEPT spectrum of 14 (CD ₃ OD).	27
Figure S39. COSY spectrum of 14 (CD ₃ OD).	27
Figure S40. HSQC spectrum of 14 (CD ₃ OD).	28
Figure S41. HMBC spectrum of 14 (CD ₃ OD).	28
Figure S42. HRESIMS spectrum of 14	29
Figure S43. UV spectrum of 14	29

ITS sequence of the strain *Aspergillus terreus* SCSIO41404.

GGTAAAGCGCTGGTCTTATGGCCACCTCCCACCCGTGACTATTGTACCTTGT
TGCTTCGGCGGGCCCGCCAGCGTTGCTGGCCGCCGGGGCGACTCGCC
CCCGGGCCCGTGCCTGCCGGAGACCCAACATGAACCTGTTCTGAAAGC
TTGCAGTCTGAGTGTGATTCTTGCAATCAGTTAAAACCTTCAACAATGGAT
CTCTGGTTCCGGCATCGATGAAGAACGCAGCGAAATGCGATAACTAATGT
GAATTGCAGAATTCACTGAGTGAATCATCGAGTCTTGAACGCACATTGCGCCCC
CTGGTATTCCGGGGGCATGCCGTCCGAGCGTCATTGCTGCCCTCAAGCC
CGGCTTGTGTGTTGGGCCCTCGTCCCCGGCTCCGGGGACGGGCCGA
AAGGCAGCGCGGCACCGCGTCCGGCTCGAGCGTATGGGGCTCGTCT
TCCGCTCCGTAGGCCCGGCCGCCGACGCATTATTGCAACTTG
TTTTTTTTCCAGGTTGACCTCGGATCAGGTAGGGATAACCGCTGAACTTAA
GCATATCAATAAGCGGAGGAA

Physicochemical data of 4–13.

Butyrolactone II (**4**): yellow oil; $[\alpha]_D^{20} = +30.5$ (*c* 0.1, MeOH); ^1H NMR (700 MHz, DMSO-*d*₆) δ_H 10.57 (1H, s, 2-OH), 9.95 (1H, s, 4'-OH), 9.22 (1H, s, 4"-OH), 7.49 (2H, d, *J* = 8.7 Hz, H-2', H-6'), 6.85 (2H, d, *J* = 8.7 Hz, H-3', H-5'), 6.56 (2H, d, *J* = 8.5 Hz, H-2'', H-6''), 6.48 (2H, d, *J* = 8.5 Hz, H-3'', H-5''), 3.71 (3H, s, 5-OCH₃), 3.37 (2H, d, *J* = 9.7 Hz, H-6); ^{13}C NMR (175 MHz, DMSO-*d*₆) δ_C 169.8 (qC, C-5), 167.9 (qC, C-1), 157.9 (qC, C-4'), 156.3 (qC, C-4''), 138.1 (qC, C-2), 131.2 (CH, C-2'', C-6''), 128.8 (CH, C-2', C-6'), 127.5 (qC, C-3), 123.2 (qC, C-1''), 121.0 (qC, C-1'), 115.9 (CH, C-3', C-5'), 114.6 (CH, C-3'', C-5''), 84.7 (qC, C-4), 53.5 (CH₃, 5-OCH₃), 38.0 (CH₂, C-6).

Methyl (*R*)-2-benzyl-4-hydroxy-3-(4-hydroxyphenyl)-5-oxo-2,5-dihydrofuran-2-carboxylate (**5**): yellow oil; $[\alpha]_D^{25} = +65.6$ (*c* 0.1, MeOH); ^1H NMR (700 MHz, CD₃OD) δ_H 7.58 (2H, d, *J* = 8.8 Hz, H-2', H-6'), 7.13 (1H, t, *J* = 7.3 Hz, H-4''), 7.09 (2H, t, *J* = 7.3 Hz, H-3'', H-5''), 6.87 (2H, d, *J* = 8.8 Hz, H-3', H-5'), 6.83 (2H d, *J* = 7.3 Hz, H-2'', H-6''), 3.79 (3H, s, 5-OCH₃), 3.56 (2H, s, H-6); ^{13}C NMR (175 MHz, CD₃OD) δ_C 171.4 (qC, C-5) 170.1 (qC, C-1), 159.4 (qC, C-4'), 139.7 (qC, C-2), 134.7 (qC, C-1''), 131.5 (CH, C-2', C-6'), 130.3 (CH, C-2'', C-6''), 129.0 (qC, C-3), 128.8 (CH, C-3'', C-5''), 128.1 (CH, C-4''), 123.0 (qC, C-1'), 116.6 (CH, C-3', C-5'), 86.5 (qC, C-4), 53.9 (CH₃, 5-OCH₃), 40.2 (CH₂, C-6).

Butyrolactone I (**6**): yellow oil; $[\alpha]_D^{20} = +64.0$ (*c* 0.2, MeOH); ^1H NMR (700 MHz, CD₃OD) δ_H 7.59 (2H, d, *J* = 8.8 Hz, H-2', H-6'), 6.87 (2H, d, *J* = 8.8 Hz, H-3', H-5'), 6.54 (1H, dd, *J* = 8.2, 2.1 Hz, H-6''), 6.50 (1H, d, *J* = 8.2 Hz, H-5''), 6.41 (1H, d,

$J = 2.1$ Hz, H-2''), 5.06 (1H, m, H-8''), 3.78 (3H, s, 5-OCH₃), 3.45 (1H, d, $J = 14.8$ Hz, H_a-6), 3.41 (1H, d, $J = 14.8$ Hz, H_b-6), 3.07 (2H, m, H-7''), 1.67 (3H, br s, H-11''), 1.57 (3H, br s, H-10''); ¹³C NMR (175 MHz, CD₃OD) δ _C 171.6 (qC, C-5), 170.4 (qC, C-1), 159.3 (qC, C-4'), 155.1 (qC, C-4''), 139.7 (qC, C-2), 133.0 (qC, C-9''), 132.4 (CH, C-2''), 130.4 (CH, C-2', C-6'), 129.8 (CH, C-6''), 129.1 (qC, C-3), 128.4 (qC, C-3''), 125.1 (qC, C-1''), 123.6 (CH, C-8''), 123.2 (qC, C-1'), 116.6 (CH, C-3', C-5'), 115.0 (CH, C-5''), 86.8 (qC, C-4), 53.8 (CH₃, 5-OCH₃), 39.6 (CH₂, C-6), 28.7 (CH₂, C-7''), 26.0 (CH₃, C-11), 17.8 (CH₃, C-10'').

Versicolactone B (**7**): white powder; $[\alpha]_D^{25} = +67.7$ (*c* 0.1, MeOH); ¹H NMR (700 MHz, CD₃OD) δ _H 7.70 (2H, d, $J = 7.5$ Hz, H-2', H-6'), 7.46 (2H, t, $J = 7.5$ Hz, H-3', H-5'), 7.38 (1H, t, $J = 7.5$ Hz, H-4'), 6.51 (1H, dd, $J = 8.2, 2.0$ Hz, H-6''), 6.49 (1H, d, $J = 8.2$ Hz, H-5''), 6.40 (1H, d, $J = 2.0$ Hz, H-2''), 5.06 (1H, m, H-8''), 3.79 (3H, s, 5-OCH₃), 3.45 (2H, br s, H-6), 3.07 (2H, m, H-7''), 1.65 (3H, br s, H-11''), 1.57 (3H, br s, H-10''); ¹³C NMR (175 MHz, CD₃OD) δ _C 171.5 (qC, C-5), 169.9 (qC, C-1), 155.2 (qC, C-4''), 141.9 (qC, C-2), 132.9 (qC, C-9''), 132.4 (CH, C-2''), 131.9 (CH, C-2', C-6'), 129.8 (CH, C-3', C-5', C-6''), 129.7 (qC, C-3), 128.6 (CH, C-4'), 128.5 (qC, C-3''), 128.0 (qC, C-1'), 125.0 (qC, C-1''), 123.6 (CH, C-8''), 115.1 (CH, C-5''), 86.9 (qC, C-4), 53.9 (CH₃, 5-OCH₃), 39.5 (CH₂, C-6), 28.8 (CH₂, C-7''), 26.0 (CH₃, C-11), 17.8 (CH₃, C-10'').

Aspernolide D (**8**): white powder; $[\alpha]_D^{25} = +61.3$ (*c* 0.1, MeOH); ¹H NMR (700 MHz, CD₃OD) δ _H 7.58 (2H, d, $J = 8.7$ Hz, H-2', H-6'), 6.87 (2H, d, $J = 8.7$ Hz, H-3', H-5'), 6.50 (1H, dd, $J = 8.1, 1.9$ Hz, H-6''), 6.48 (1H, d, $J = 8.1$ Hz, H-5''), 6.47 (1H, d, $J = 1.9$ Hz, H-2''), 5.39 (1H, m, H-8''), 3.91 (2H, br s, H-10''), 3.78 (3H, s, 5-OCH₃), 3.45 (1H, d, $J = 14.6$ Hz, H_a-6), 3.41 (1H, d, $J = 14.6$ Hz, H_b-6), 3.15 (2H, d, $J = 7.4$ Hz, H-7''), 1.65 (3H, br s, H-11''); ¹³C NMR (175 MHz, CD₃OD) δ _C 171.6 (qC, C-5), 170.4 (qC, C-1), 159.4 (qC, C-4'), 155.2 (qC, C-4''), 139.8 (qC, C-2), 136.3 (qC, C-9''), 132.7 (CH, C-2''), 130.4 (CH, C-2', C-6'), 129.9 (CH, C-6''), 129.2 (qC, C-3), 127.9 (qC, C-3''), 125.3 (CH, C-8''), 125.2 (qC, C-1''), 123.2 (qC, C-1'), 116.6 (CH, C-3', C-5'), 115.1 (CH, C-5''), 86.9 (qC, C-4), 69.1 (CH₂, C-10''), 53.9 (CH₃, 5-OCH₃), 39.5 (CH₂, C-6), 28.6 (CH₂, C-7''), 13.8 (CH₃, C-11).

Aspernolide A (**9**): yellow oil; $[\alpha]_D^{25} = +38.6$ (*c* 0.1, MeOH); ¹H NMR (700 MHz, CD₃OD) δ _H 7.56 (2H, d, $J = 8.9$ Hz, H-2', H-6'), 6.87 (2H, d, $J = 8.9$ Hz, H-3', H-5'), 6.51 (1H, dd, $J = 8.3, 2.1$ Hz, H-6''), 6.48 (1H, d, $J = 2.1$ Hz, H-2''), 6.43 (1H, d, $J = 8.3$ Hz, H-5''), 3.79 (3H, s, 5-OCH₃), 3.44 (2H, s, H-6), 2.58 (2H, m, H-7''), 1.72 (2H,

t , $J = 6.8$ Hz, H-8''), 1.25(3H, s, H-11''), 1.24 (3H, s, H-10''); ^{13}C NMR (175 MHz, CD₃OD) δ_{C} 171.5 (qC, C-5), 170.3 (qC, C-1), 159.4 (qC, C-4'), 154.3 (qC, C-4''), 139.7 (qC, C-2), 132.6 (CH C-2''), 130.4 (CH, C-2', C-6'), 130.2 (CH, C-6''), 129.3 (qC, C-3), 125.5 (qC, C-3''), 123.1 (qC, C-1''), 121.4 (qC, C-1'), 117.4 (CH, C-5''), 116.6 (CH, C-3', C-5'), 86.8 (qC, C-4), 75.1 (qC, C-9''), 53.9 (CH₃, 5-OCH₃), 39.6 (CH₂, C-6), 33.7 (CH₂, C-8''), 27.0 (CH₃, C-10''), 26.9 (CH₃, C-11''), 23.2 (CH₂, C-7'').

Butyrolactone V (**10**): yellow oil; $[\alpha]_{\text{D}}^{20} = +70.0$ (c 0.1, MeOH); ^1H NMR (700 MHz, CDCl₃) δ_{H} 7.59 (2H, d, $J = 8.6$ Hz, H-2', H-6'), 6.90 (2H, d, $J = 8.6$ Hz, H-3', H-5'), 6.59 (1H, br s, H-2''), 6.54 (2H, overlapped, H-5'', H-6''), 3.78 (3H, s, 5-OCH₃), 3.76 (1H, t, $J = 4.9$ Hz, H-8''), 3.54 (1H, d, $J = 14.8$ Hz, H_a-6), 3.45 (1H, d, $J = 14.8$ Hz, H_b-6), 2.87 (1H, dd, $J = 16.8, 4.9$ Hz, H_a-7''), 2.62 (1H, dd, $J = 16.8, 4.9$ Hz, H_b-7''), 1.31(3H, s, H-10''), 1.24 (3H, s, H-11''); ^{13}C NMR (175 MHz, CDCl₃) δ_{C} 169.9 (qC, C-5), 169.4 (qC, C-1), 156.7 (qC, C-4'), 152.1 (qC, C-4''), 137.5 (qC, C-2), 132.2 (CH C-2''), 129.8 (CH, C-6''), 129.7 (CH, C-2', C-6'), 128.3 (qC, C-3), 124.9 (qC, C-1''), 122.4 (qC, C-1'), 118.3 (qC, C-3''), 116.9 (CH, C-5''), 116.2 (CH, C-3', C-5'), 86.1 (qC, C-4), 76.9 (qC, C-9''), 69.8 (CH, C-8''), 53.7 (CH₃, 5-OCH₃), 38.8 (CH₂, C-6), 31.2 (CH₂, C-7''), 24.8 (CH₃, C-10''), 22.5 (CH₃, C-11'').

Terrelactone (**11**): yellow oil; $[\alpha]_{\text{D}}^{25} = +54.1$ (c 0.1, MeOH); ESIMS m/z 465.5 [M + Na]⁺; ^1H NMR (700 MHz, CD₃OD) δ_{H} 7.58 (2H, d, $J = 8.8$ Hz, H-2', H-6'), 6.87 (2H, d, $J = 8.8$ Hz, H-3', H-5'), 6.50 (1H, dd, $J = 8.1, 2.1$ Hz, H-6''), 6.48 (1H, d, $J = 8.1$ Hz, H-5''), 6.45 (1H, d, $J = 2.1$ Hz, H-2''), 3.79 (3H, s, 5-OCH₃), 3.45 (1H, d, $J = 14.7$ Hz, H_a-6), 3.41 (1H, d, $J = 14.7$ Hz, H_b-6), 2.49 (1H, m, H_a-7''), 2.40 (1H, m, H_b-7''), 1.53 (2H, m, H-8''), 1.20 (3H, s, H-10''), 1.19 (3H, s, H-11''); ^{13}C NMR (175 MHz, CD₃OD) δ_{C} 171.6 (qC, C-5), 170.4 (qC, C-1), 159.4 (qC, C-4'), 155.2 (qC, C-4''), 139.7 (qC, C-2), 132.9 (CH, C-2''), 130.4 (CH, C-2', C-6'), 129.7 (CH, C-6''), 129.6 (qC, C-3), 129.2 (qC, C-3''), 125.2 (qC, C-1''), 123.2 (qC, C-1'), 116.6 (CH, C-3', C-5'), 115.2 (CH, C-5''), 86.9 (qC, C-4), 71.5 (qC, C-9''), 53.9 (CH₃, 5-OCH₃), 44.7 (CH₂, C-8''), 39.5 (CH₂, C-6), 29.3 (CH₃, C-11''), 29.0 (CH₃, C-10''), 25.8 (CH₂, C-7'').

Butyrolactone VI (**12**): white solid; $[\alpha]_{\text{D}}^{25} = +38.2$ (c 0.1, MeOH); ^1H NMR (700 MHz, CD₃OD): δ_{H} 7.58 (2H, d, $J = 8.9$ Hz, H-2', H-6'), 6.87 (2H, d, $J = 8.9$ Hz, H-3', H-5'), 6.61 (1H, d, $J = 2.0$ Hz, H-2''), 6.52 (1H, d, $J = 8.2$ Hz, H-5''), 6.49 (1H, dd, $J = 8.2, 2.0$ Hz, H-6''), 3.79 (3H, s, 5-OCH₃), 3.45 (2H, s, H-6), 3.44 (1H, m, H-8''), 2.68

(1H, dd, $J = 14.1, 2.2$ Hz, H_a-7''), 2.54 (1H, dd, $J = 14.1, 10.0$ Hz, H_b-7''), 1.18 (3H, s, H-10''), 1.17 (3H, s, H-11''); ¹³C NMR (175 MHz, CD₃OD) δ_C 171.6 (qC, C-5), 170.4 (qC, C-1), 159.4 (qC, C-4'), 155.9 (qC, C-4''), 139.8 (qC, C-2), 134.3 (CH, C-2''), 130.5 (CH C-6''), 130.4 (CH, C-2', C-6'), 129.3 (qC, C-3), 127.3 (qC, C-3''), 125.5 (qC, C-1''), 123.1 (qC, C-1'), 116.6 (CH, C-3', C-5'), 115.9 (CH, C-5''), 86.8 (qC, C-4), 80.6 (CH, C-8''), 73.8 (qC, C-9''), 53.9 (CH₃, 5-OCH₃), 39.5 (CH₂, C-6), 34.0 (CH₂, C-7''), 25.5 (CH₃, C-10''), 25.1 (CH₃, C-11'').

