Supplementary Materials

Triterpenoid Saponins and Flavonoid Glycosides from the Flower of *Camellia flavida* and Their Cytotoxic and α-Glycosidase Inhibitory Activities

Siyuan Ma [1,†], Yuxin Wu [1,†], Hanfeng Min [1], Li Ge [1,*], and Kedi Yang [1,*]

[1] Medical College of Guangxi University, Nanning 530004, China

***** Correspondence: geli_2009@163.com (L.G.); kdyang@163.com (K.Y.); Tel.: +86-771-3949953 (K.Y.)

† These authors contributed equally to this work.

CONTENTS

1. Spectroscopic data for compound **1** 1

2. Spectroscopic data for compound **2** 6

3. Spectroscopic data for compound **3** 11

4. Spectroscopic data for compound **4** 17

5. Spectroscopic data for compound **5** 22

6. Spectroscopic data for compound **6** 27

7. Spectroscopic data for compound **7** 32

8. Spectroscopic data for compound **8** 36

9. Spectroscopic data for compound **9** 41

10. Spectroscopic data for compound **10** 46

11. ^{1}H and ^{13}C NMR spectroscopic data for compound **11**−**15** 51

12. Molecular docking results of compounds **1**−**7** and **9**−**10** with α-Glycosidase..... 56

1. Spectroscopic data for compound **1**

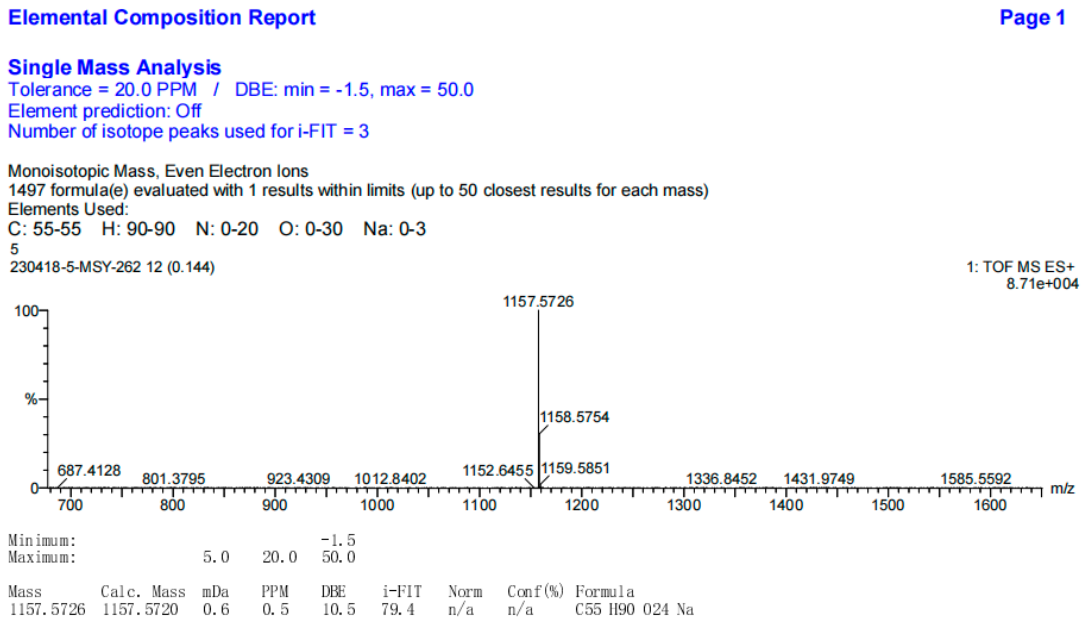

Figure S1. The HR-ESI-MS of compound **1**.

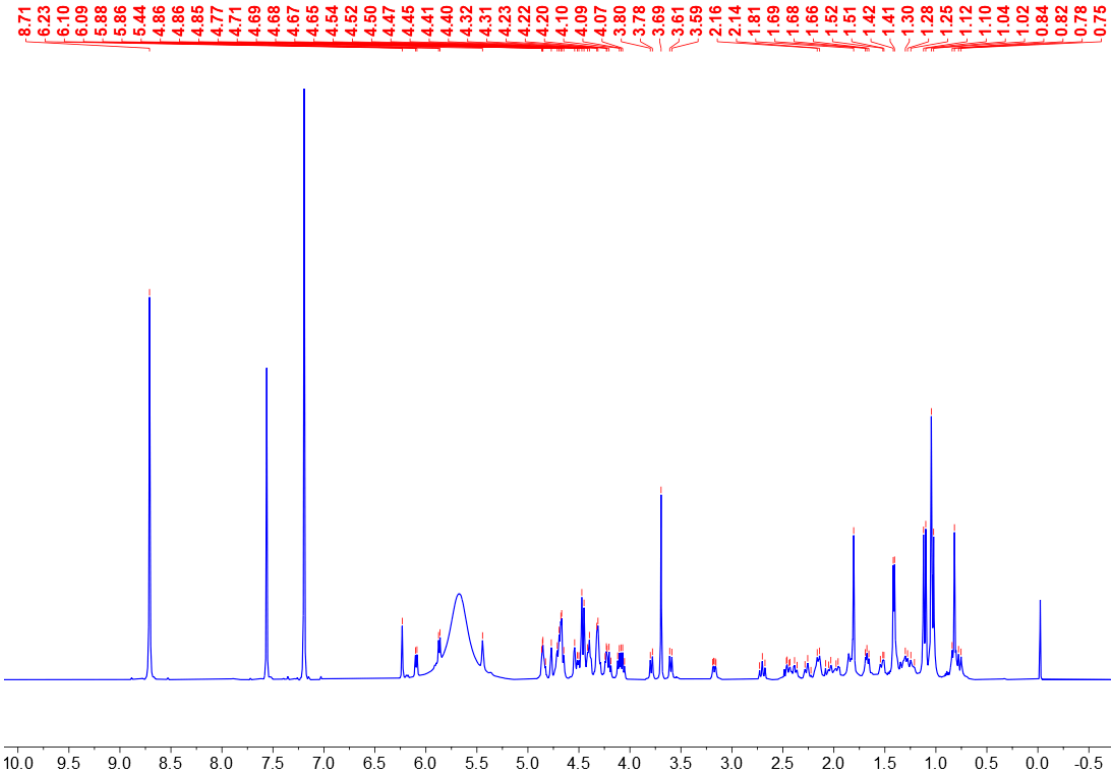

Figure S2. The ^{1}H NMR spectrum of compound **1** (600 MHz, Pyr-d_5).

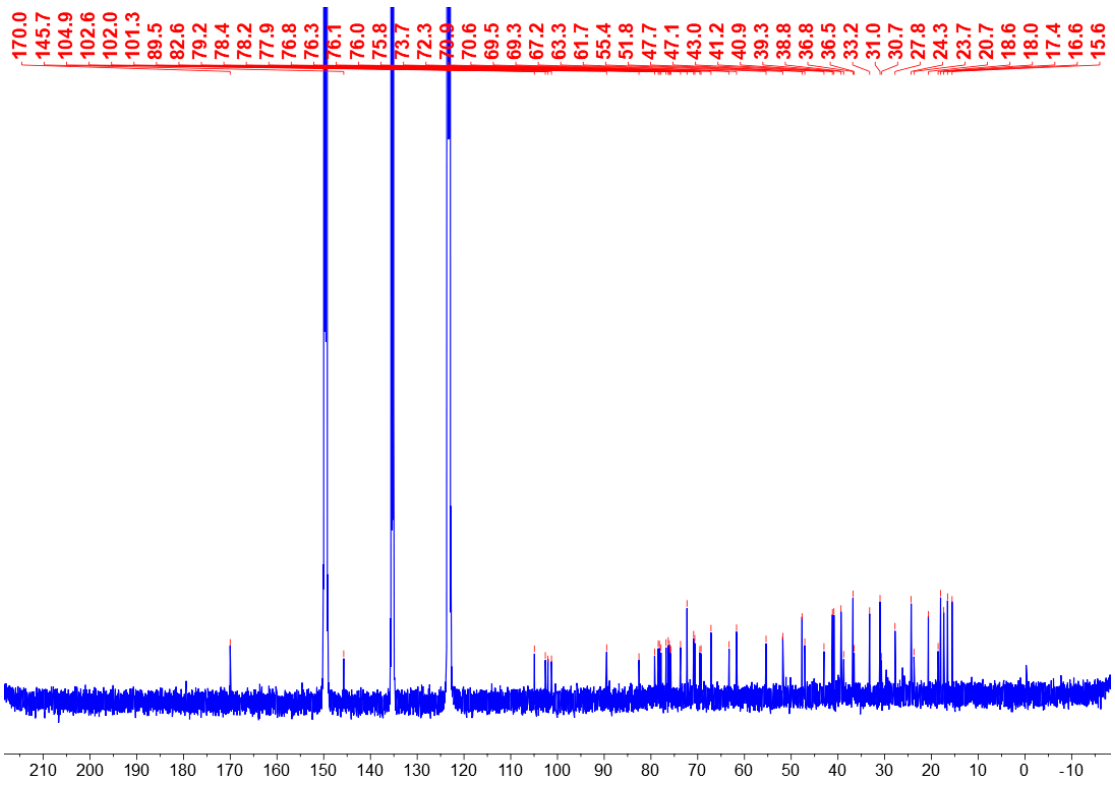

Figure S3. The ^{13}C NMR spectrum of compound **1** (151 MHz, Pyr-d_5).

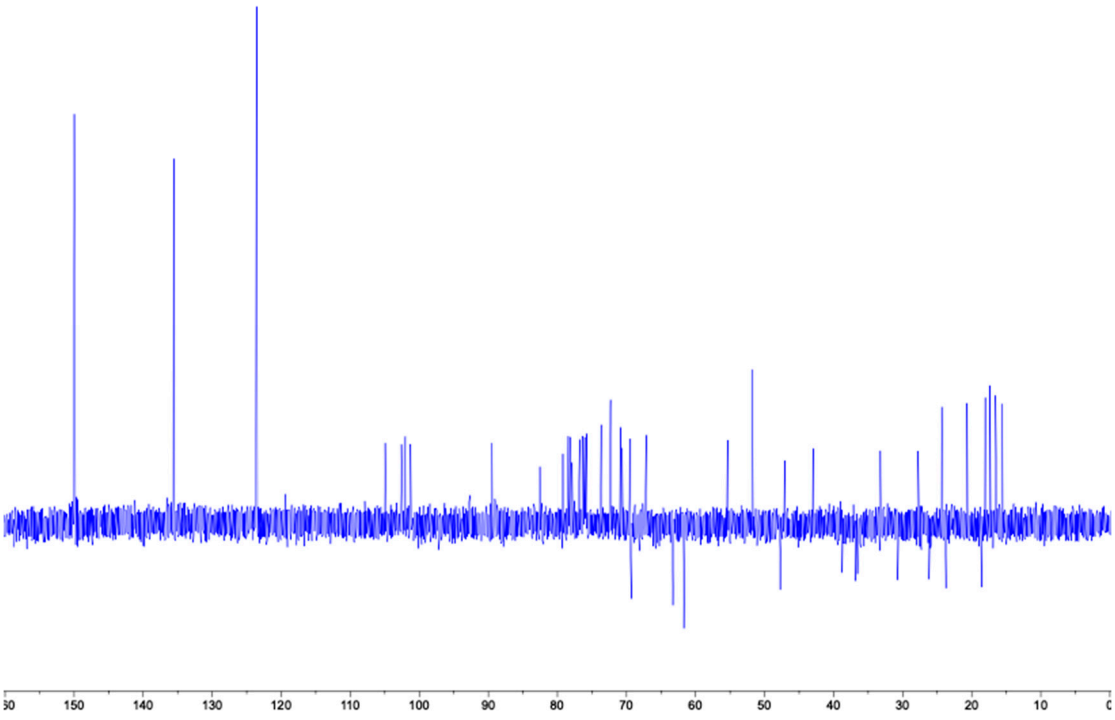

Figure S4. The DEPT 135 spectrum of compound **1** (151 MHz, Pyr-d_5).