Butyrolactone IV (**13**): yellow oil; $[\alpha]_D^{20} = +40.0$ (*c* 0.1, MeOH); ¹H NMR (700 MHz, CD₃OD) δ_H 7.58 (2H, d, $J = 8.9$ Hz, H-2', H-6'), 6.87 (2H, d, $J = 8.9$ Hz, H-3', H-5'), 6.61 (1H, br s, H-2''), 6.54 (1H, dd, $J = 8.2, 1.6$ Hz, H-6''), 6.46 (1H, d, $J = 8.2$ Hz, H-5''), 4.50 (1H, dd, $J = 9.4, 8.5$ Hz, H-8''), 3.79 (3H, s, 5-OCH₃), 3.47 (2H, s, H-6), 3.03 (1H, dd, $J = 15.8, 8.5$ Hz, H_a-7''), 2.97 (1H, dd, $J = 15.8, 9.4$ Hz, H_b-7''), 1.19 (3H, s, H-10''), 1.16 (3H, s, H-11''); ¹³C NMR (175 MHz, CD₃OD) δ_C 171.5 (qC, C-5), 170.2 (qC, C-1), 160.5 (qC, C-4''), 159.4 (qC, C-4'), 139.7 (qC, C-2), 131.0 (CH, C-6''), 130.4 (CH, C-2', C-6'), 129.1 (qC, C-3), 128.1 (qC, C-3''), 127.9 (CH C-2''), 126.2 (qC, C-1''), 123.1 (qC, C-1'), 116.6 (CH, C-3', C-5'), 109.1 (CH, C-5''), 90.4 (CH, C-8''), 86.8 (qC, C-4), 72.5 (qC, C-9''), 53.9 (CH₃, 5-OCH₃), 39.7 (CH₂, C-6), 31.3 (CH₂, C-7''), 25.3 (CH₃, C-10''), 25.2 (CH₃, C-11'').

Table S1. X-ray crystallographic data for **1**

Empirical formula	C ₁₆ H ₁₂ O ₄
Formula weight	269.08
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2/c
a/Å	23.6601(13)
b/Å	5.4446(3)
c/Å	21.0558(17)
α/°	90
β/°	99.555(7)
γ/°	90
Volume/Å ³	2674.8(3)
Z	4
ρ _{calc} g/cm ³	1.412
μ/mm ⁻¹	0.856
F(000)	1192.0
Crystal size/mm ³	0.4 × 0.1 × 0.05
Radiation	CuKα ($\lambda = 1.54184$)
2Θ range for data collection/°	8.518 to 148.942
Index ranges	-29 ≤ h ≤ 28, -6 ≤ k ≤ 6, -7 ≤ l ≤ 26
Reflections collected	5257
Independent reflections	5257 [R _{int} = ?, R _{sigma} = 0.0622]
Data/restraints/parameters	5257/0/389
Goodness-of-fit on F ²	1.061
Final R indexes [I>=2σ (I)]	R ₁ = 0.1083, wR ₂ = 0.2959
Final R indexes [all data]	R ₁ = 0.1280, wR ₂ = 0.3097
Largest diff. peak/hole / e Å ⁻³	0.62/-0.48

Table S2. The primer sequences for the genes.

Gene	Forward(5'-3' sequence)	Reverse (5'-3' sequence)
GAPDH	GCTCTCTGCTCCTCCTGTTC	ACGACCAAATCCGTTGACTC
LXR α	TCAGCATCTTCTCTGCAGACCGG	TCATTAGCATCCGTGGAAACA
ABCA1	ACCCACCCTATGAACAAACATGA	GAGTCGGGTAACGGAAACAGG
UGT1A1	CATGCTGGGAAGATACTGTTGAT	GCCCAGAGACTAACAAAAGACTCT
TNF α	CAAGCCTGTAGCCCATGTTGTA	ACCAGCTGGTTATCTCTCAGCT
CXCL10	GTGGCATTCAAGGAGTACCTC	TGATGGCCTTCGATTCTGGATT
CYP3A5	AATGTTTGTCCTATCGTCAGGG	AGACCTTCGATTGTGAAGACAG
CYP3A7	AAACTTGGCCGTGGAAACCT	CAGCATAAGGCTGTTGACAGTC
ALDH3A1	CTCTGTGACCCCTCGATCCA	GCATCTTCCCCGTAGAACTCTT
UGT2B10	GAAATGGACTACAGTTCTGCTGA	GTGGATGAGTCGTTGGATCA
CYP1A1	TCGGCCACGGAGTTCTTC	GGTCAGCATGTGCCAATCA
GSTA2	TACTCCAATATACGGGGCAGAA	TCCTCAGGTTGACTAAAGGGC
gapdh	CTTGGCATTGTGGAAGGGC	TGCAGGGATGATGTTCTGGG
Il6	TAGTCCTTCCTACCCCAATTCC	TTGGTCCTTAGCCACTCCTTC
Cxcl10	CTCATCCTGCTGGGTCTGAG	CCTATGGCCCTCATTCTCAC
Bcl2	GCTACCGTCGTGACTTCGC	CCCCACCGAACTCAAAGAAGG
Bax	AGACAGGGGCCTTTGCTAC	AATTGCCCCGAGACACTCG
Pcna	TTGCACGTATATGCCGAGACC	GGTGAACAGGCTATTCTCATCT
Tnf α	GACGTGGAACTGGCAGAAGAG	TTGGTGGTTGTGAGTGTGAG
Ccl2	CCTGCTGTTCACAGTTGCC	ATTGGGATCATCTGCTGGT
Lx α	AGGAGTGTGACTTCGCAAA	CTCTTCTGCCGTTCAAGTT

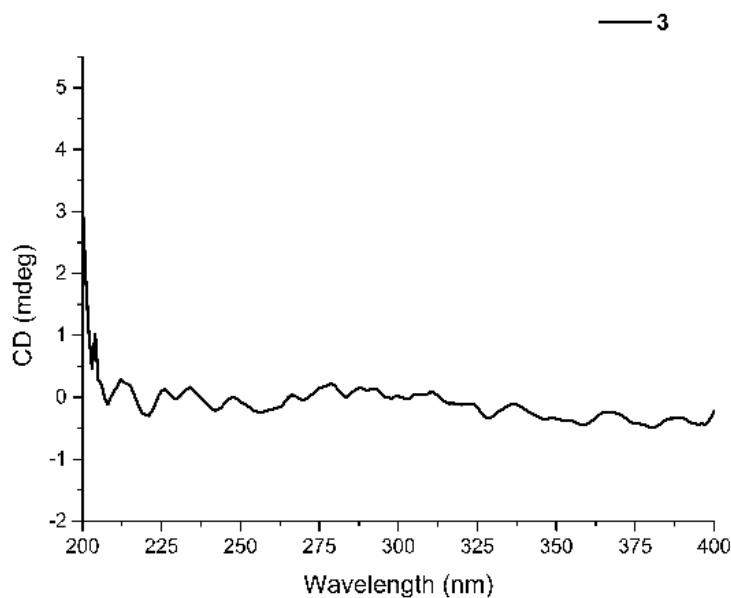


Figure S1. Experimental ECD spectrum of **3**.

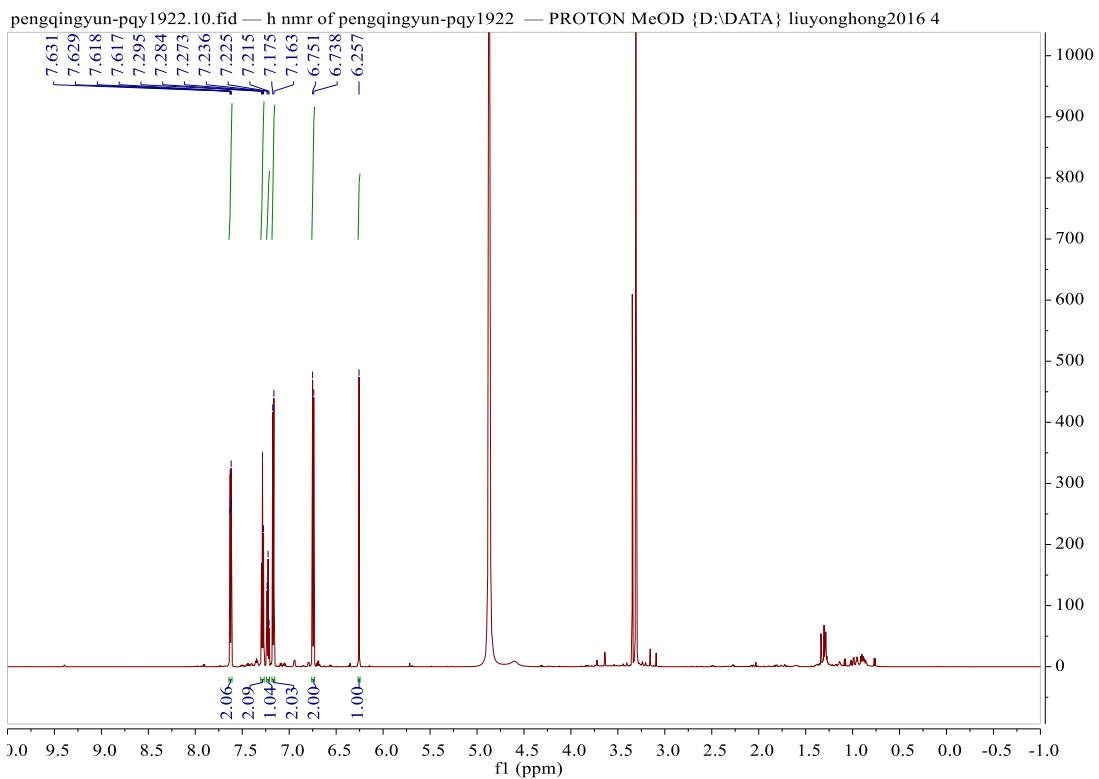


Figure S2. ^1H NMR spectrum of **1** (CD_3OD , 700 MHz)

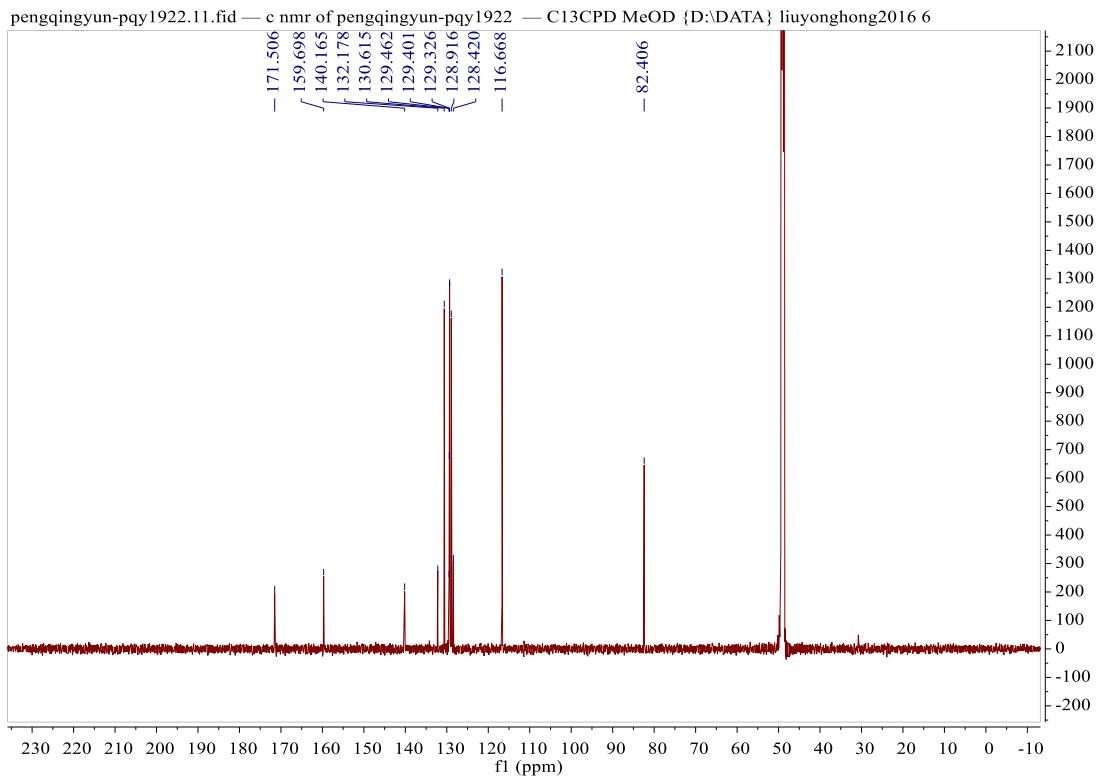


Figure S3. ^{13}C NMR spectrum of **1** (CD_3OD , 175 MHz).

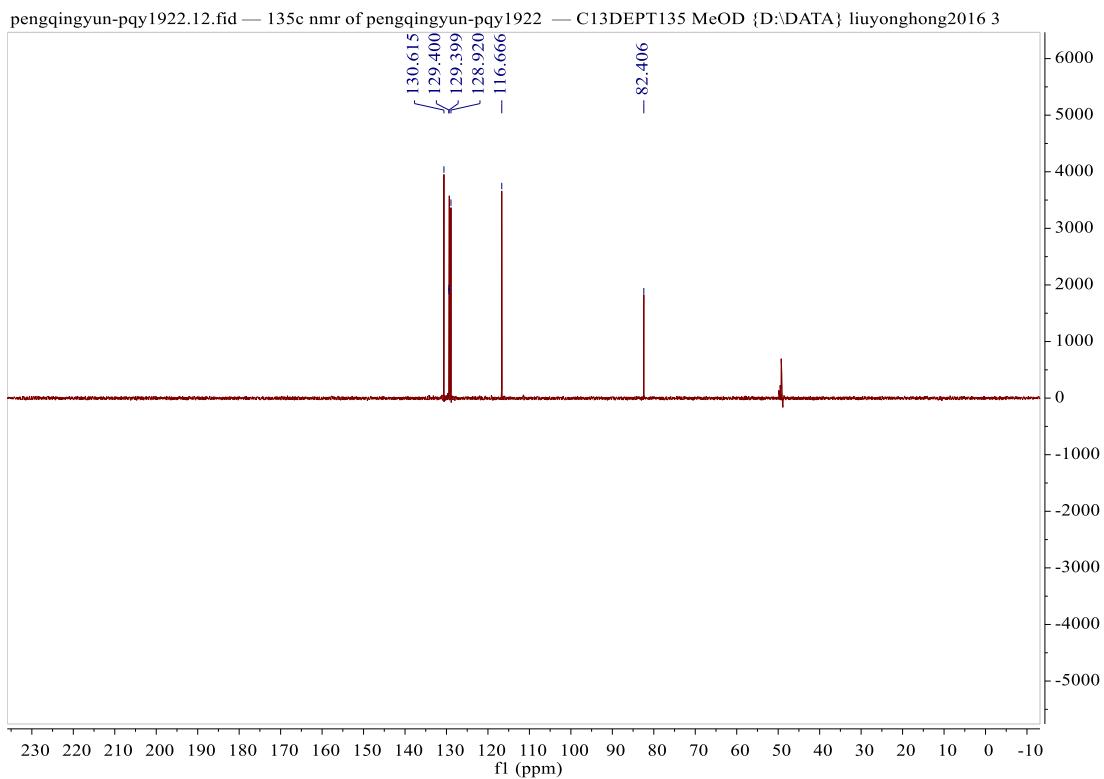


Figure S4. DEPT spectrum of **1** (CD_3OD).