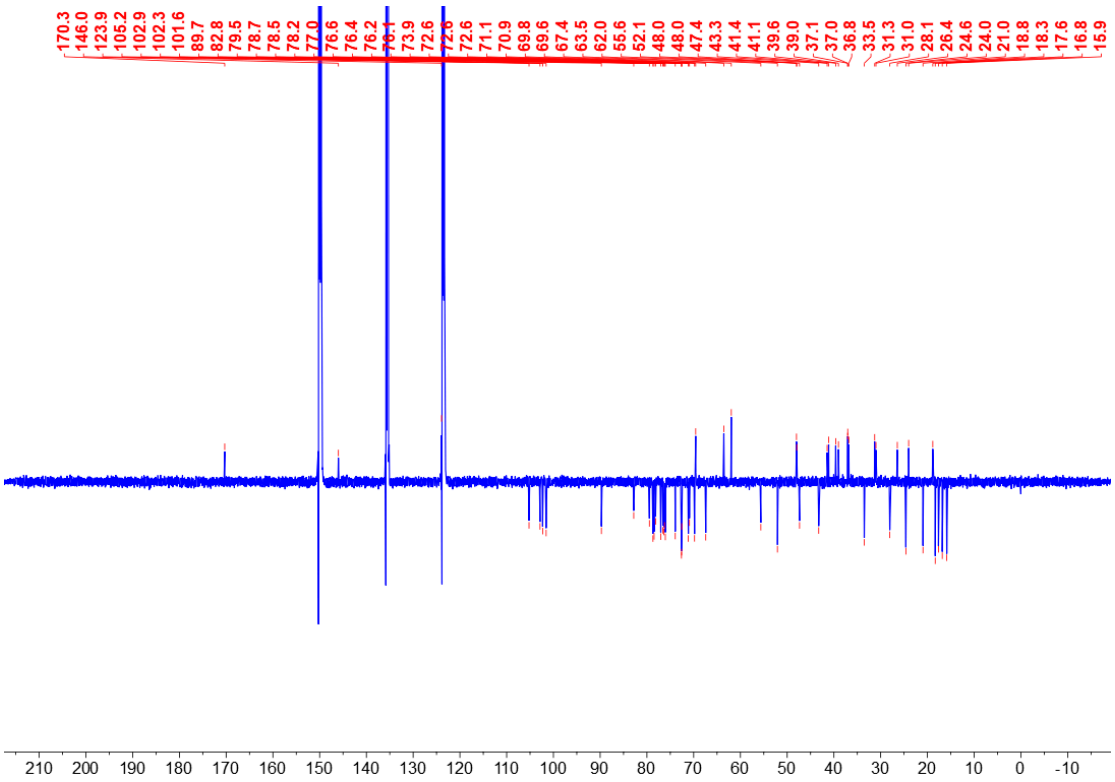

Figure S5. The DEPTQ spectrum of compound **1** (151 MHz, Pyr-d_5).

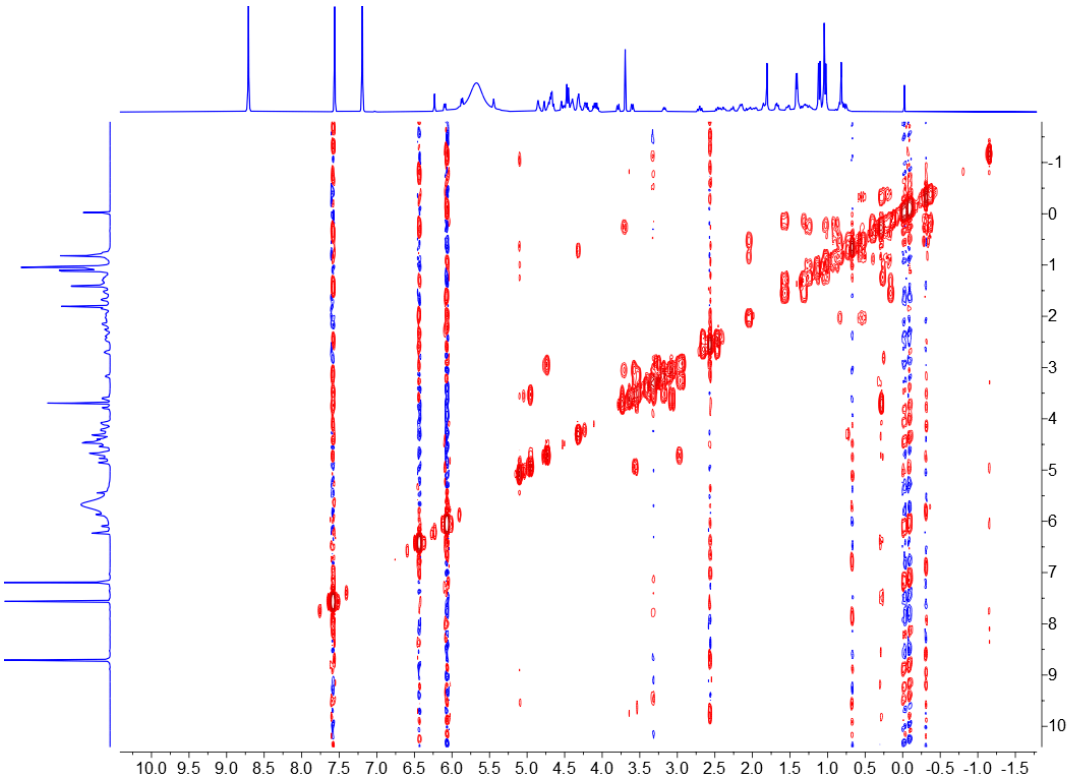

Figure S6. The ^{1}H-^{1}H COSY spectrum of compound **1** (600 MHz, Pyr-d_5).

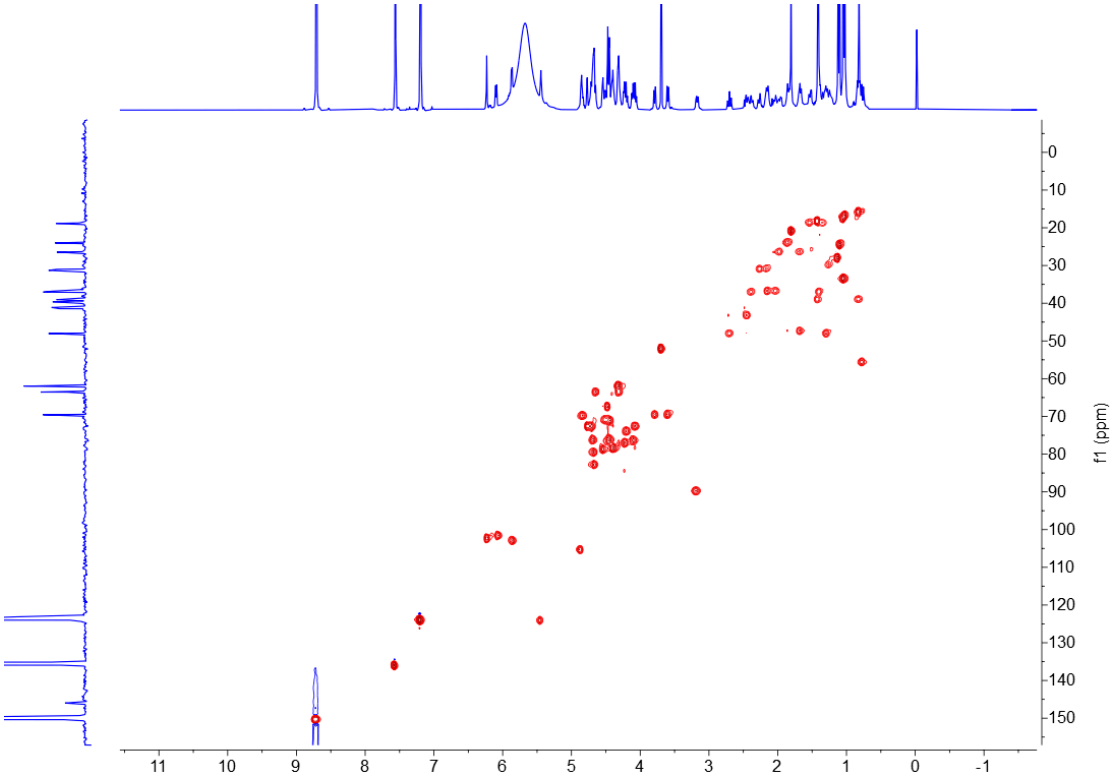

Figure S7. The HSQC spectrum of compound **1** (600/151 MHz, Pyr-d_5).

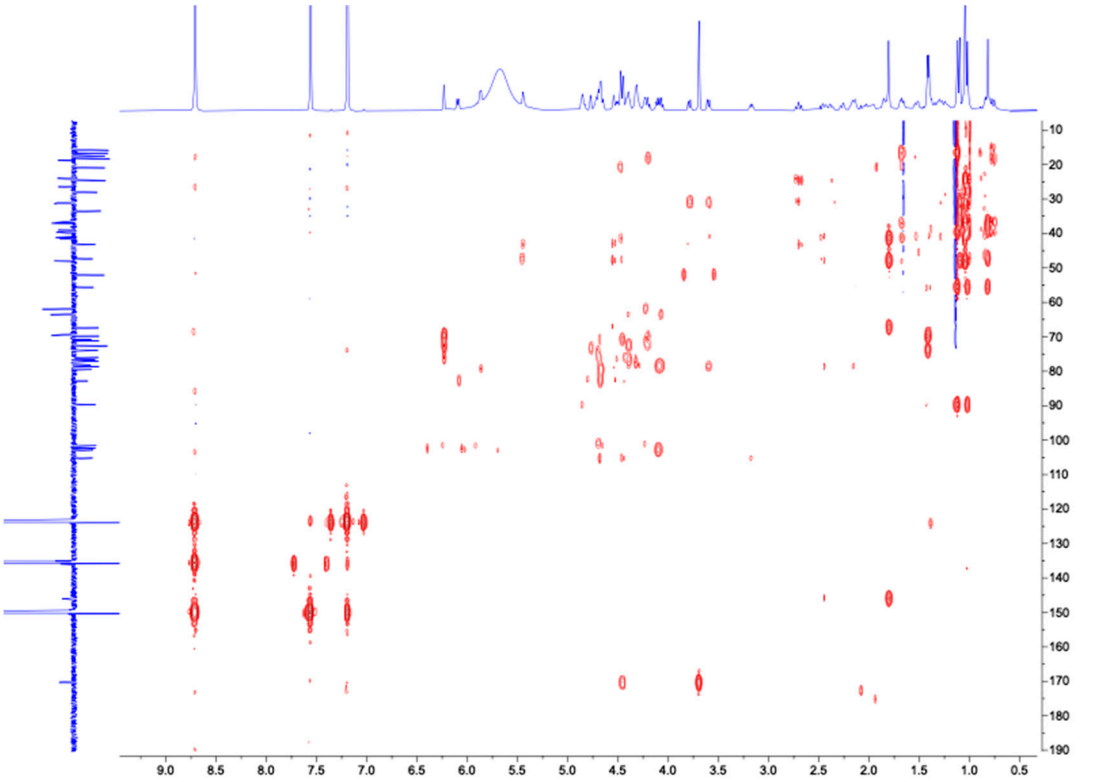

Figure S8. The HMBC spectrum of compound **1** (600/151 MHz, Pyr-d_5).

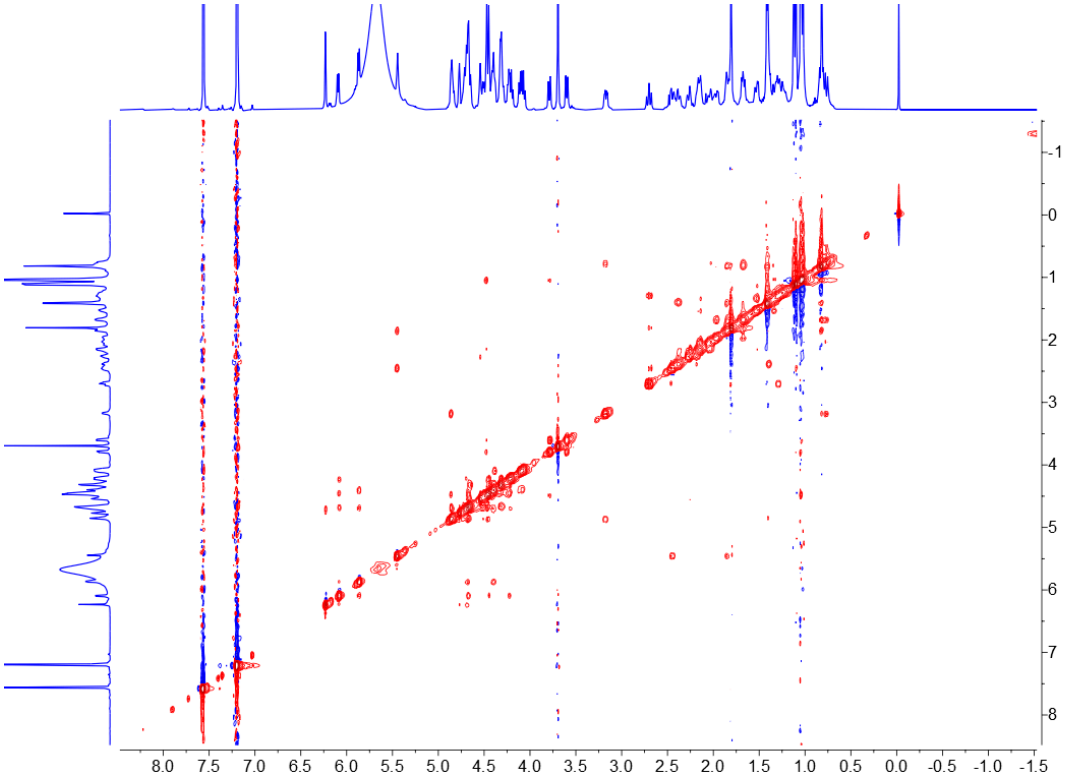

Figure S9. The NOESY spectrum of compound **1** (600 MHz, Pyr-d_5).