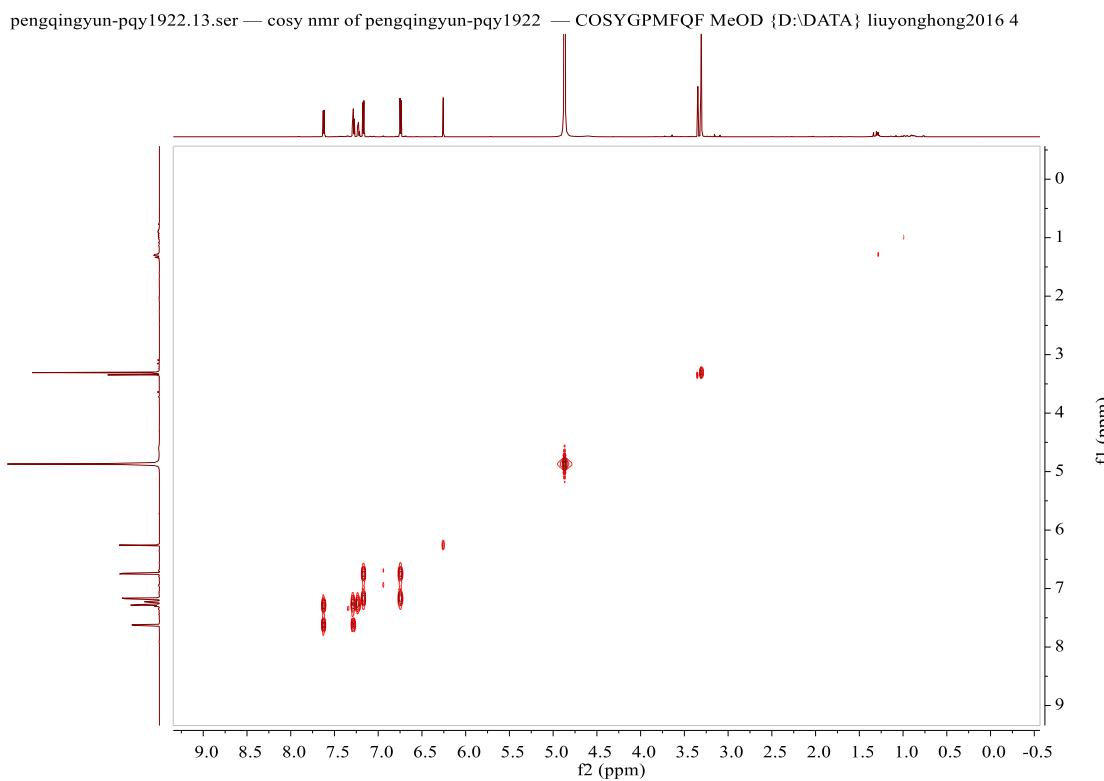


Figure S5. COSY spectrum of **1** (CD_3OD).

pengqingyun-pqy1922.15.ser — qc nmr of pengqingyun-pqy1922 — HSQCEDETGP MeOD {D:\DATA} liuyonghong2016 4

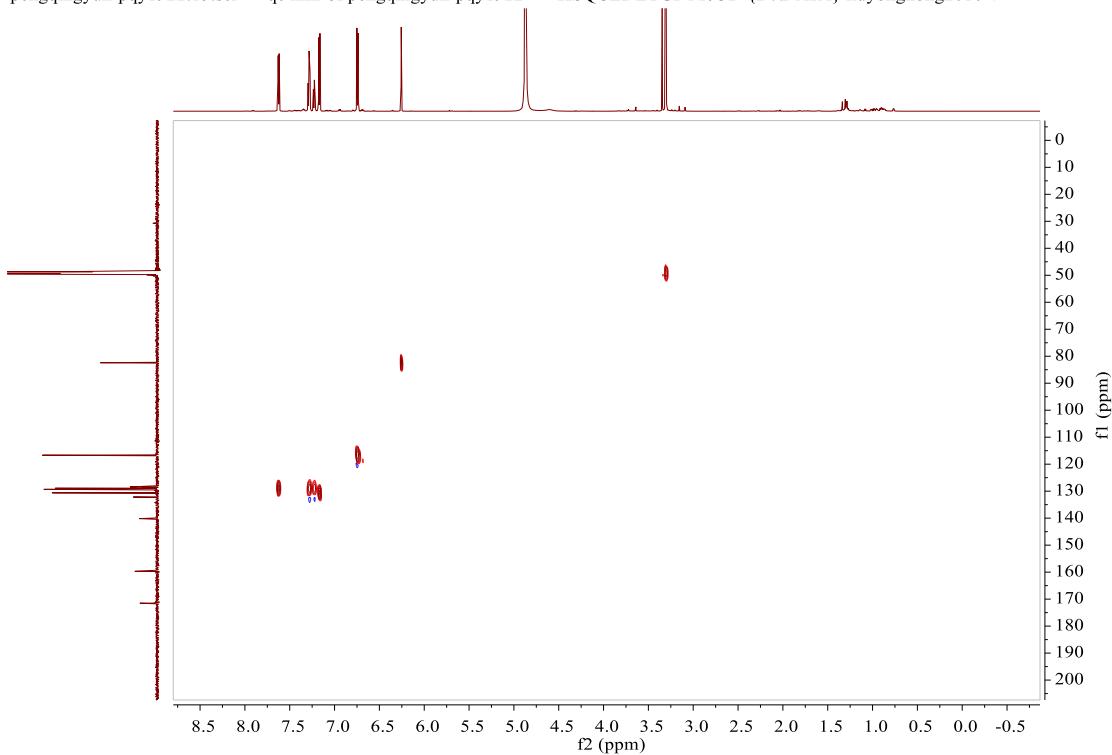


Figure S6. HSQC spectrum of **1** (CD_3OD).

pengqingyun-pqy1922.16.ser — bc nmr of pengqingyun-pqy1922 — hmbcetgpl3nd MeOD {D:\DATA} liuyonghong2016 4

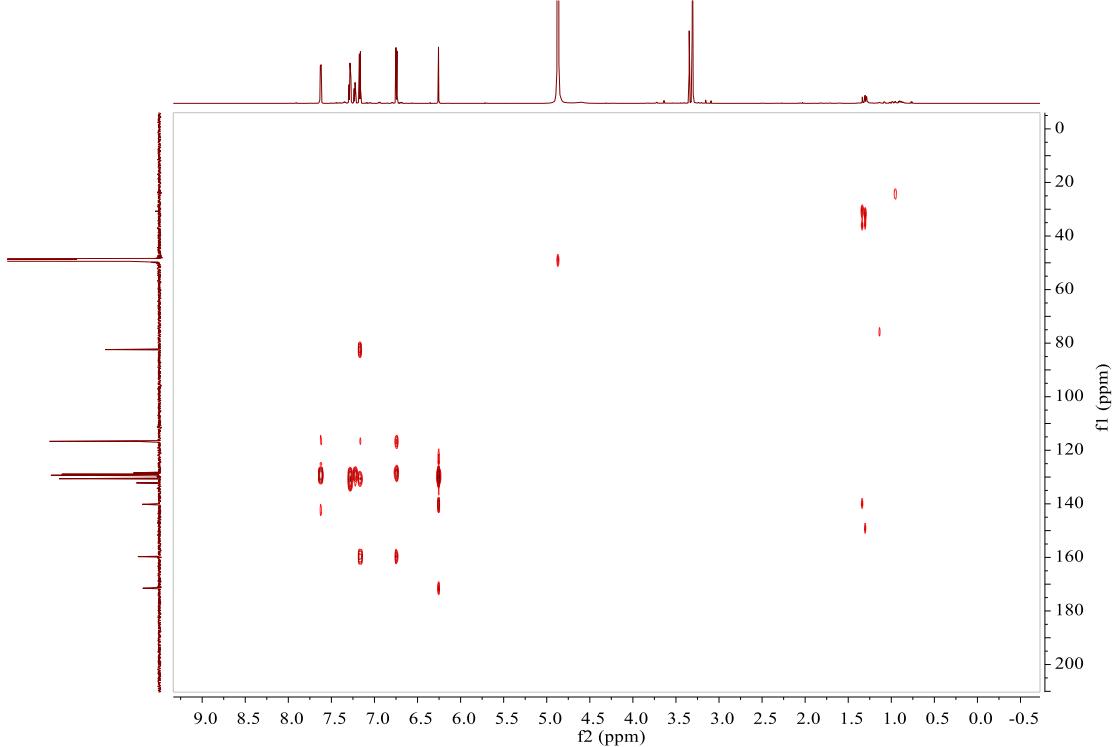


Figure S7. HMBC spectrum of **1** (CD_3OD).

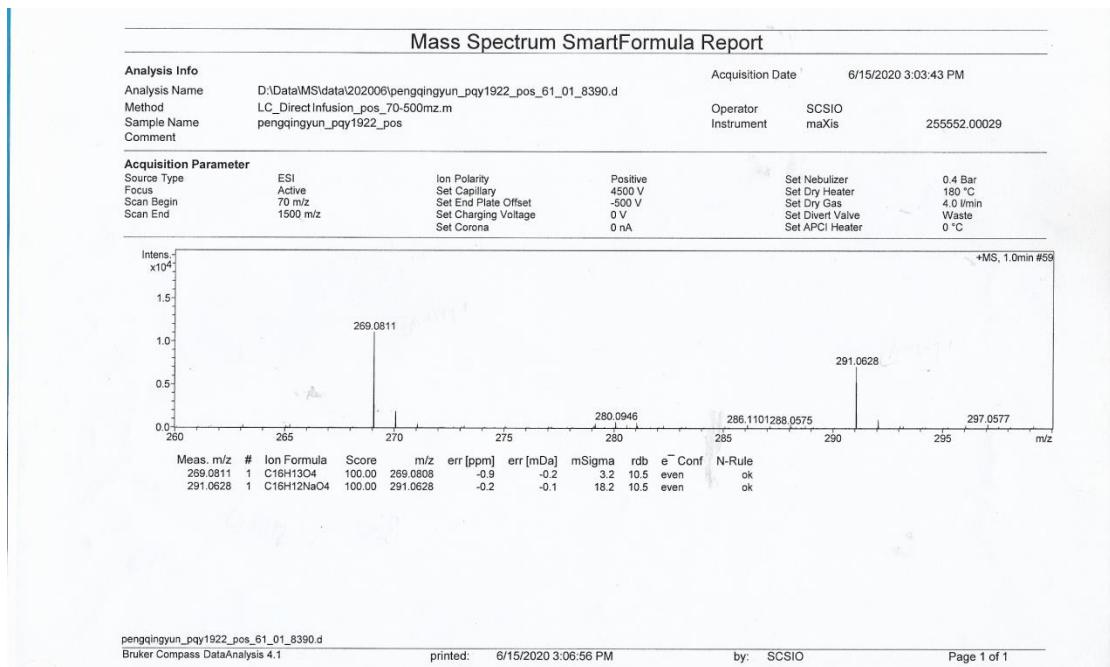


Figure S8. HRESIMS spectrum of **1**.

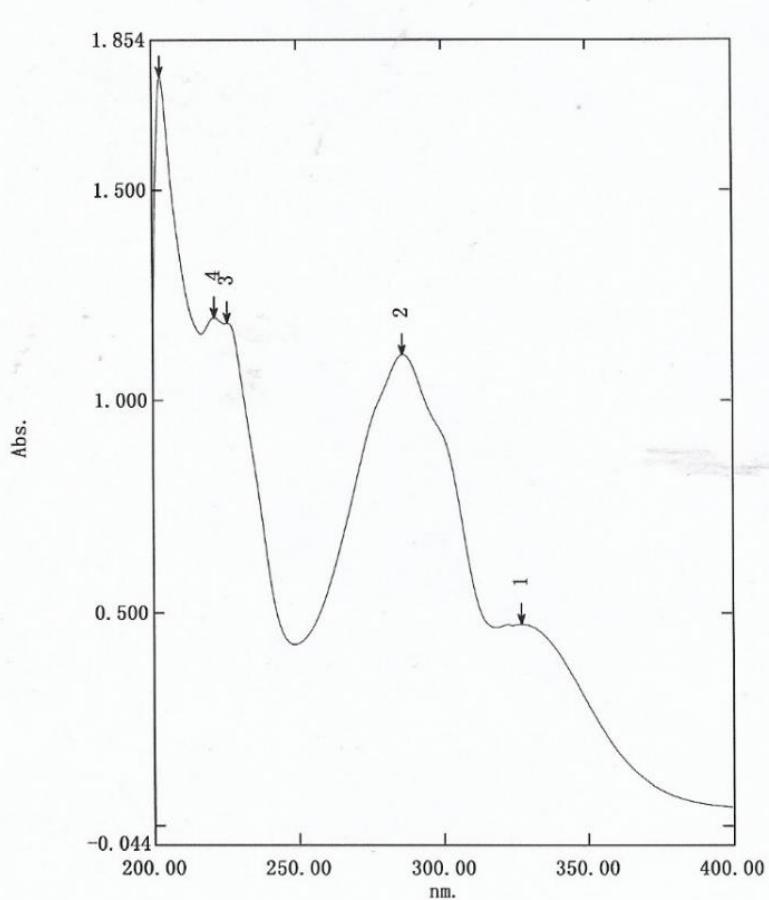


Figure S9. UV spectrum of **1**.

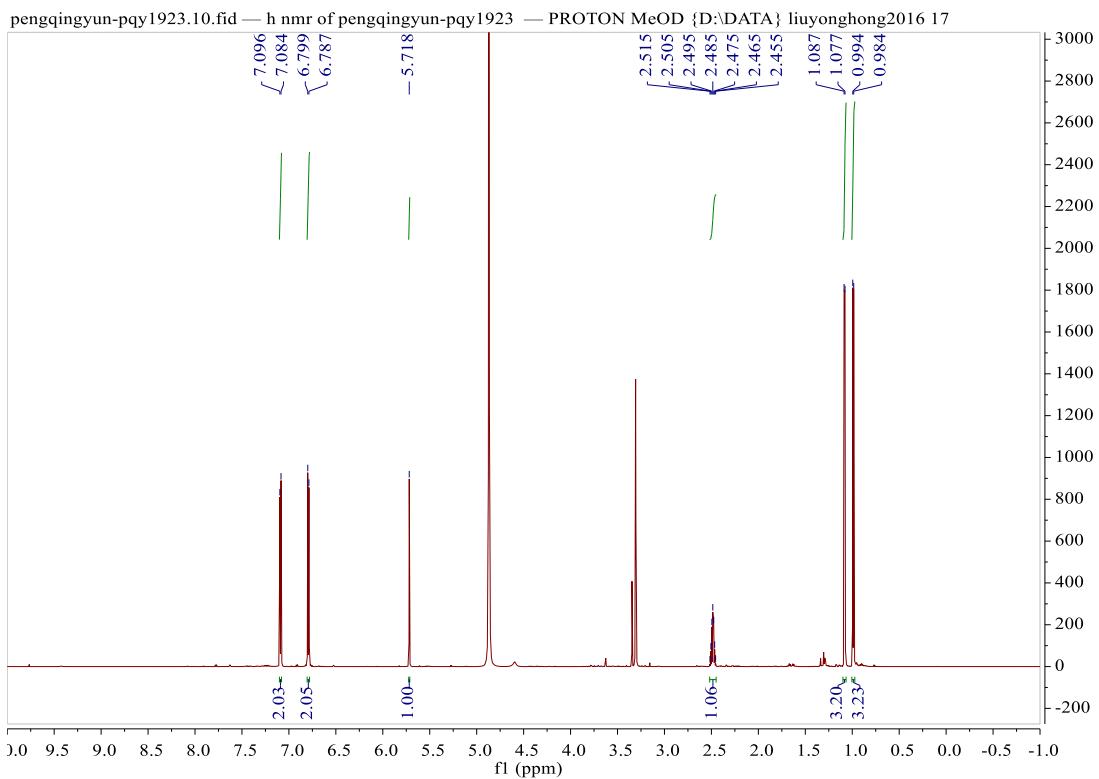


Figure S10. ^1H NMR spectrum of **2** (CD_3OD , 700 MHz).

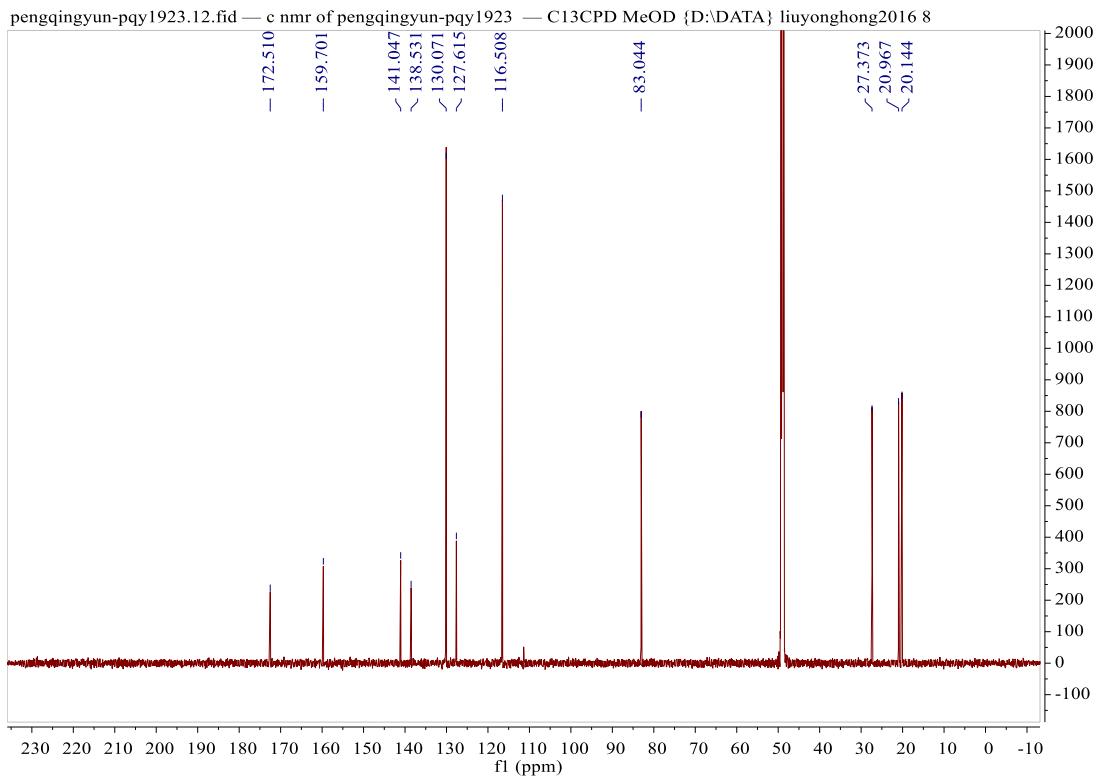


Figure S11. ^{13}C NMR spectrum of **2** (CD_3OD , 175 MHz).

pengqingyun-pqy1923.17.fid — 135c nmr of pengqingyun-pqy1923 — C13DEPT135 MeOD {D:\DATA} liuyonghong2016 14

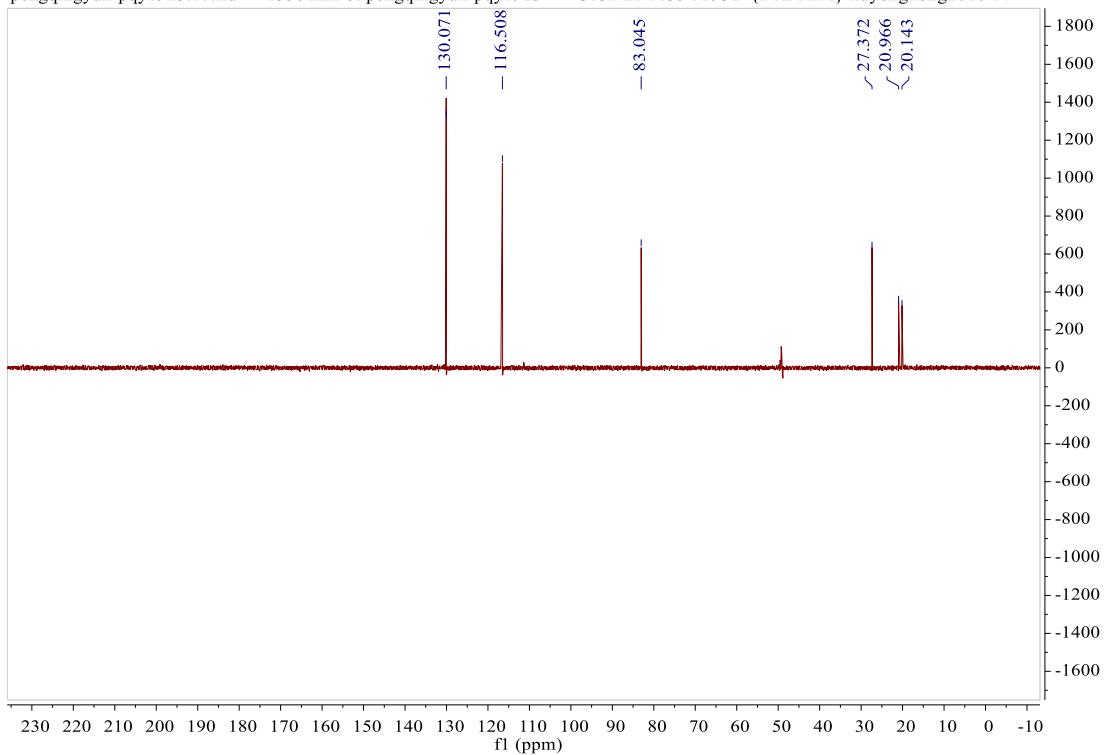


Figure S12. DEPT spectrum of **2** (CD_3OD).

pengqingyun-pqy1923.13.ser — cosy nmr of pengqingyun-pqy1923 — COSYGPMFQF MeOD {D:\DATA} liuyonghong2016 13

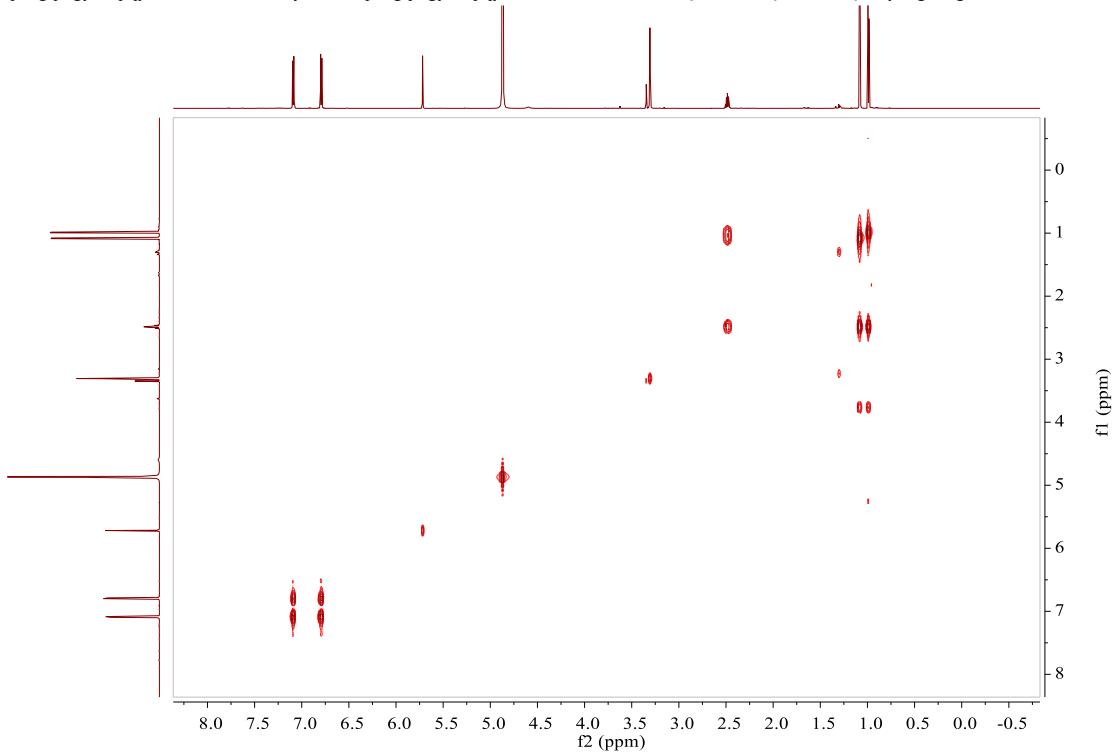


Figure S13. COSY spectrum of **2** (CD_3OD).

pengqingyun-pqy1923.15.ser — qc nmr of pengqingyun-pqy1923 — HSQCETGP MeOD {D:\DATA} liuyonghong2016 13

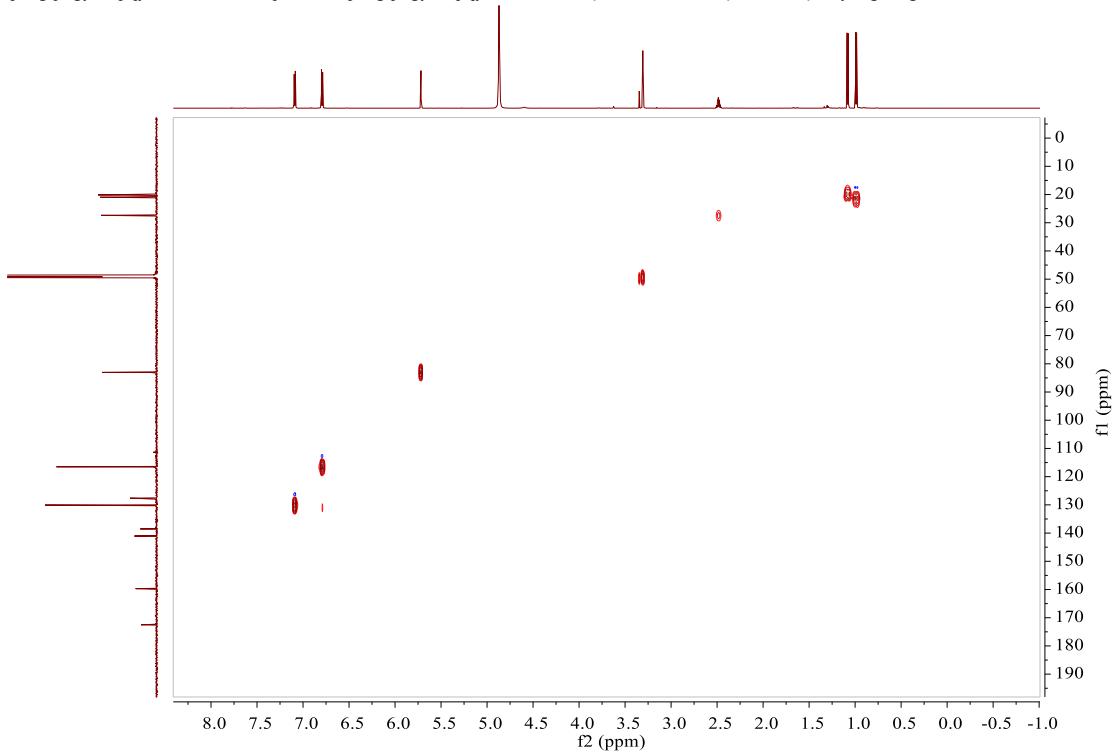


Figure S14. HSQC spectrum of **2** (CD_3OD).

pengqingyun-pqy1923.16.ser — bc nmr of pengqingyun-pqy1923 — HMBCETGPL3ND MeOD {D:\DATA} liuyonghong2016 13

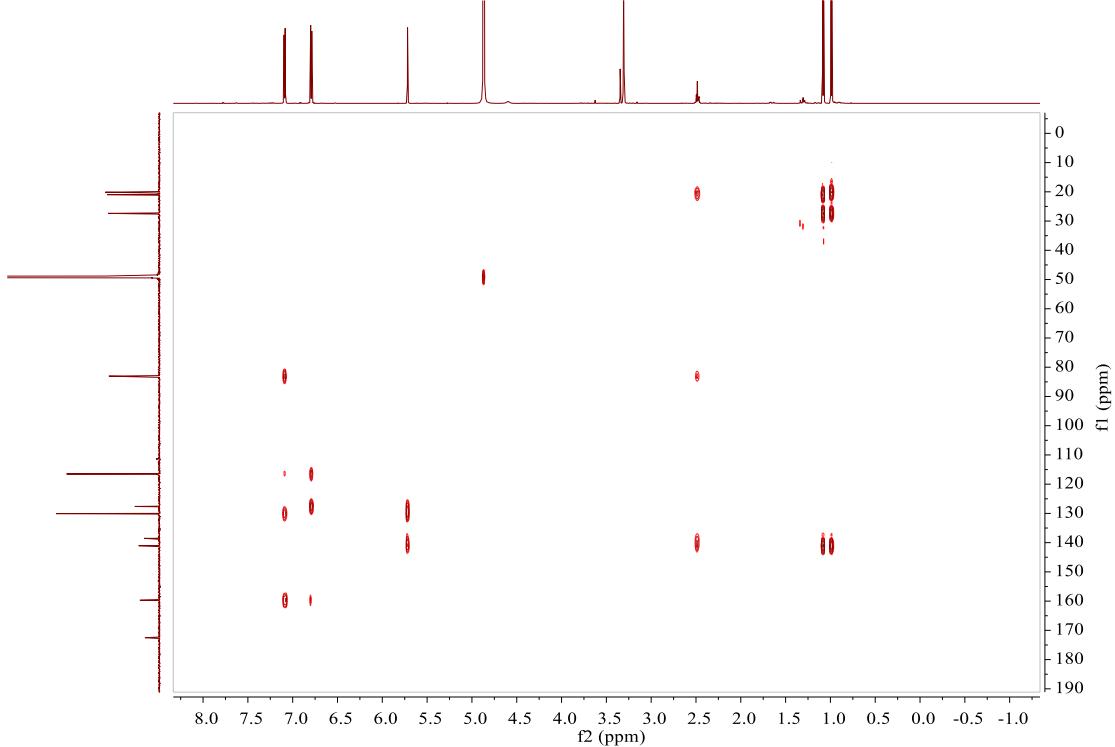


Figure S15. HMBC spectrum of **2** (CD_3OD).

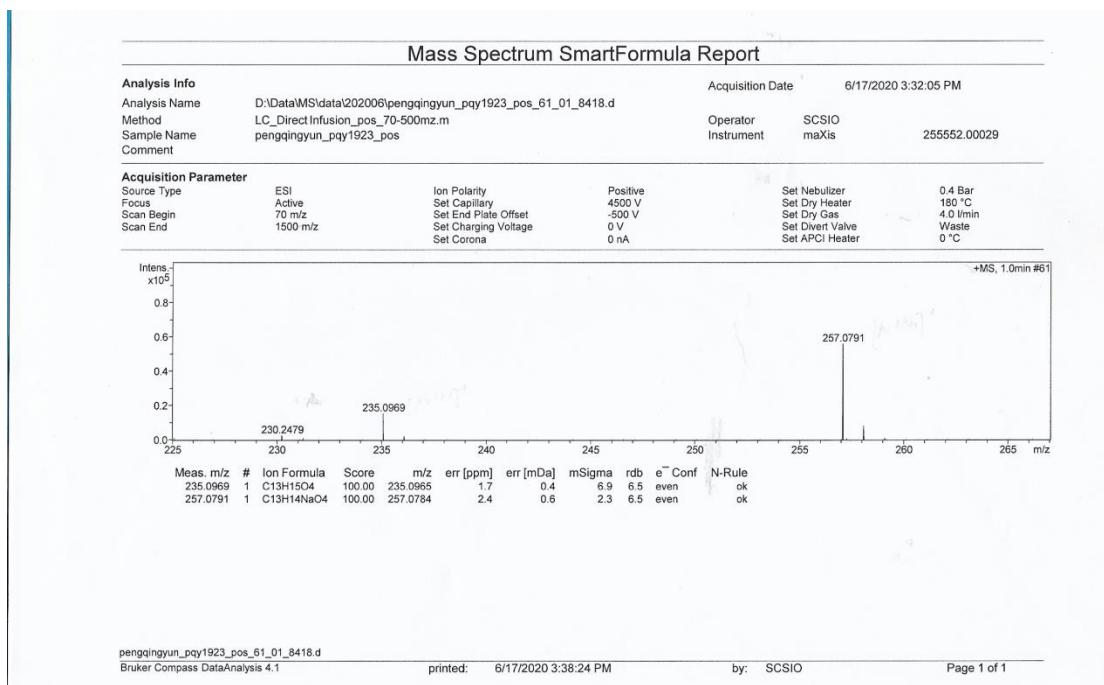


Figure S16. HRESIMS spectrum of 2.

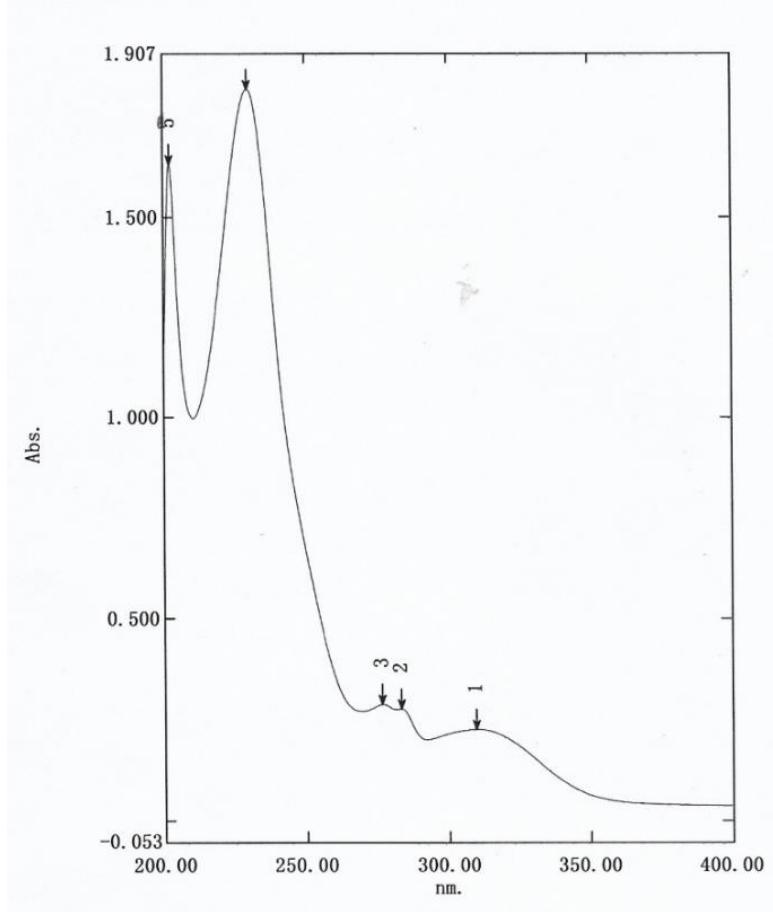


Figure S17. UV spectrum of 2.

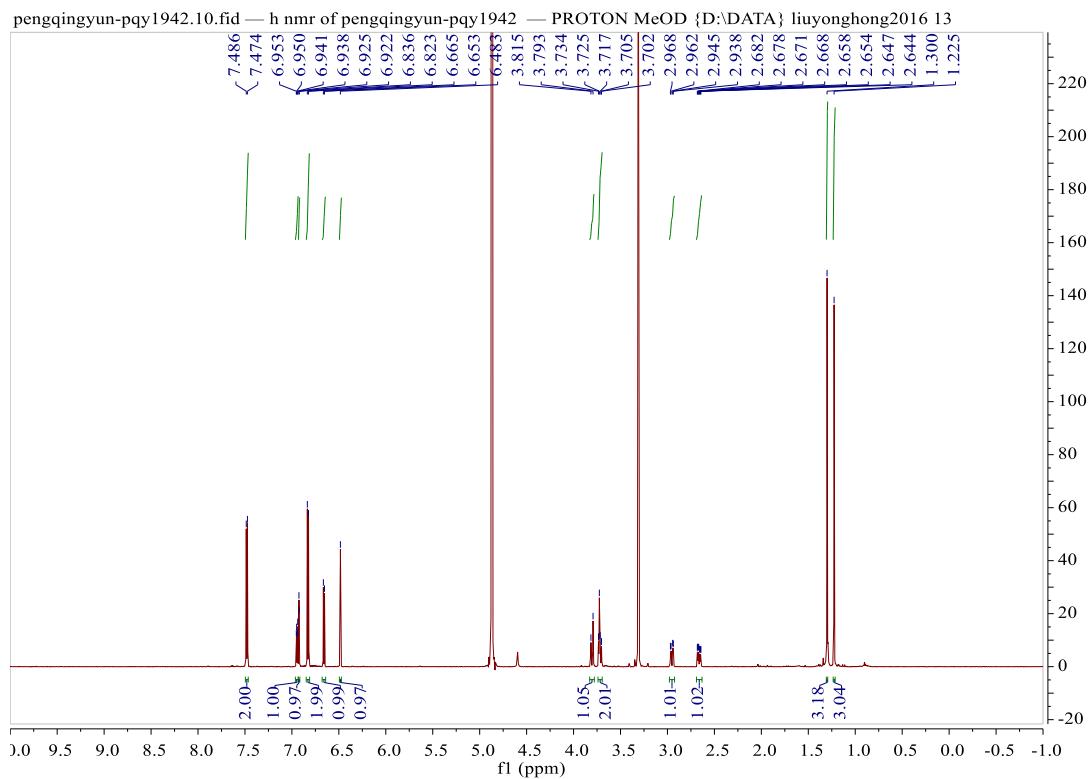


Figure S18. ^1H NMR spectrum of **3** (CD_3OD , 700 Hz).