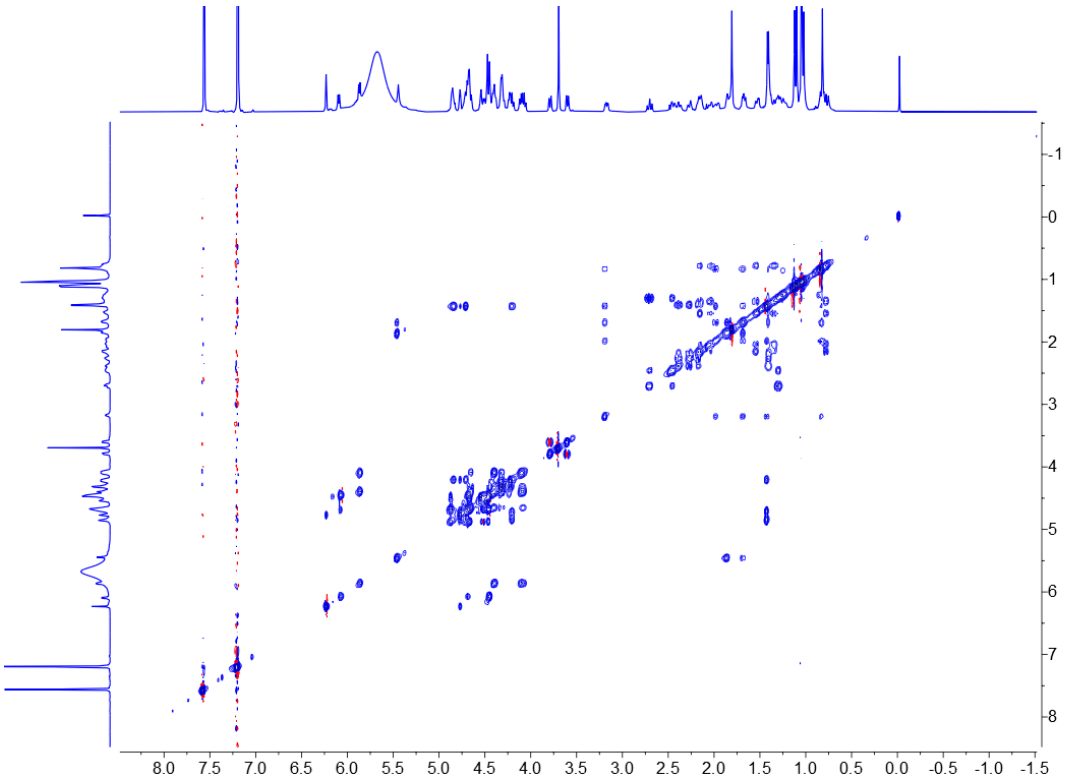

Figure S10. The TOCSY spectrum of compound **1** (600 MHz, Pyr-d_5).

2. Spectroscopic data for compound **2**

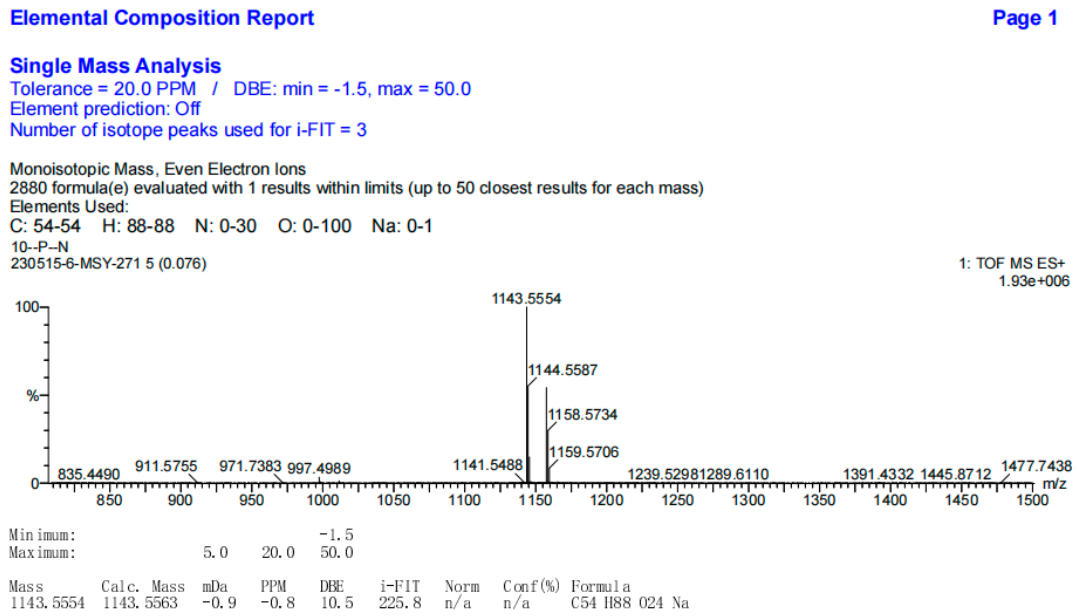

Figure S11. The HR-ESI-MS of compound **2**.

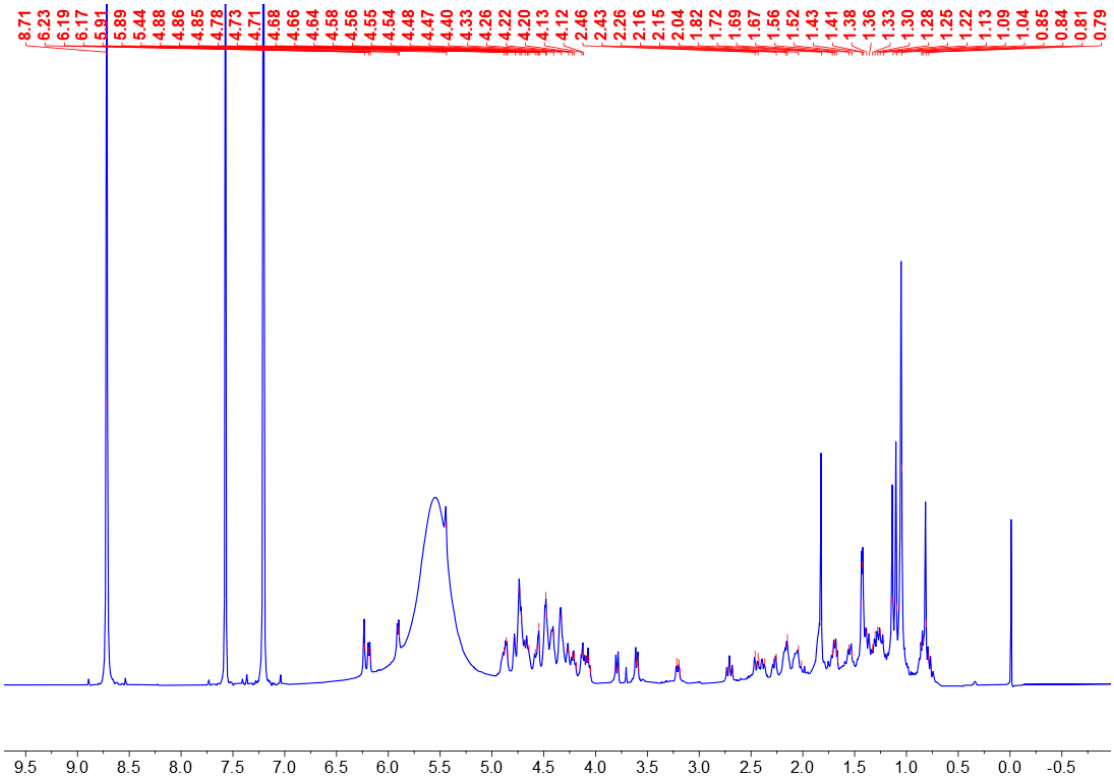

Figure S12. The ^{1}H NMR spectrum of compound **2** (600 MHz, Pyr-d_5).

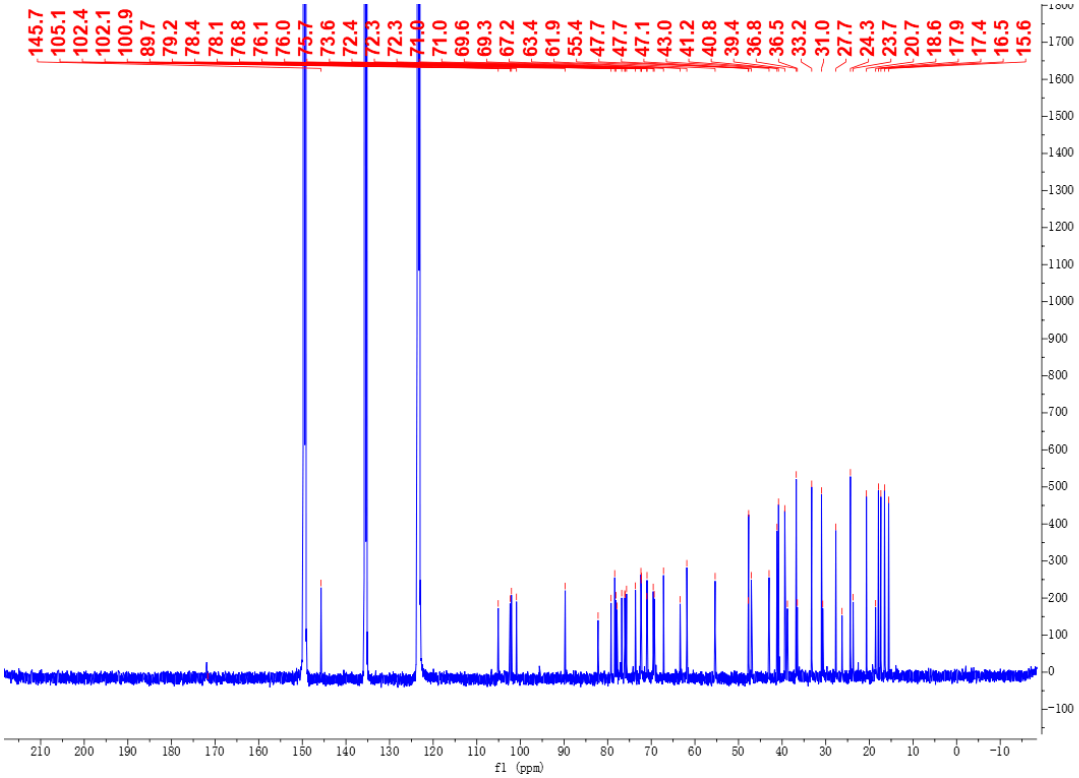

Figure S13. The ^{13}C NMR spectrum of compound **2** (151 MHz, Pyr-d_5).