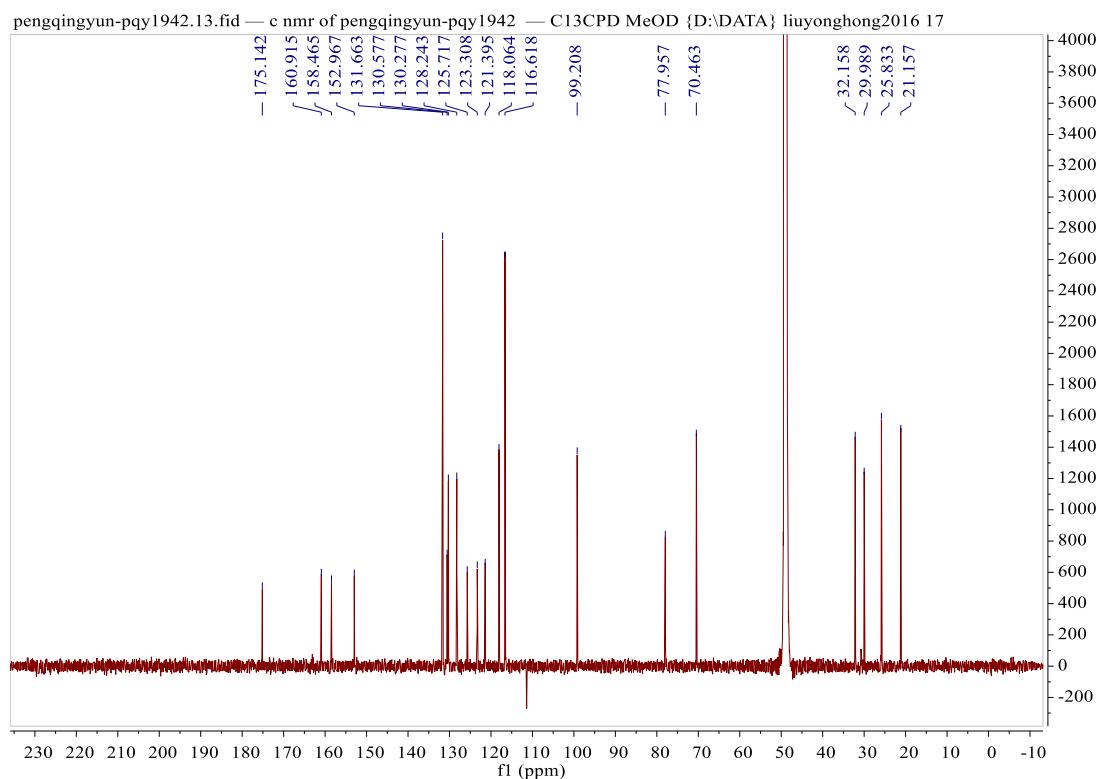


Figure S19. ^{13}C NMR spectrum of **3** (CD_3OD , 175 Hz).

pengqingyun-pqy1942.12.fid — 135c nmr of pengqingyun-pqy1942 — C13DEPT135 MeOD {D:\DATA} liuyonghong2016 17

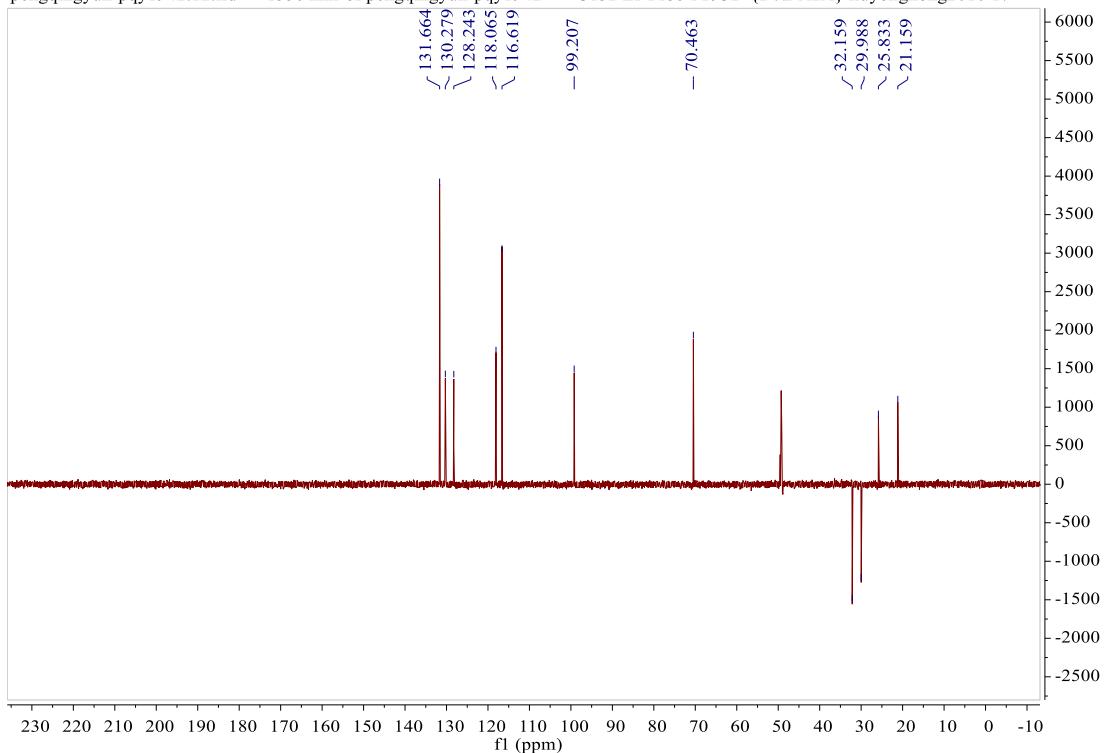


Figure S20. DEPT spectrum of **3** (CD_3OD).

pengqingyun-pqy1942.18.ser — cosy nmr of pengqingyun-pqy1942 — COSYGPMFQF MeOD {D:\DATA} liuyonghong2016 17

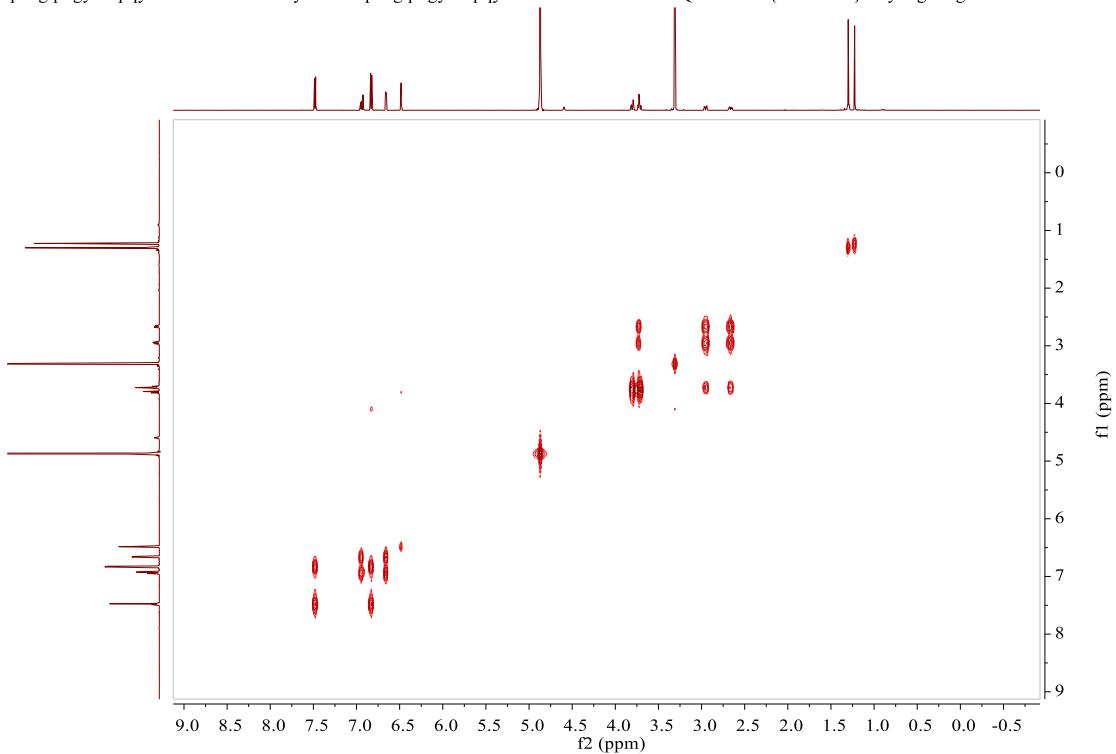


Figure S21. COSY of spectrum of **3** (CD_3OD).

pengqingyun-pqy1942.16.ser — qc nmr of pengqingyun-pqy1942 — HSQCETGP MeOD {D:\DATA} liuyonghong2016 18

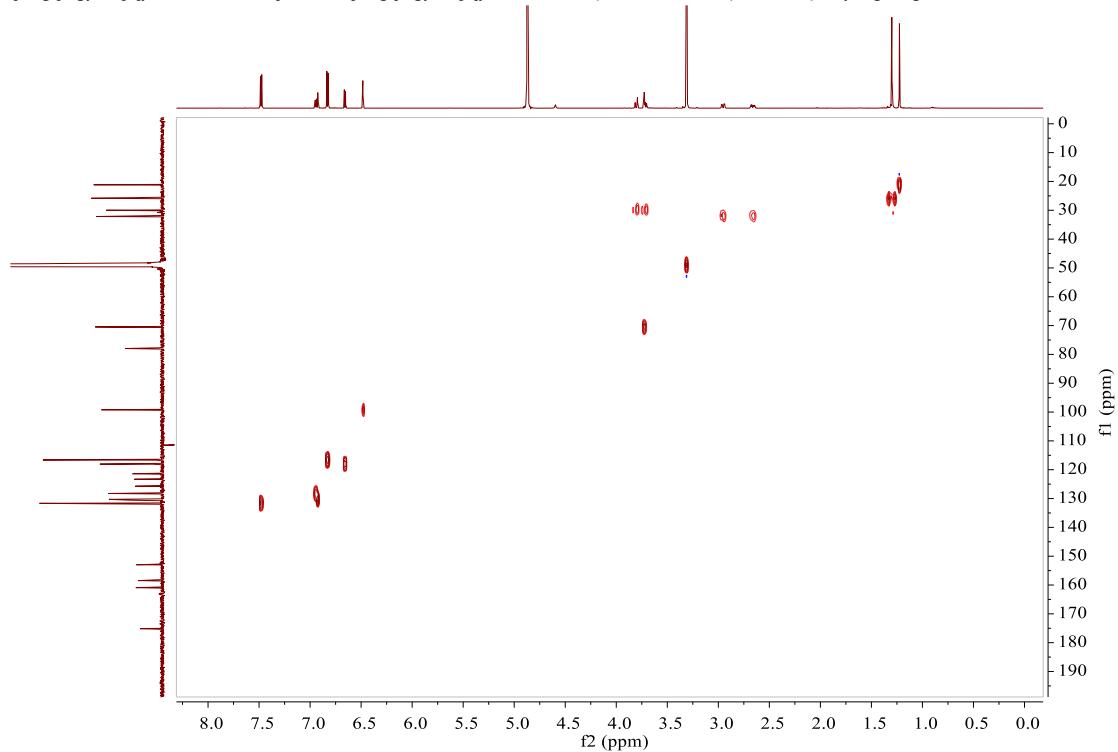


Figure S22. HSQC of spectrum of **3** (CD_3OD).

pengqingyun-pqy1942.15.ser — bc nmr of pengqingyun-pqy1942 — HMBCETGPL3ND MeOD {D:\DATA} liuyonghong2016 18

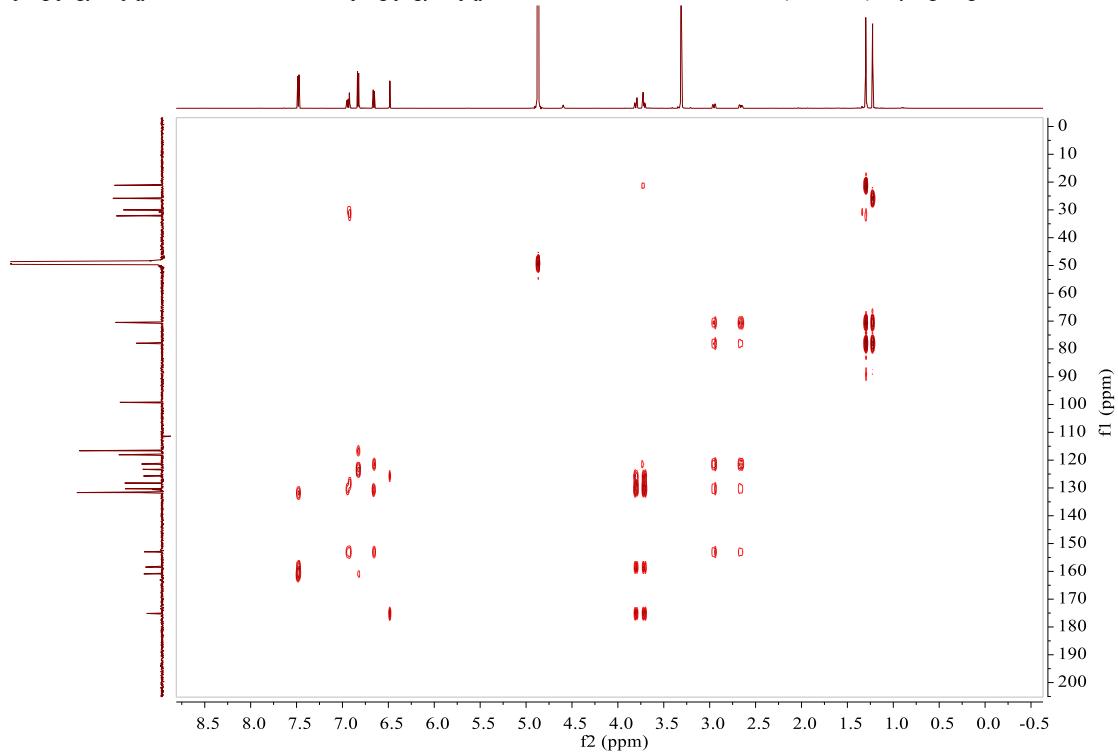


Figure S23. HMBC of spectrum of **3** (CD_3OD).

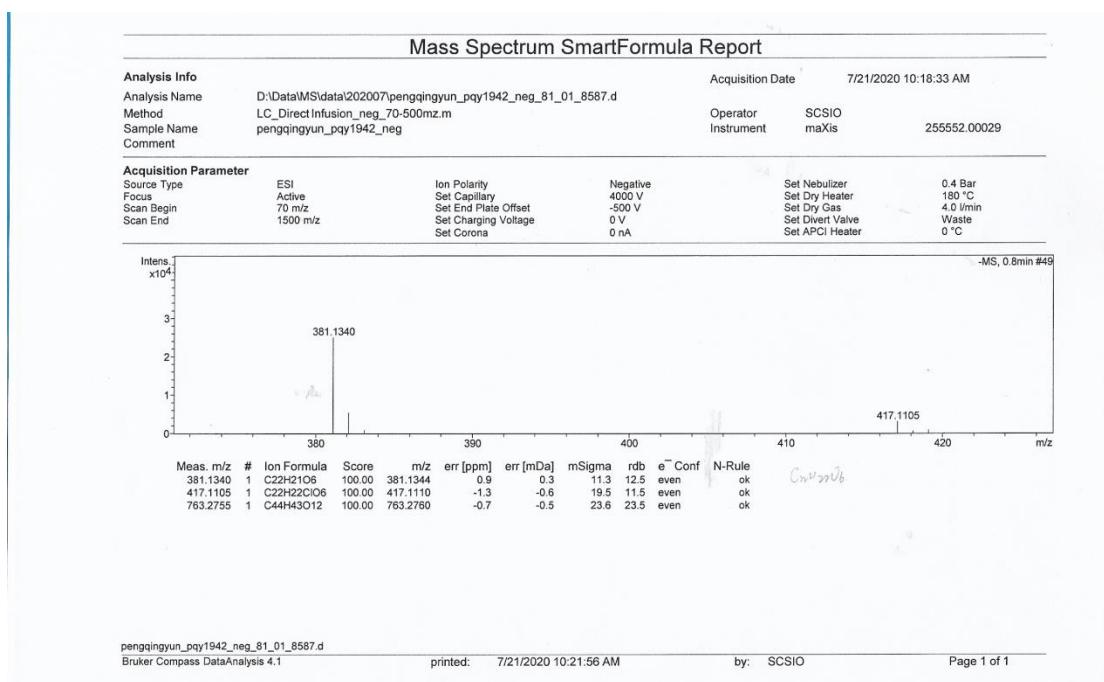


Figure S24. HRESIMS spectrum of 3.

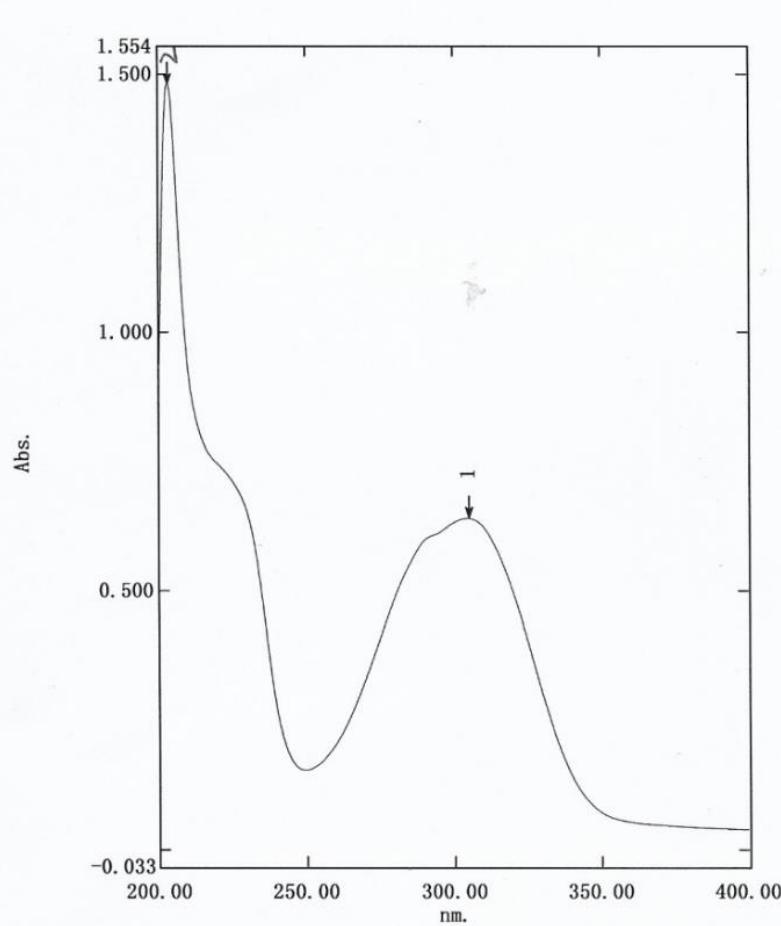
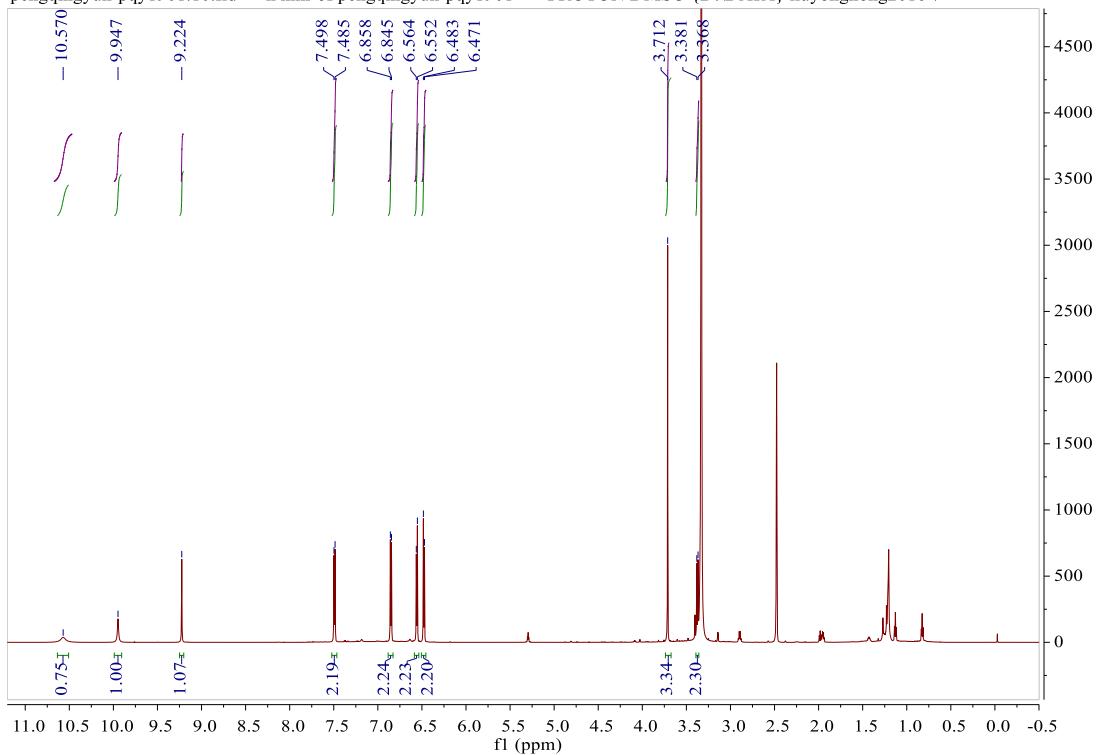
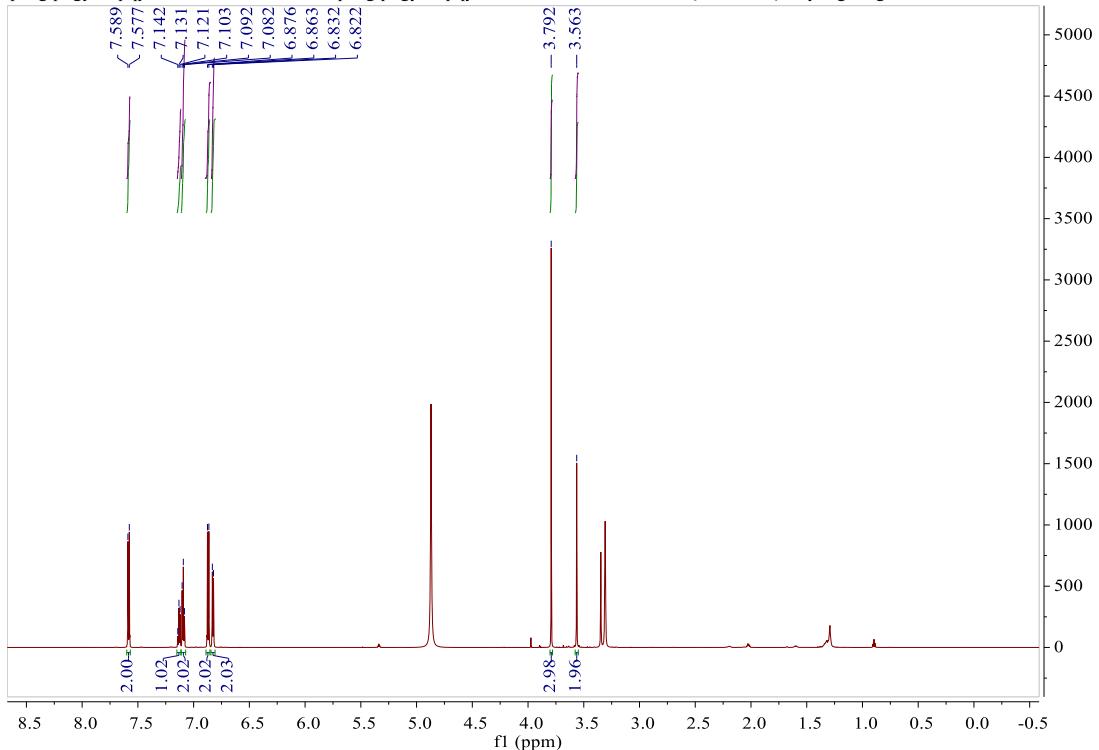


Figure S25. UV spectrum of 3.

**Figure S26.** ^1H NMR spectrum of **4** ($\text{DMSO}-d_6$, 700 MHz).**Figure S27.** ^1H NMR spectrum of **5** (CD_3OD , 700 MHz).

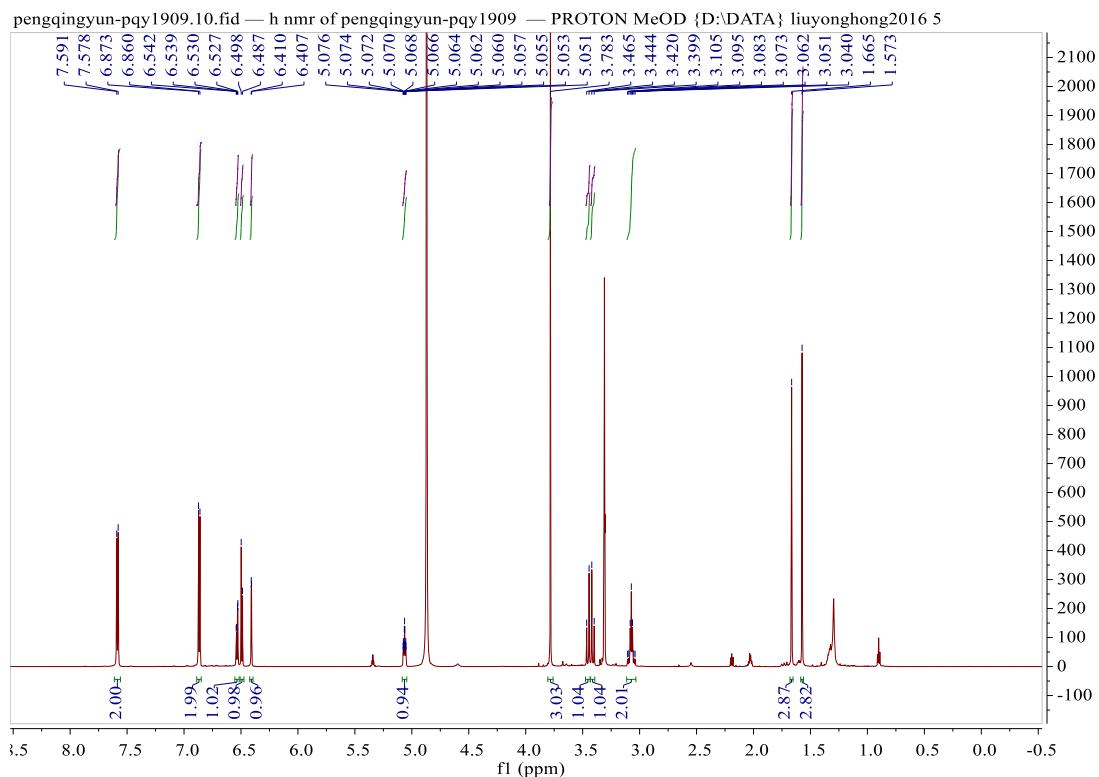


Figure S28. ^1H NMR spectrum of **6** (CD_3OD , 700 MHz).

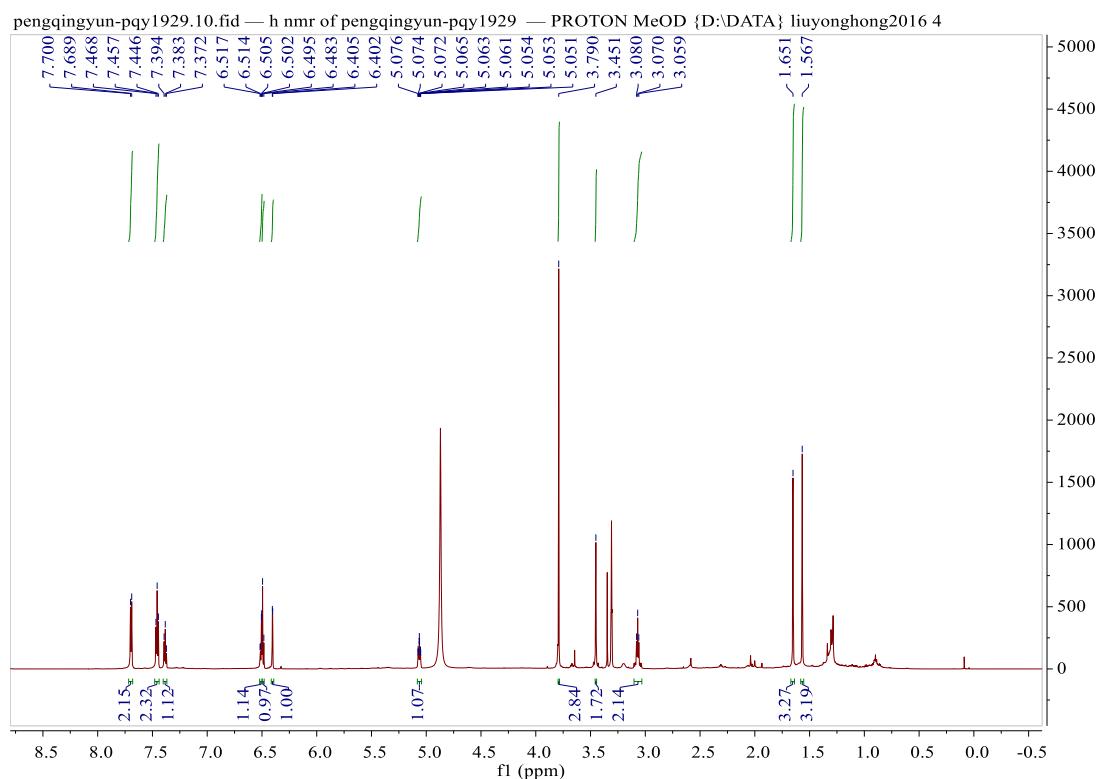


Figure S29. ^1H NMR spectrum of **7** (CD_3OD , 700 MHz).

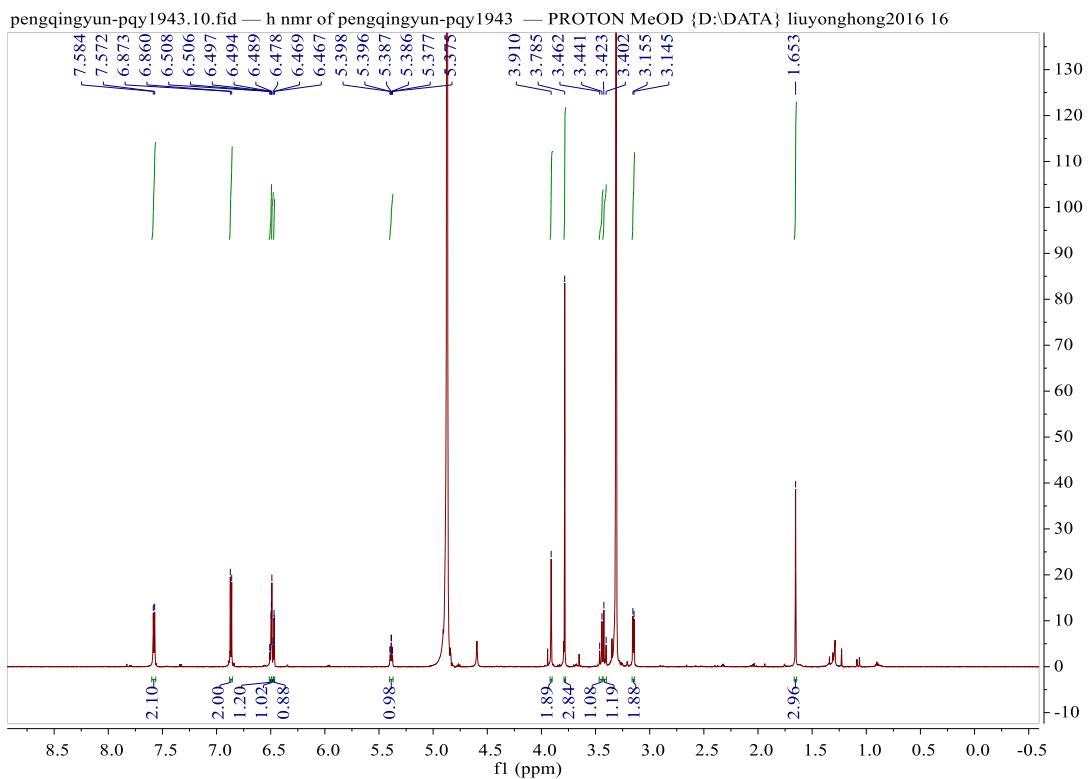


Figure S30. ^1H NMR spectrum of **8** (CD_3OD , 700 MHz).