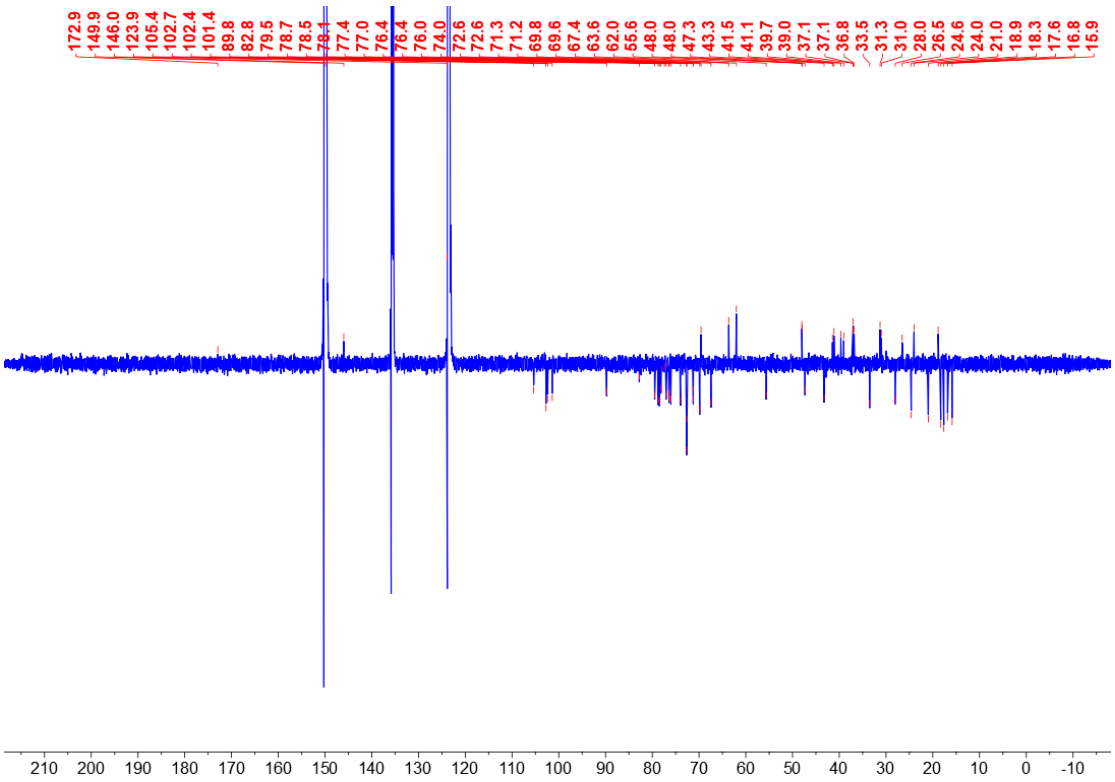

Figure S14. The DEPTQ spectrum of compound **2** (151 MHz, Pyr-d_5).

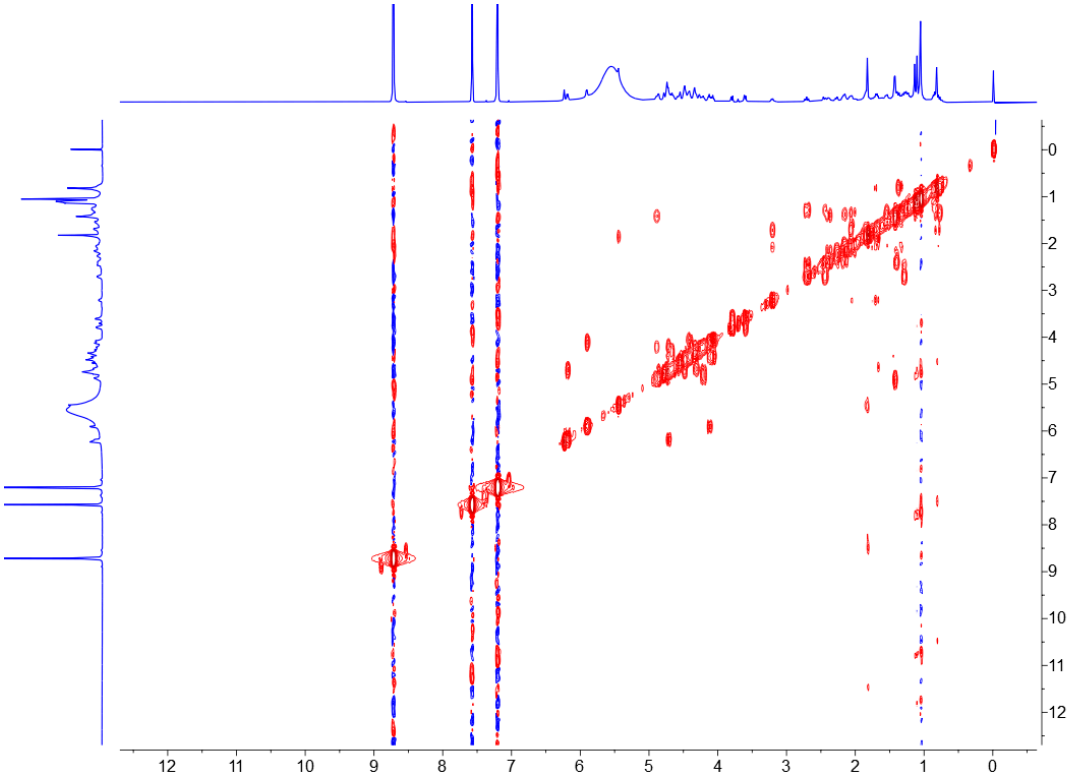

Figure S15. The ^{1}H-^{1}H COSY spectrum of compound **2** (600 MHz, Pyr-d_5).

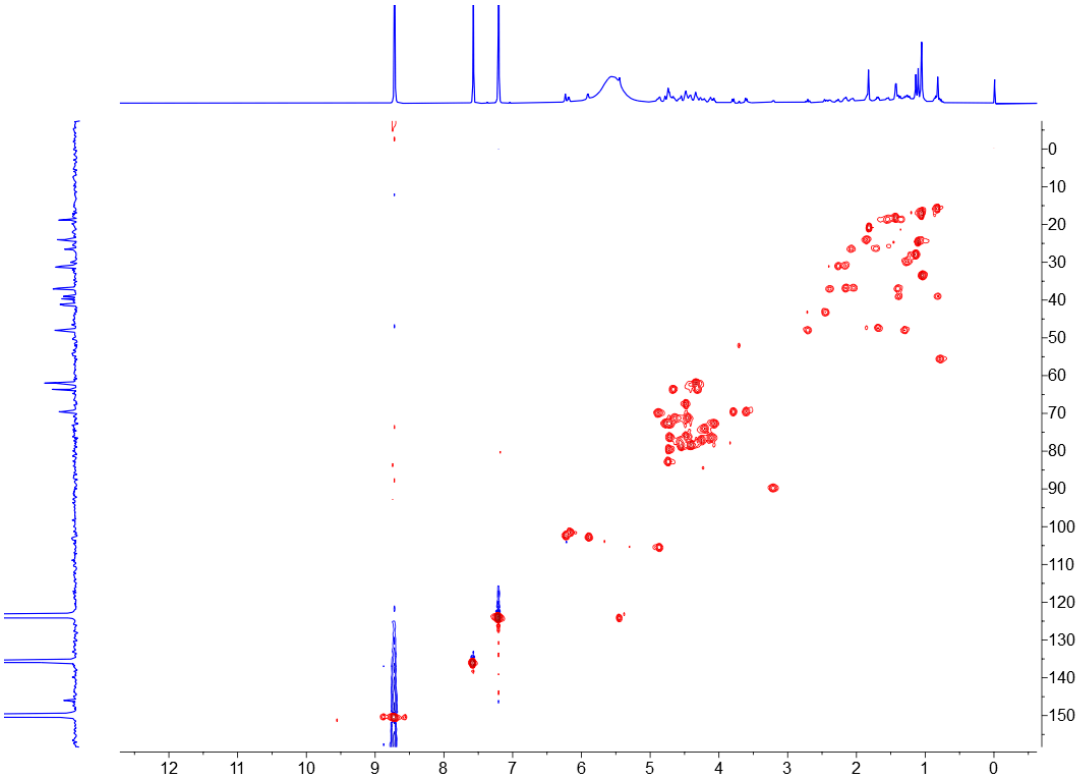

Figure S16. The HSQC spectrum of compound **2** (600/151 MHz, Pyr-d_5).

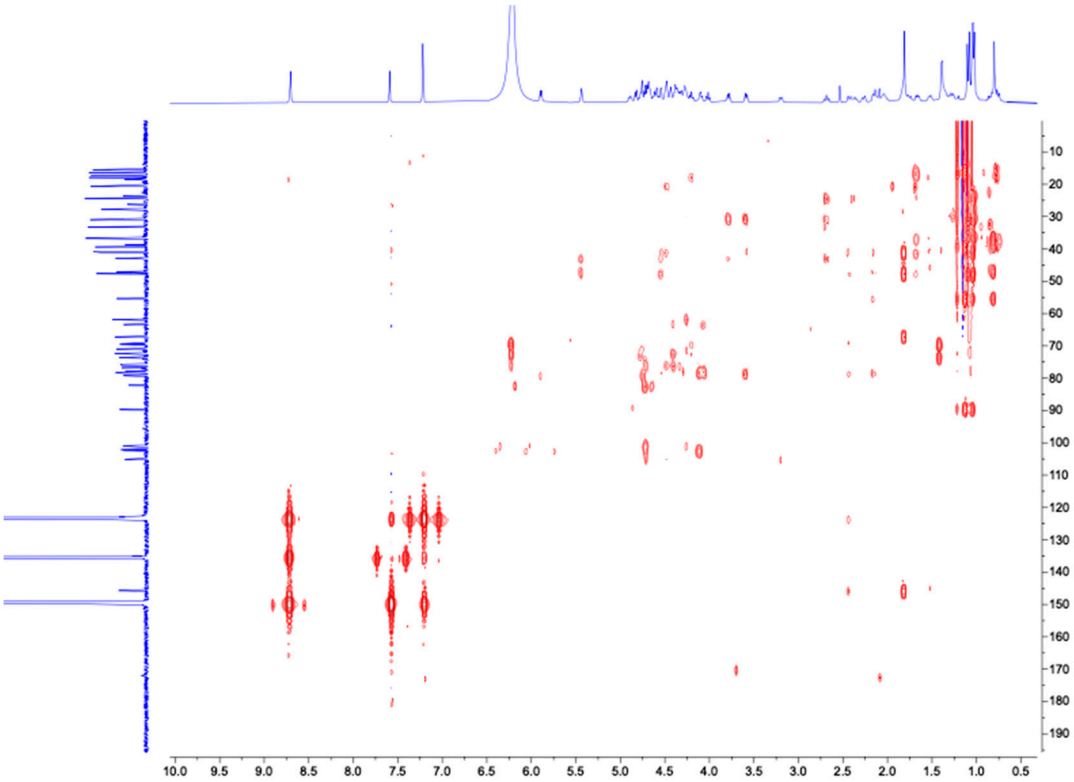

Figure S17. The HMBC spectrum of compound **2** (600/151 MHz, Pyr-d_5).

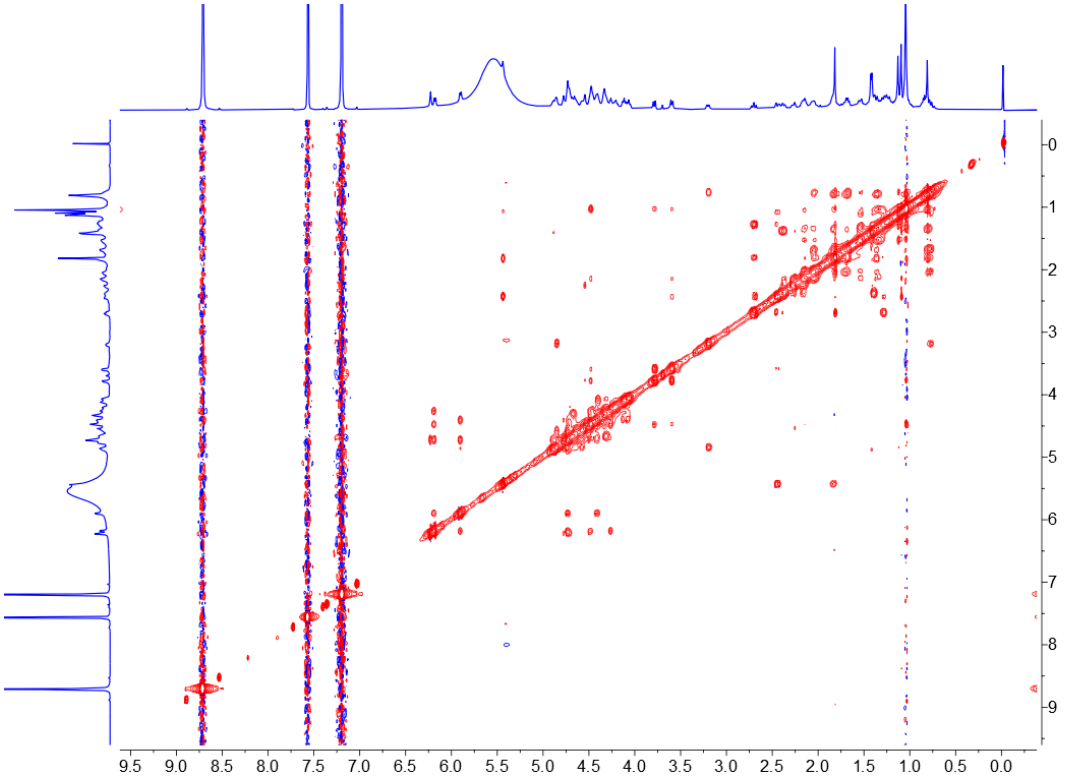

Figure S18. The NOESY spectrum of compound **2** (600 MHz, Pyr-d_5).