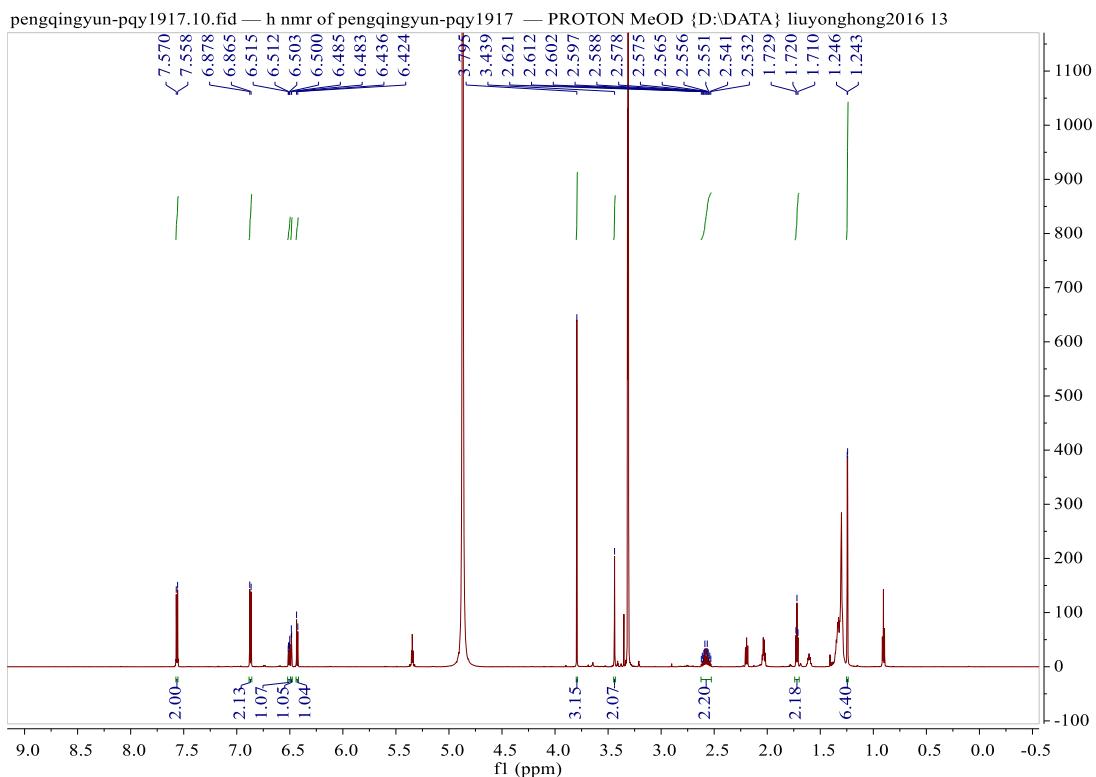


Figure S31. ^1H NMR spectrum of **9** (CD_3OD , 700 MHz).

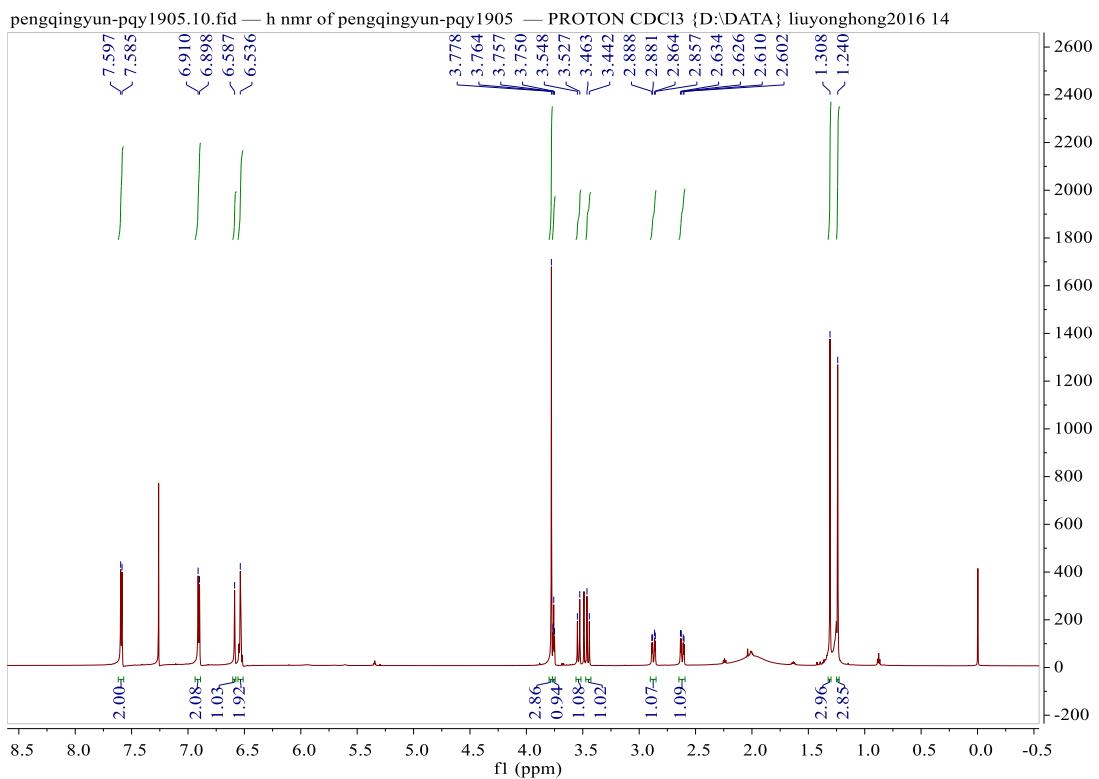


Figure S32. ¹H NMR spectrum of **10** (CDCl₃, 700 MHz).

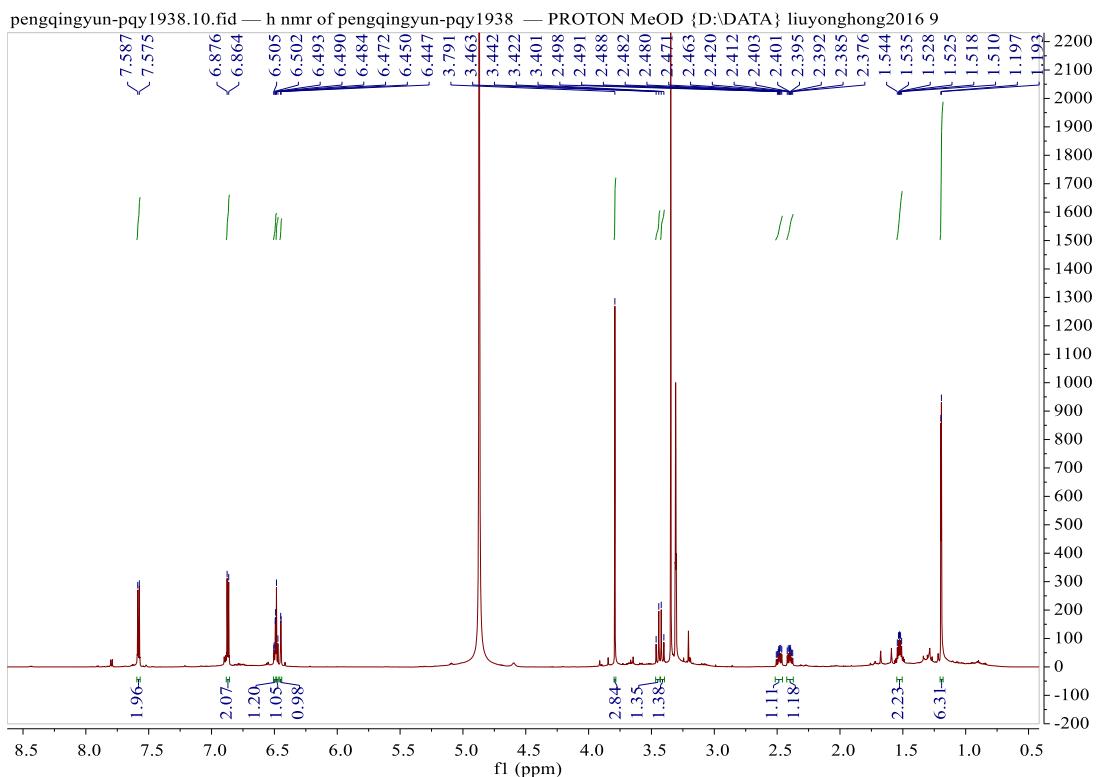


Figure S33. ¹H NMR spectrum of **11** (CD₃OD, 700 MHz).

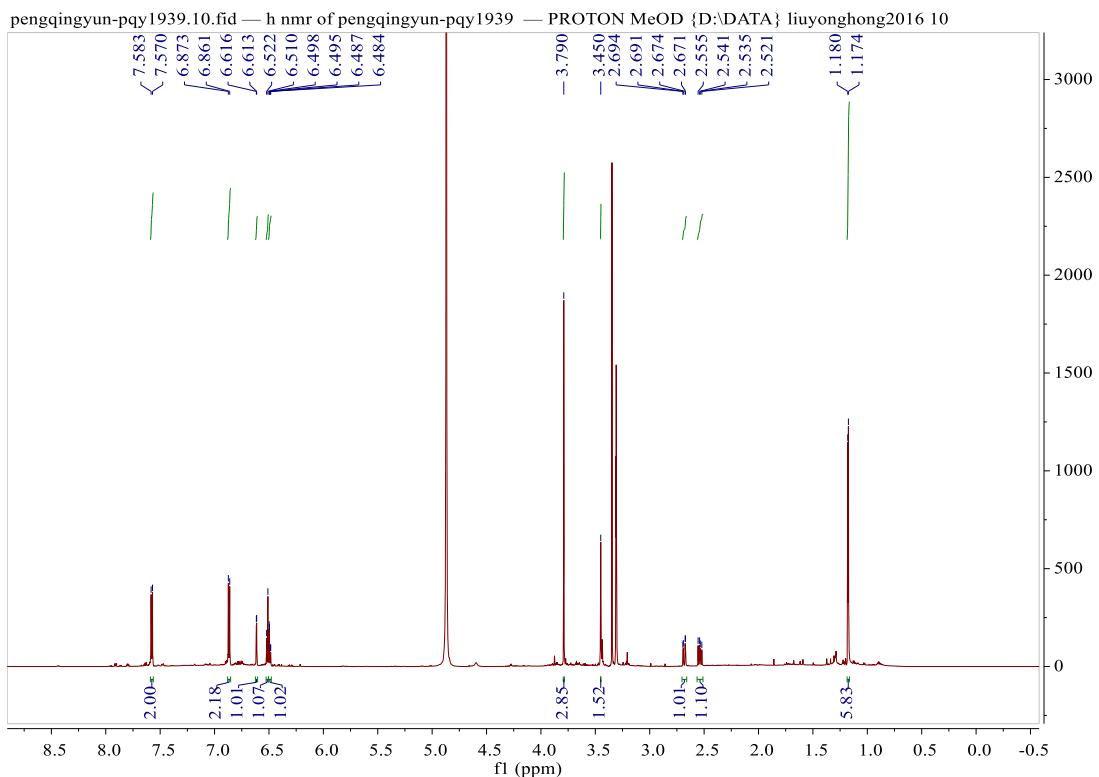


Figure S34. ^1H NMR spectrum of **12** (CD_3OD , 700 MHz).

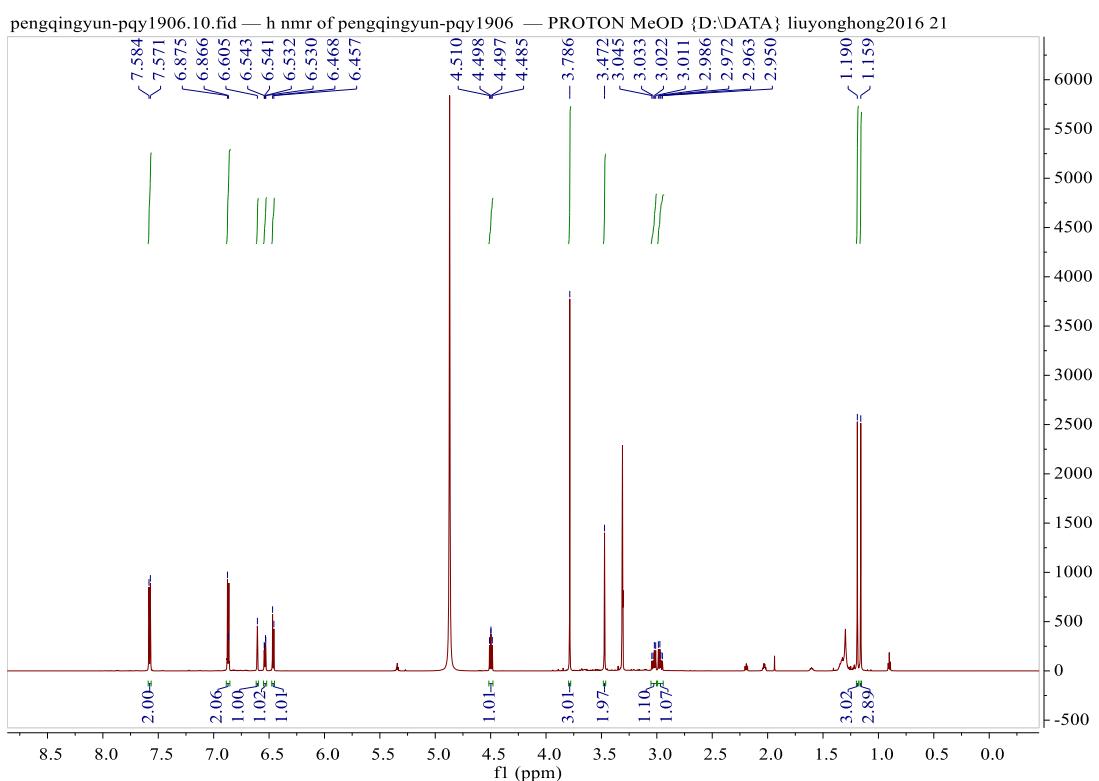


Figure S35. ^1H NMR spectrum of **13** (CD_3OD , 700 MHz).

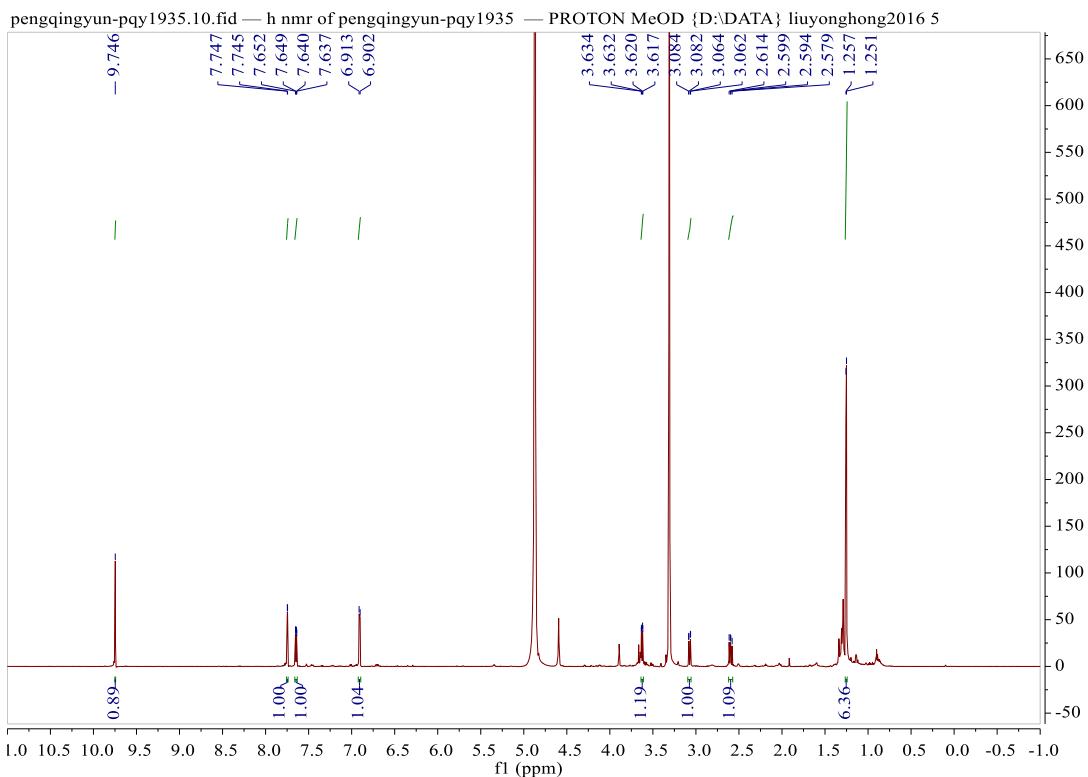


Figure S36. ^1H NMR spectrum of **14** (CD_3OD , 700 MHz).

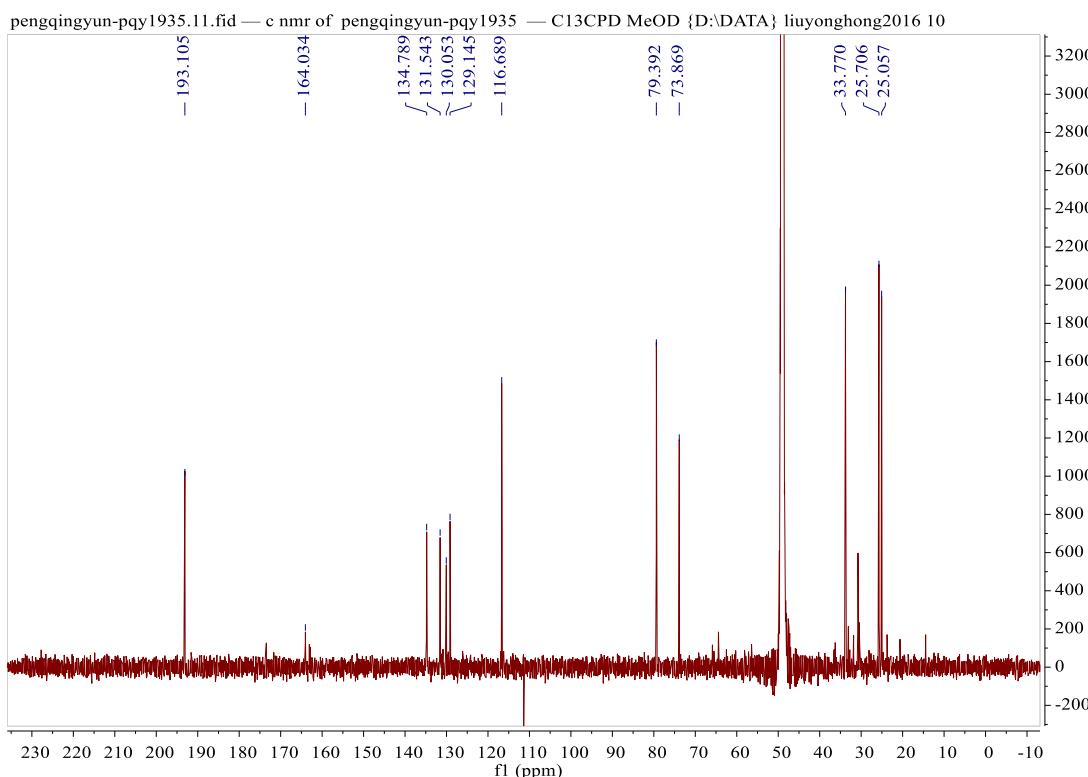


Figure S37. ^{13}C NMR spectrum of **14** (CD_3OD , 175 MHz).

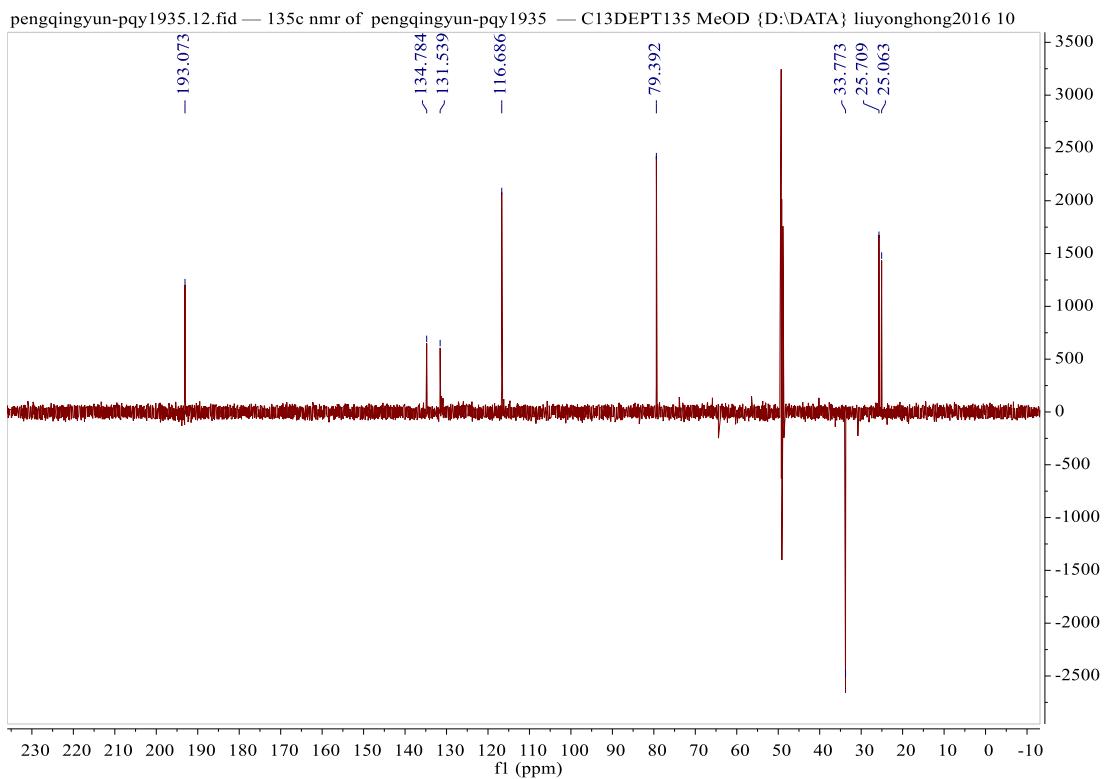


Figure S38. DEPT spectrum of **14** (CD_3OD).

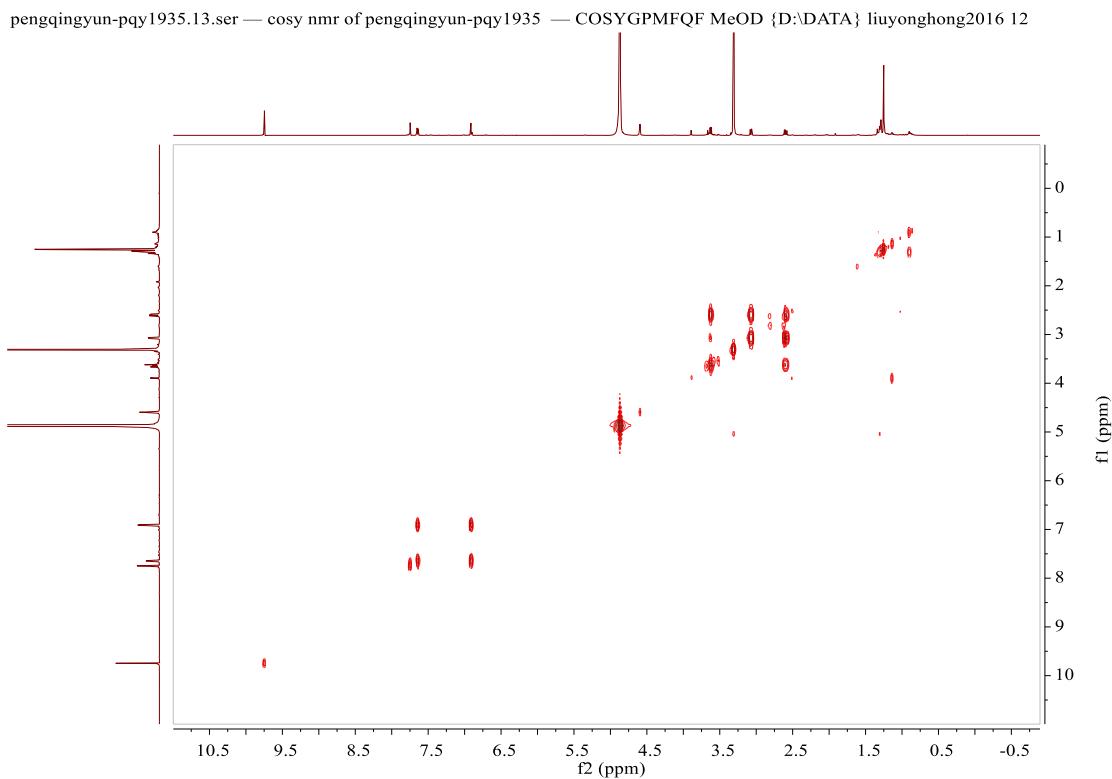


Figure S39. COSY spectrum of **14** (CD_3OD).

pengqingyun-pqy1935.15.ser — qc nmr of pengqingyun-pqy1935 — HSQCEDETGP MeOD {D:\DATA} liuyonghong2016 12

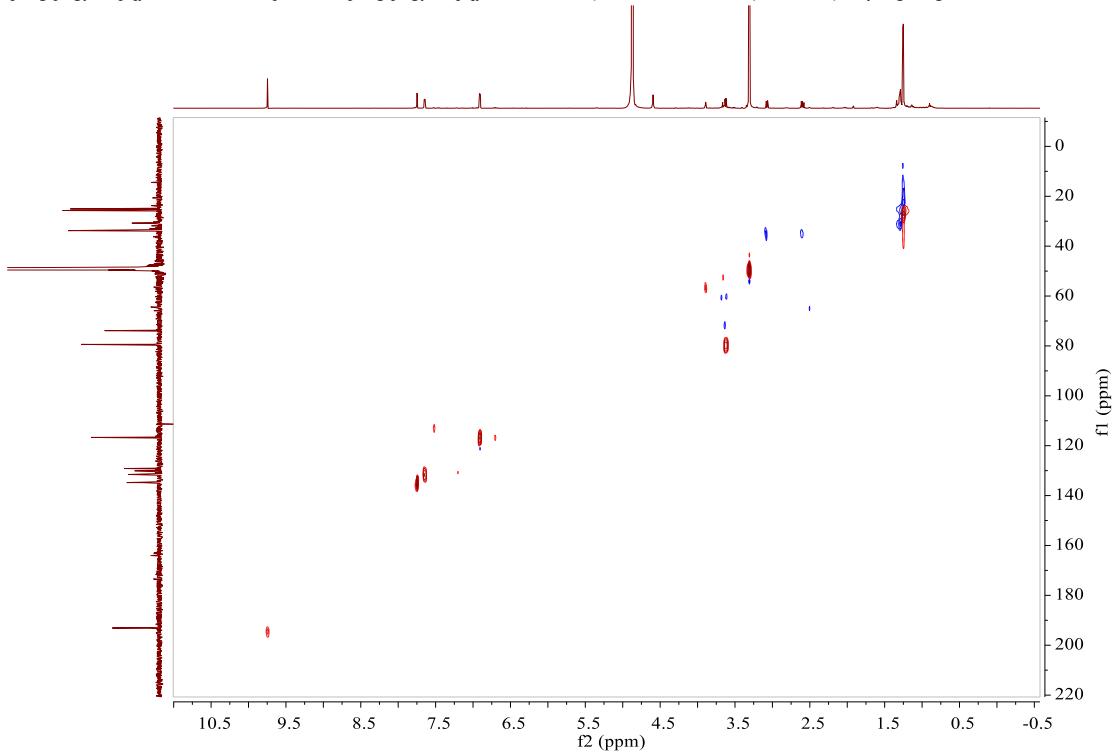


Figure S40. HSQC spectrum of **14** (CD_3OD).

pengqingyun-pqy1935.16.ser — bc nmr of pengqingyun-pqy1935 — HMBCETGPL3ND MeOD {D:\DATA} liuyonghong2016 12

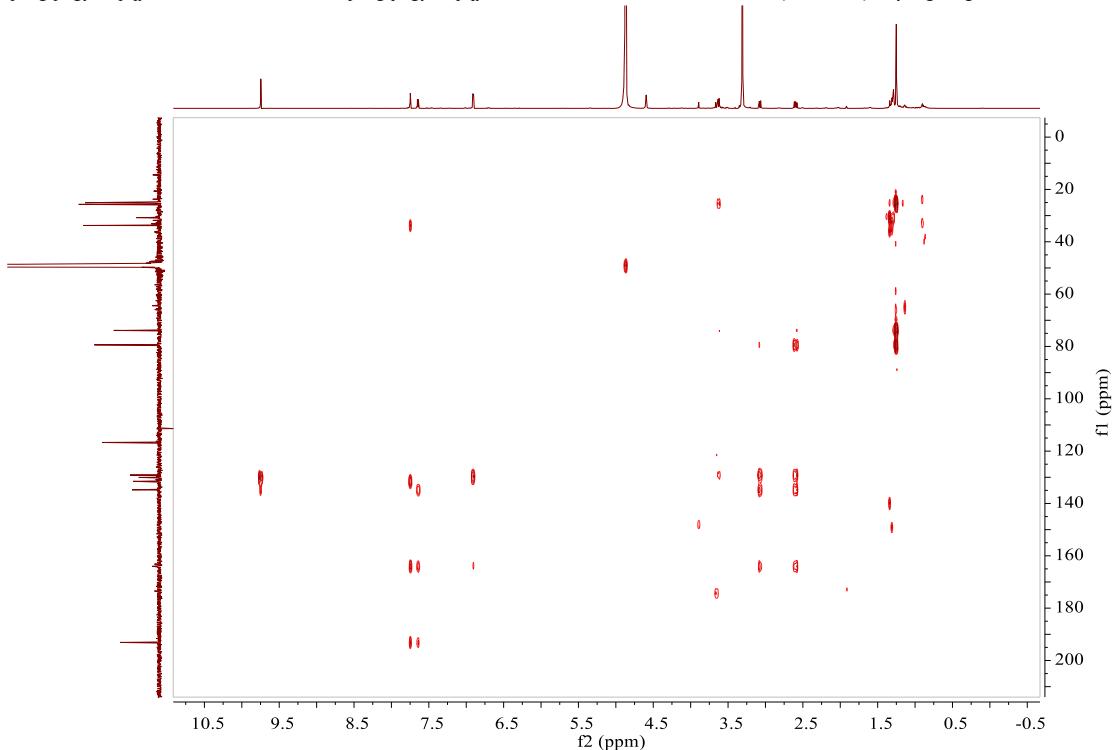


Figure S41. HMBC spectrum of **14** (CD_3OD).

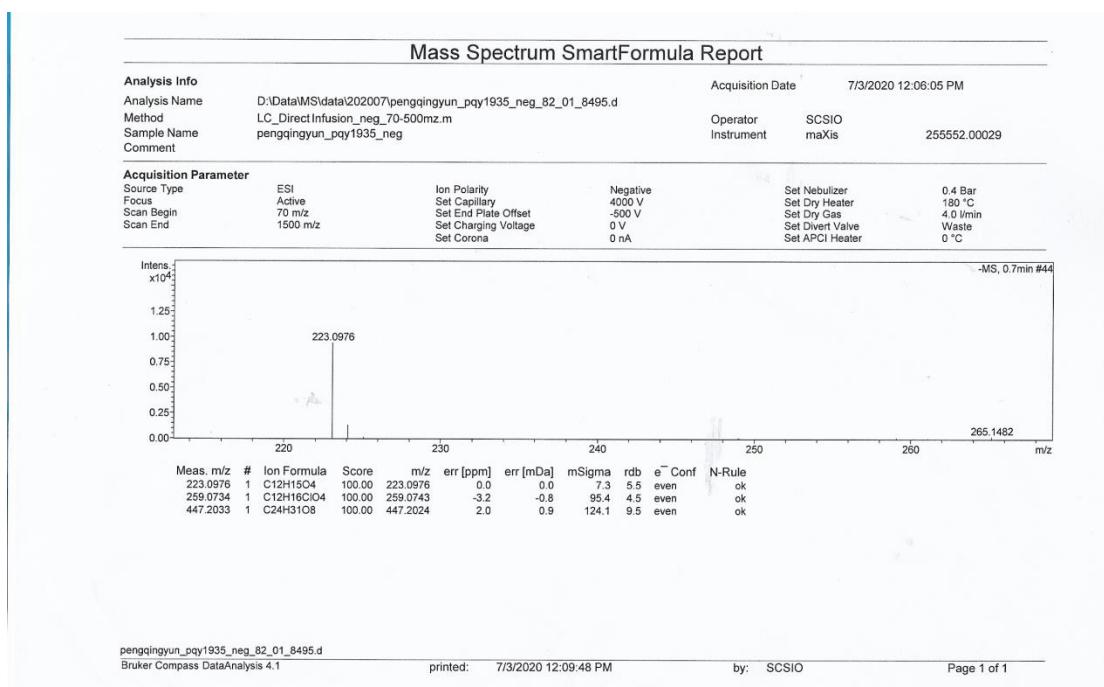


Figure S42. HRESIMS spectrum of **14**.

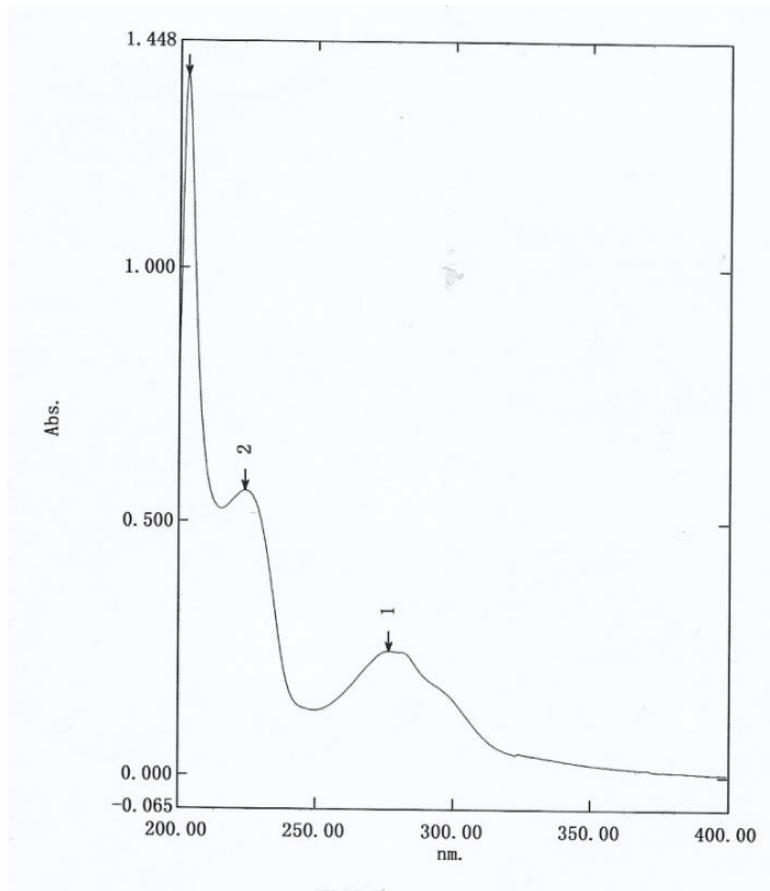


Figure S43. UV spectrum of **14**.