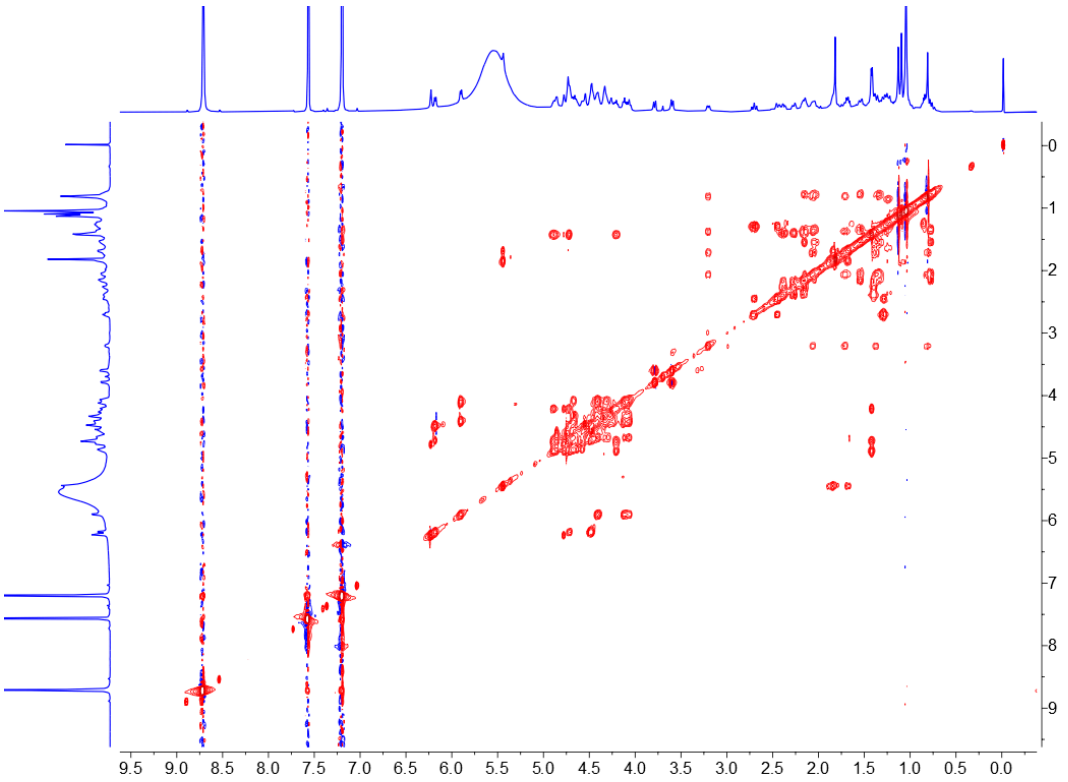

Figure S19. The TOCSY spectrum of compound **2** (600 MHz, Pyr-d_5).

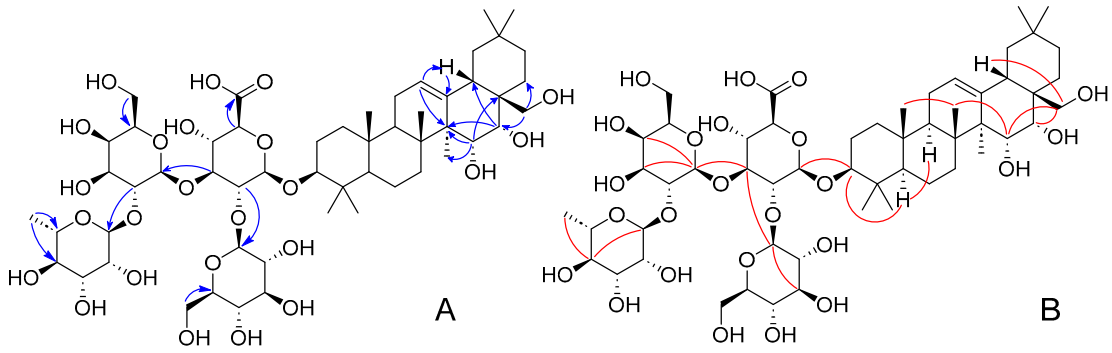

Figure S20. Key HMBC (A) and NOESY (B) correlations of compound **2**.

3. Spectroscopic data for compound **3**

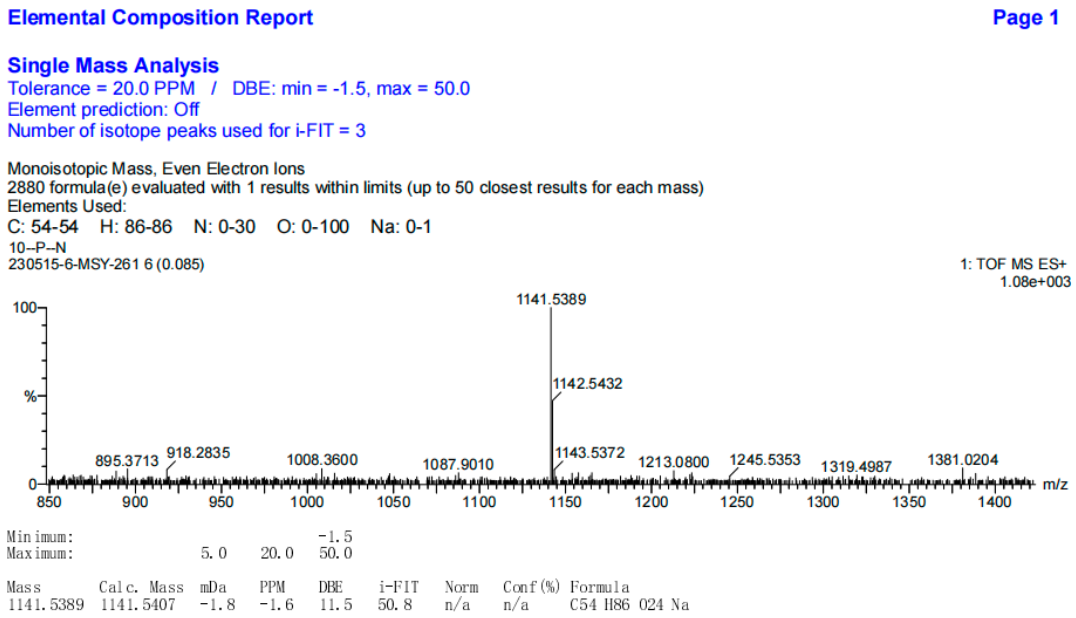

Figure S21. The HR-ESI-MS of compound **3**.

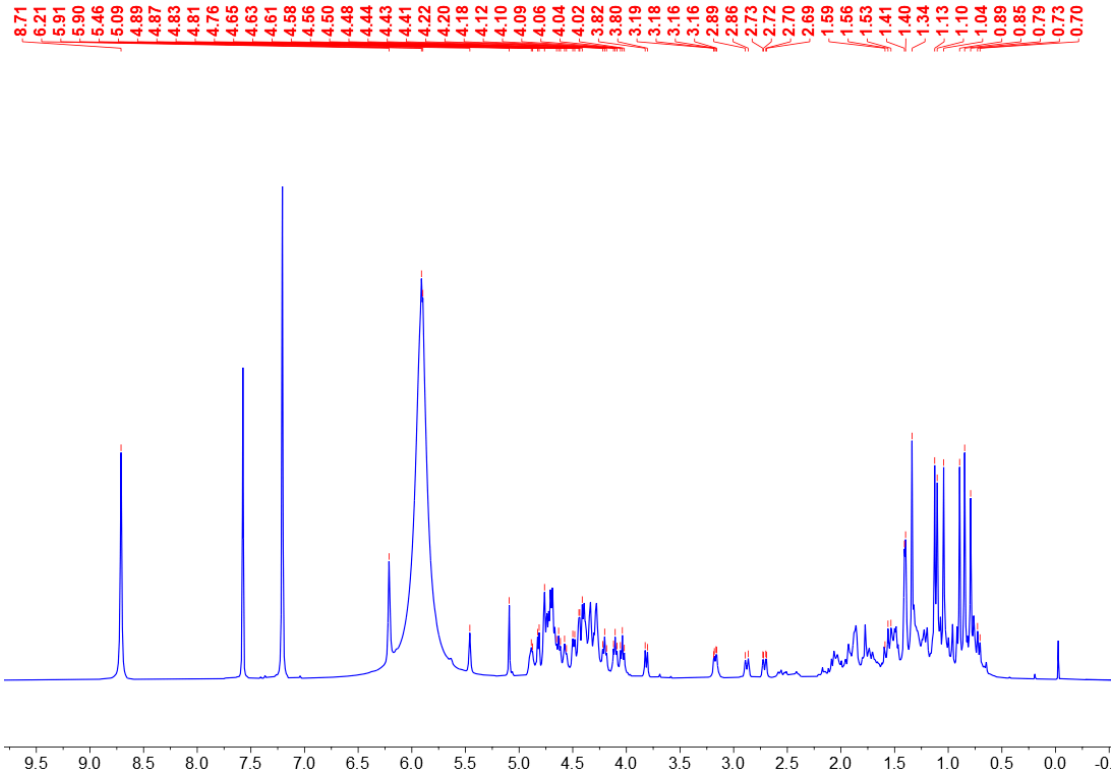

Figure S22. The ^{1}H NMR spectrum of compound **3** (600 MHz, Pyr-d_5).

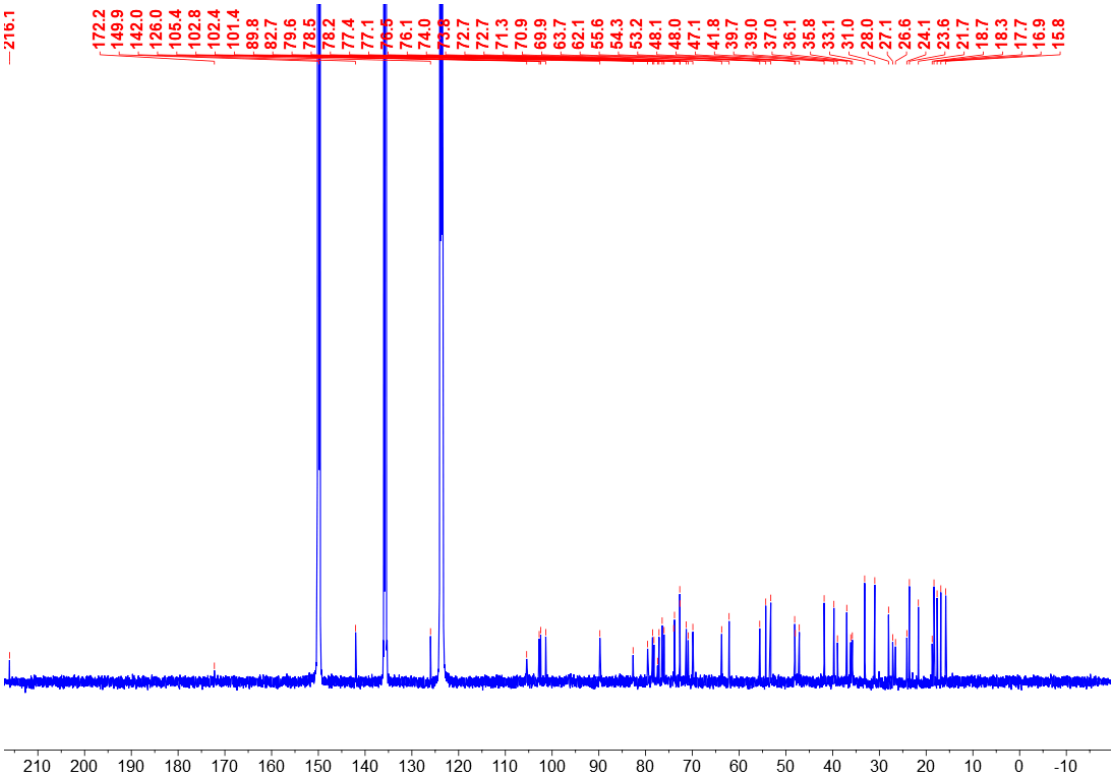

Figure S23. The ^{13}C NMR spectrum of compound **3** (151 MHz, Pyr-d_5).

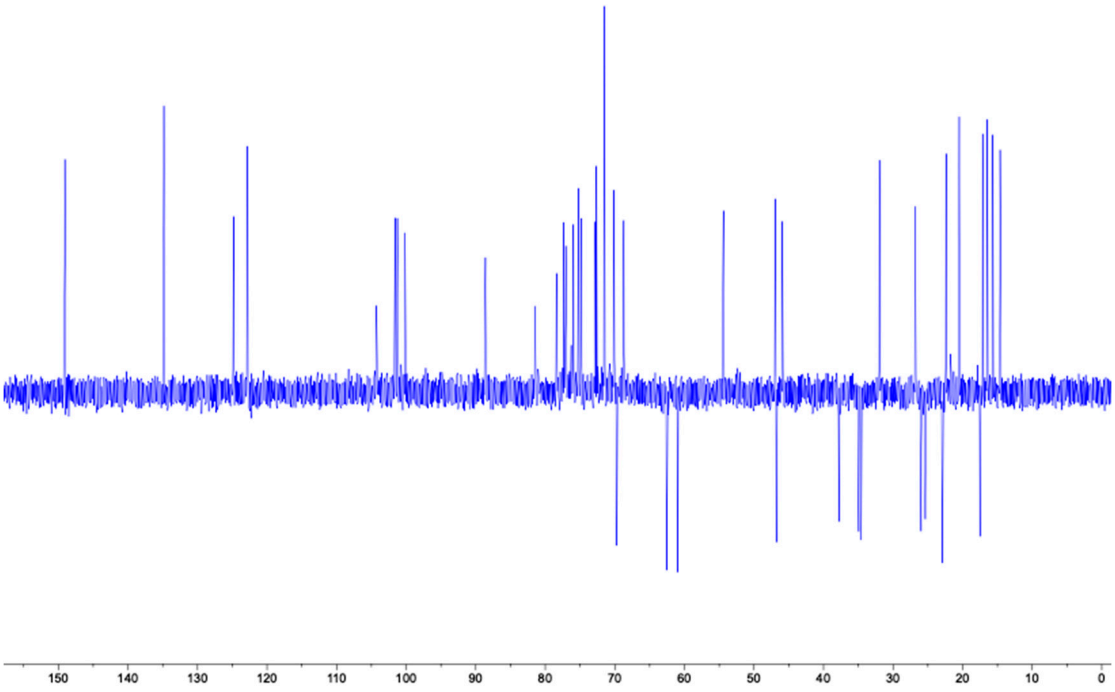

Figure S24. The DEPT 135 spectrum of compound **3** (151 MHz, Pyr-d_5).

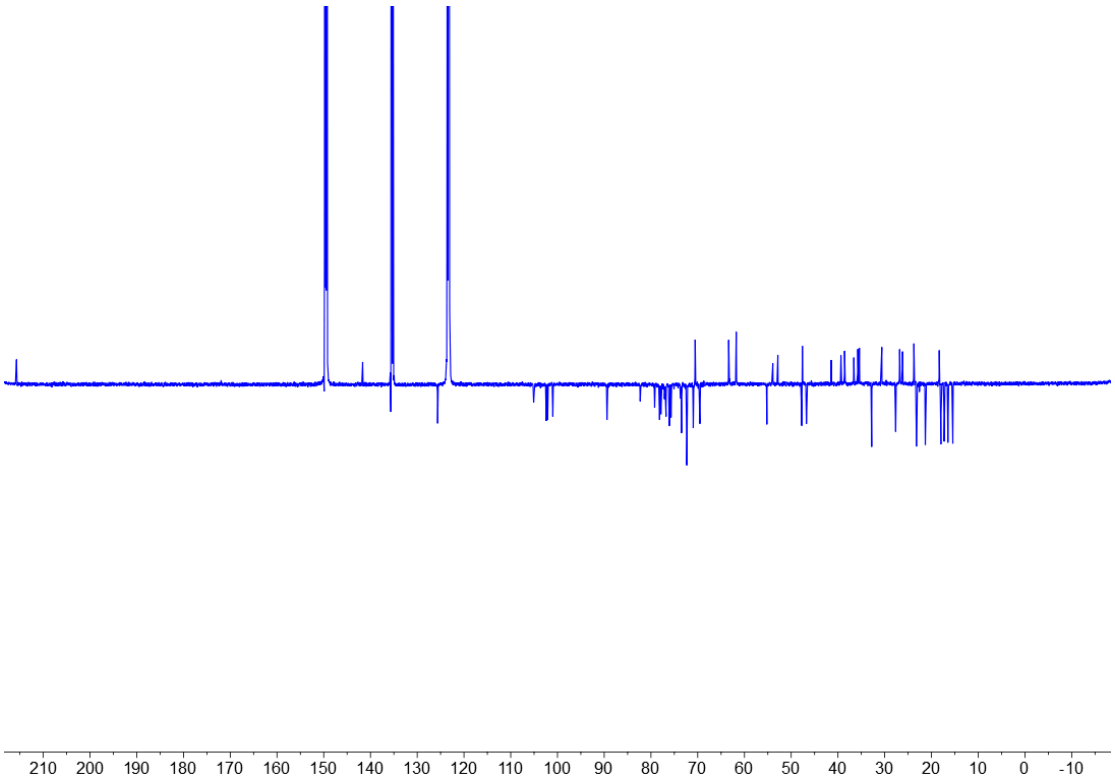

Figure S25. The DEPTQ spectrum of compound **3** (151 MHz, Pyr-d_5).

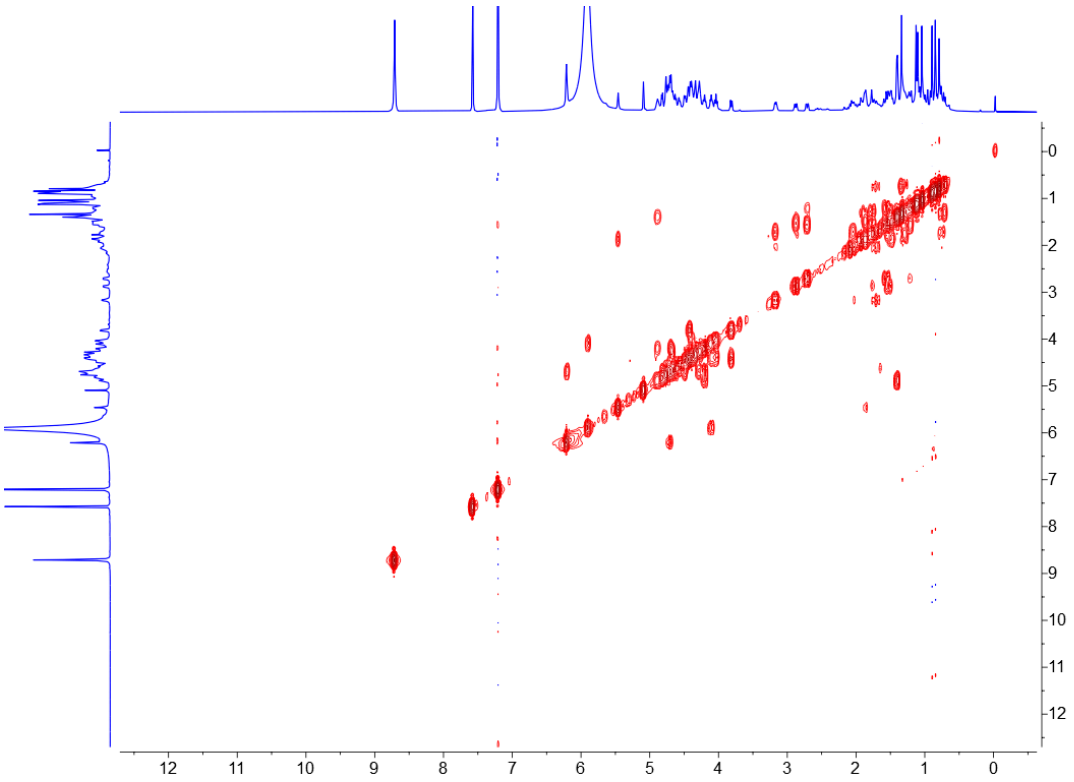

Figure S26. The ^{1}H-^{1}H COSY spectrum of compound **3** (600 MHz, Pyr-d_5).

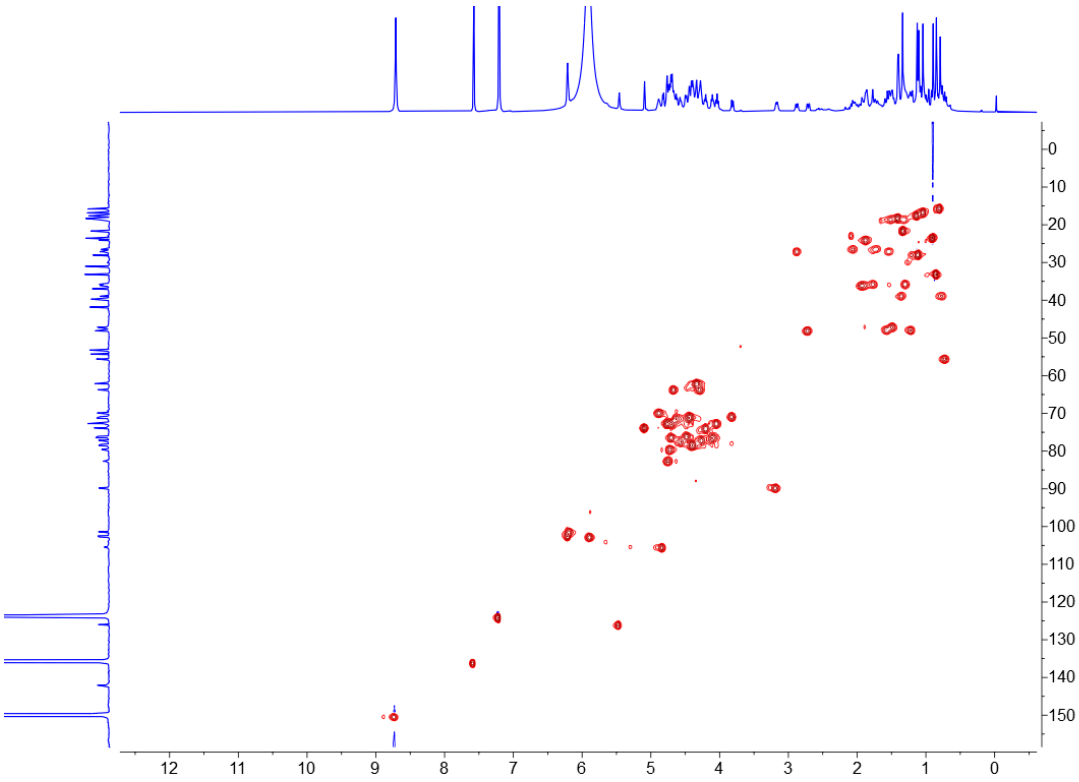

Figure S27. The HSQC spectrum of compound **3** (600/151 MHz, Pyr-d_5).

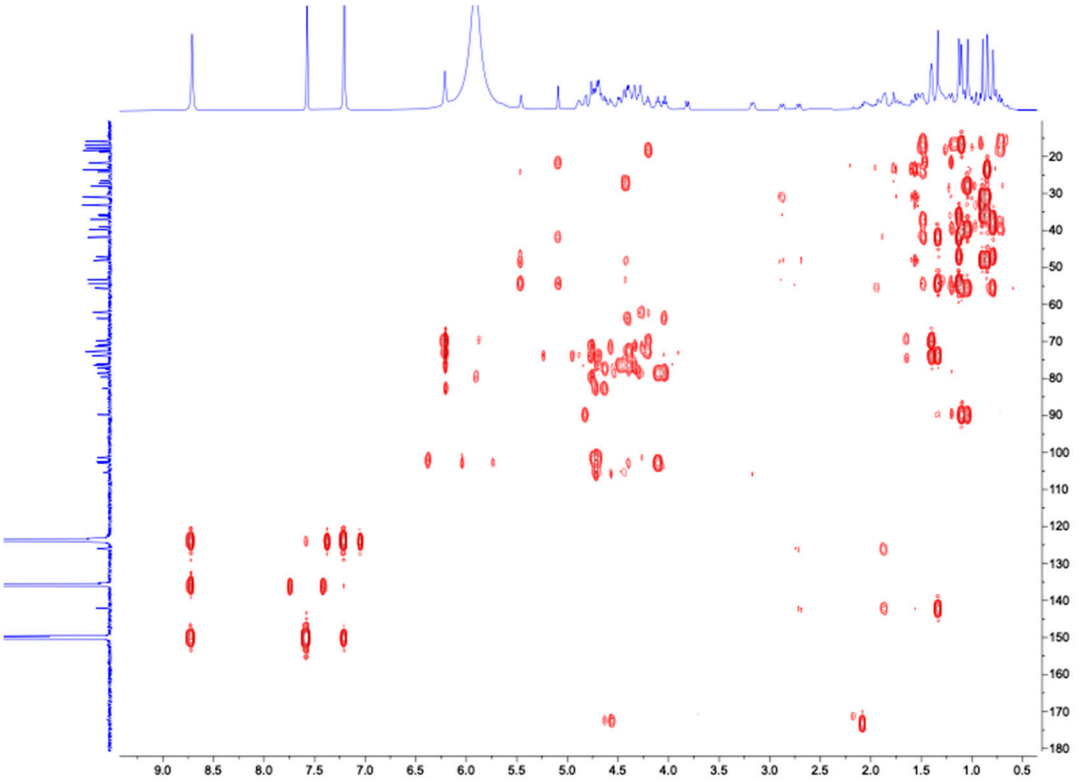

Figure S28. The HMBC spectrum of compound **3** (600/151 MHz, Pyr-d_5).

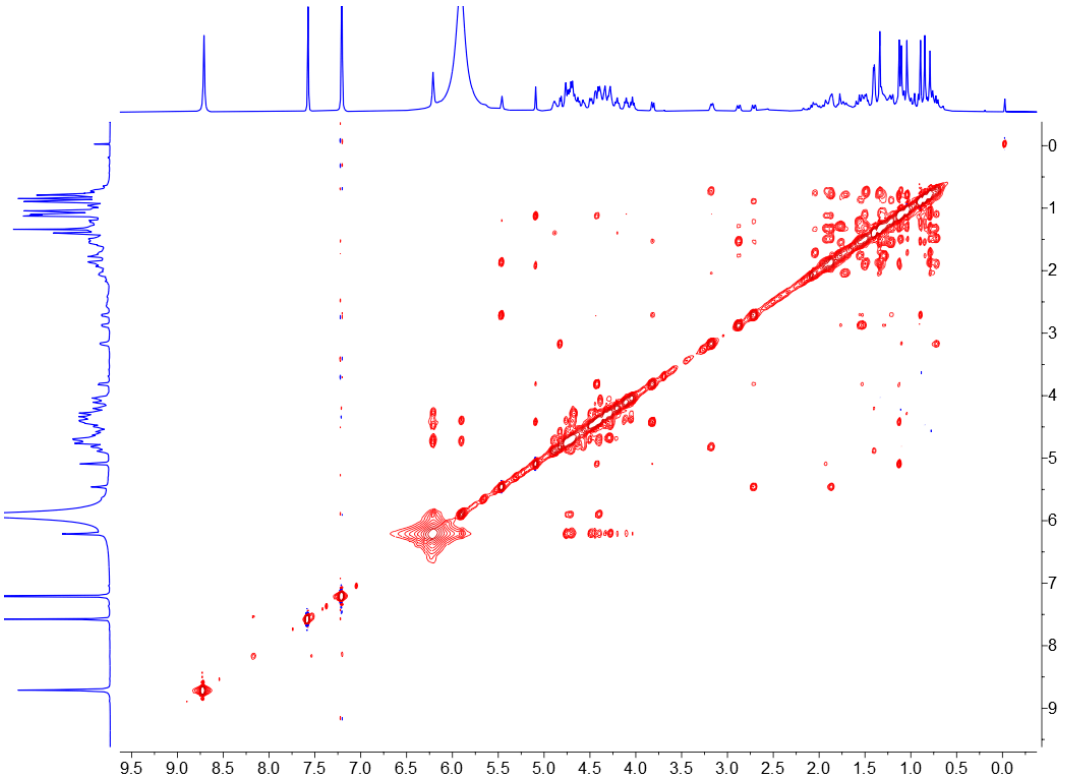

Figure S29. The NOESY spectrum of compound **3** (600 MHz, Pyr-d_5).

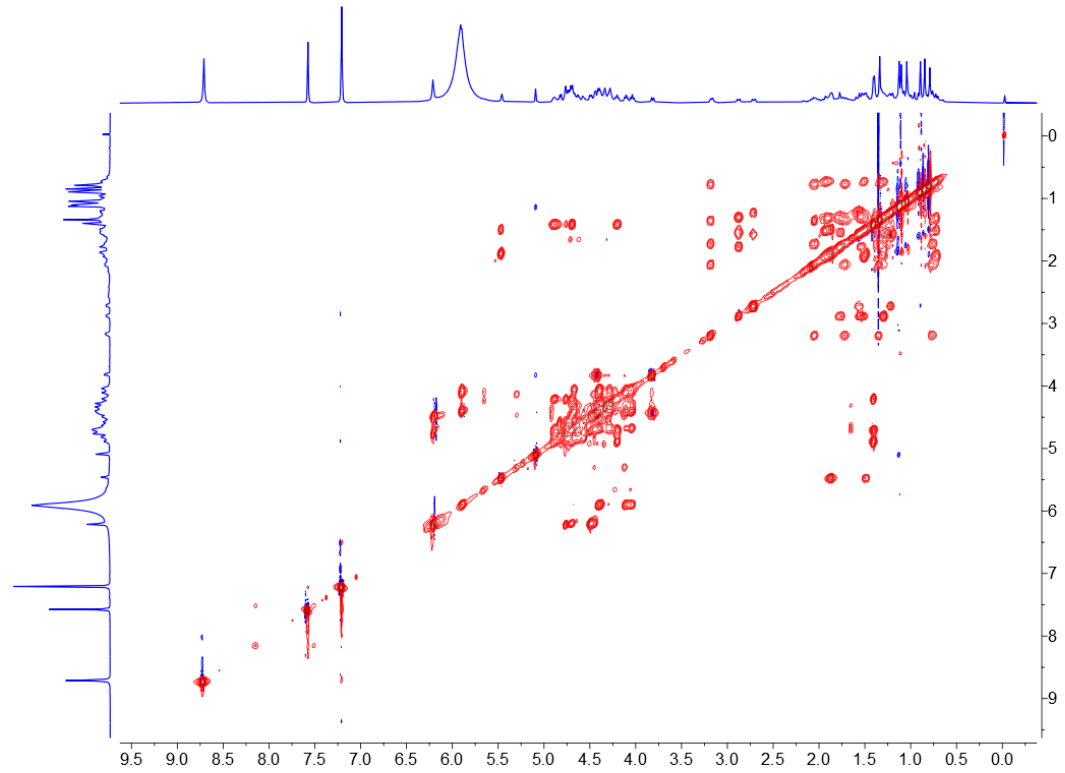

Figure S30. The TOCSY spectrum of compound **3** (600 MHz, Pyr-d_5).

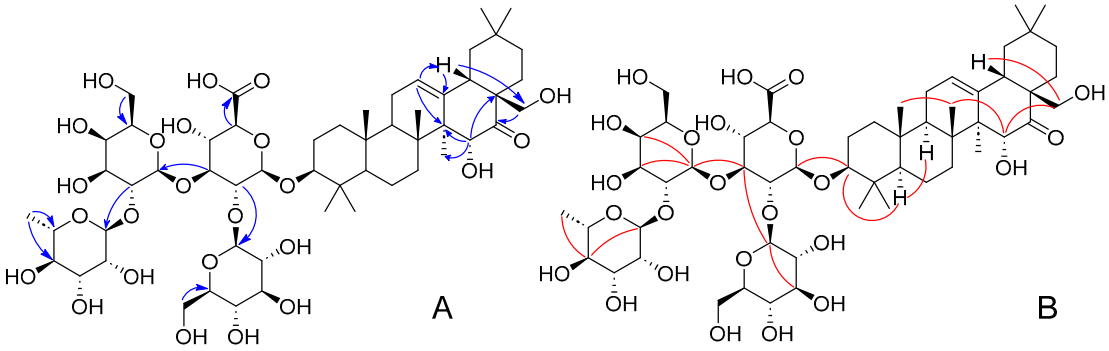

Figure S31. Key HMBC (A) and NOESY (B) correlations of compound **3**.

4. Spectroscopic data for compound **4**

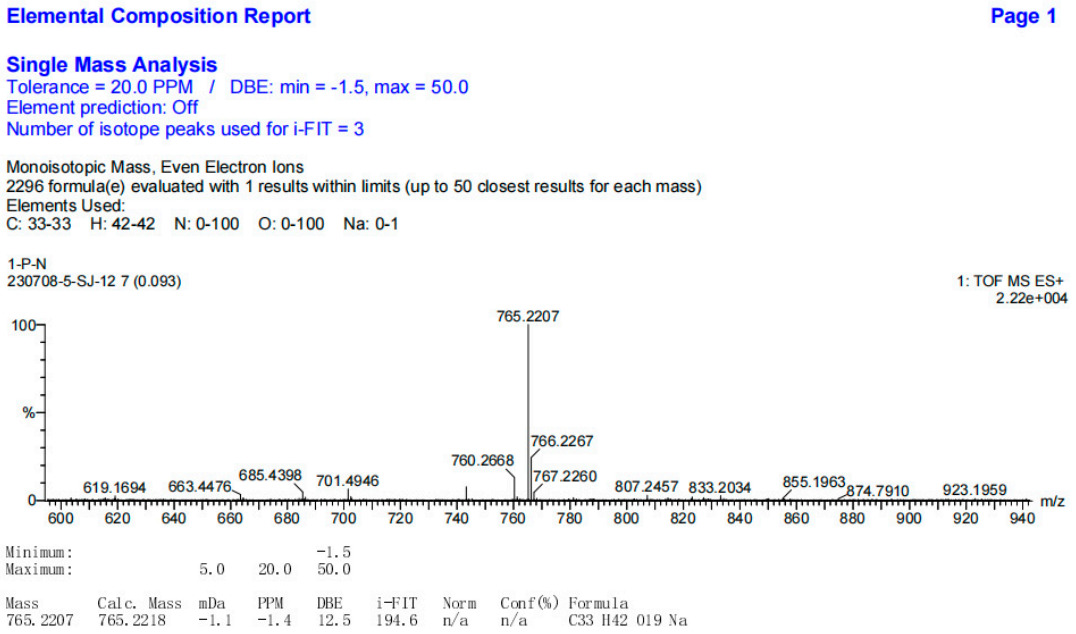

Figure S32. The HR-ESI-MS of compound **4**.

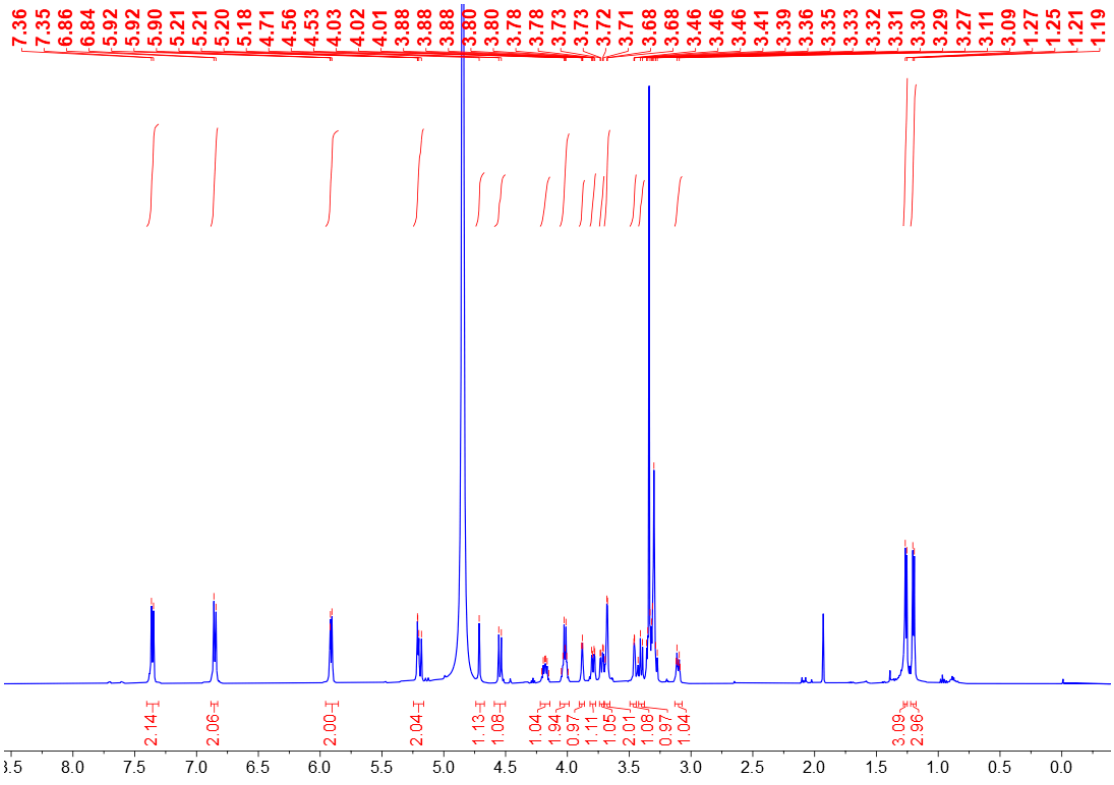

Figure S33. The ^{1}H NMR spectrum of compound **4** (600 MHz, CD_3OD).

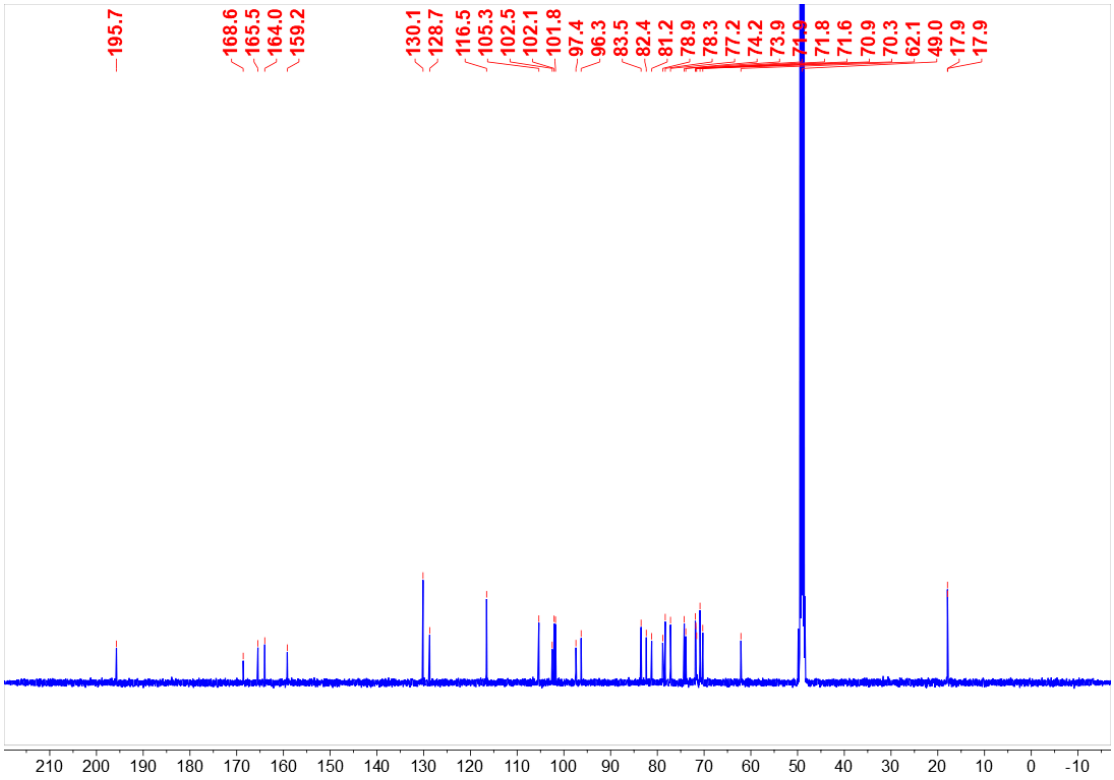

Figure S34. The ^{13}C NMR spectrum of compound **4** (151 MHz, CD_3OD).

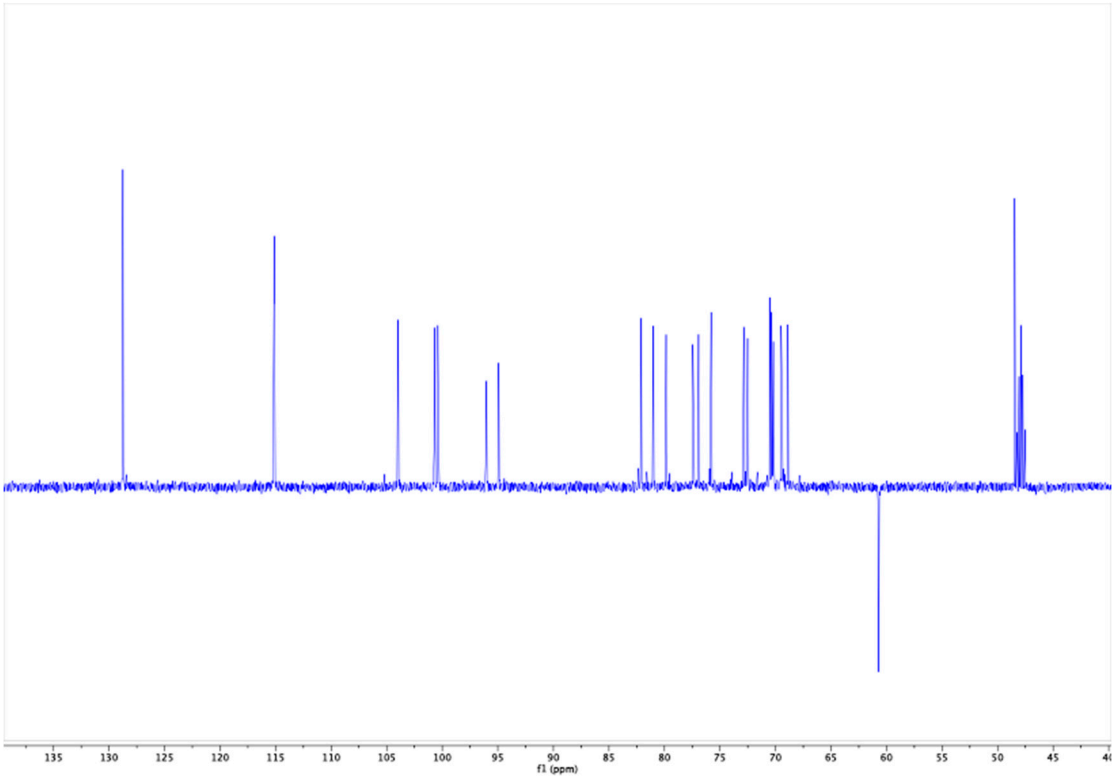

Figure S35. The DEPT 135 spectrum of compound **4** (151 MHz, CD_3OD).

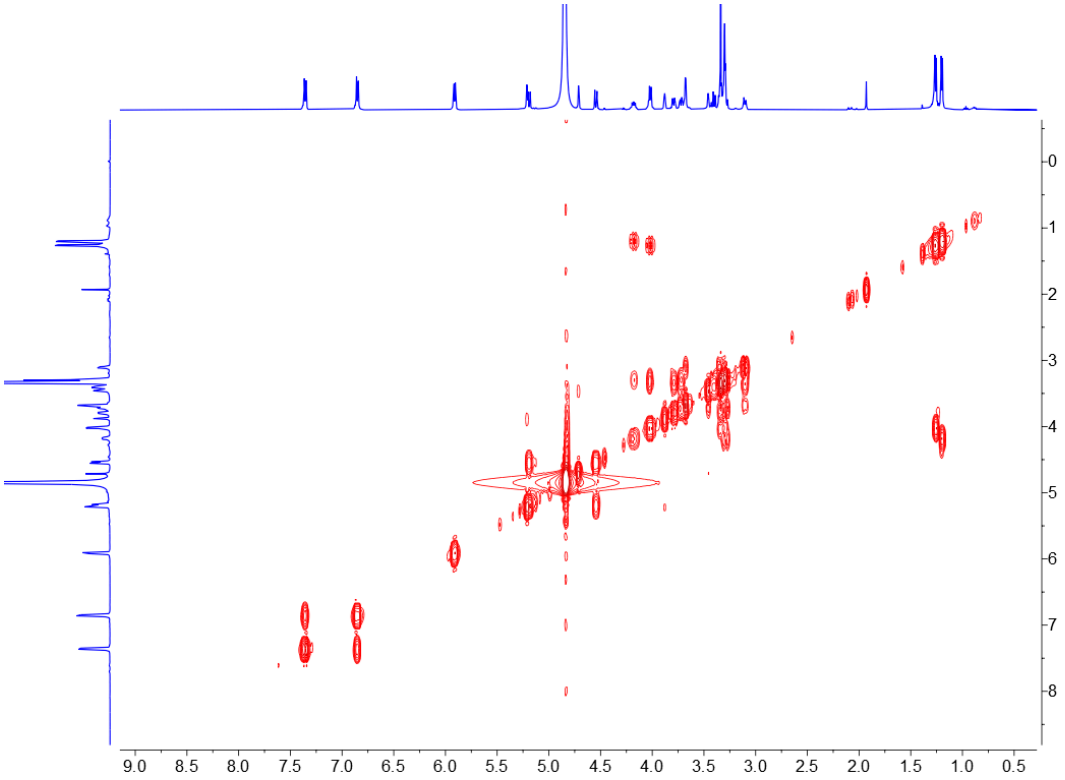

Figure S36. The ^{1}H-^{1}H COSY spectrum of compound **4** (600 MHz, CD_3OD).

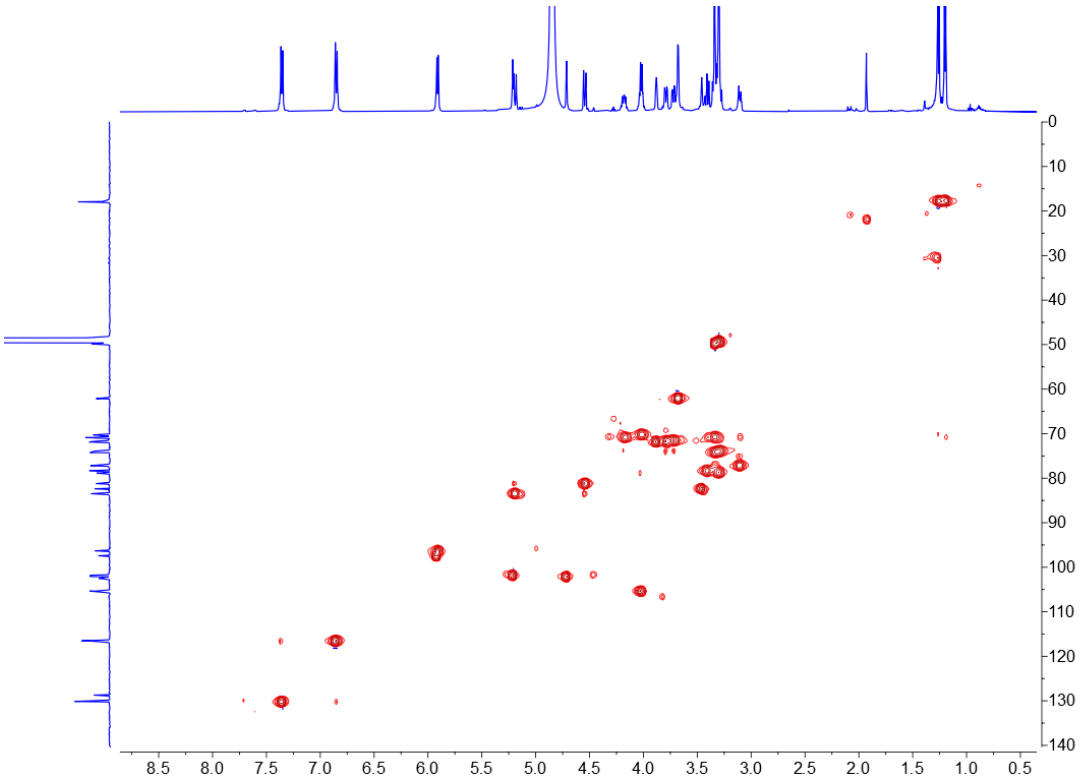

Figure S37. The HSQC spectrum of compound **4** (600/151 MHz, CD_3OD).

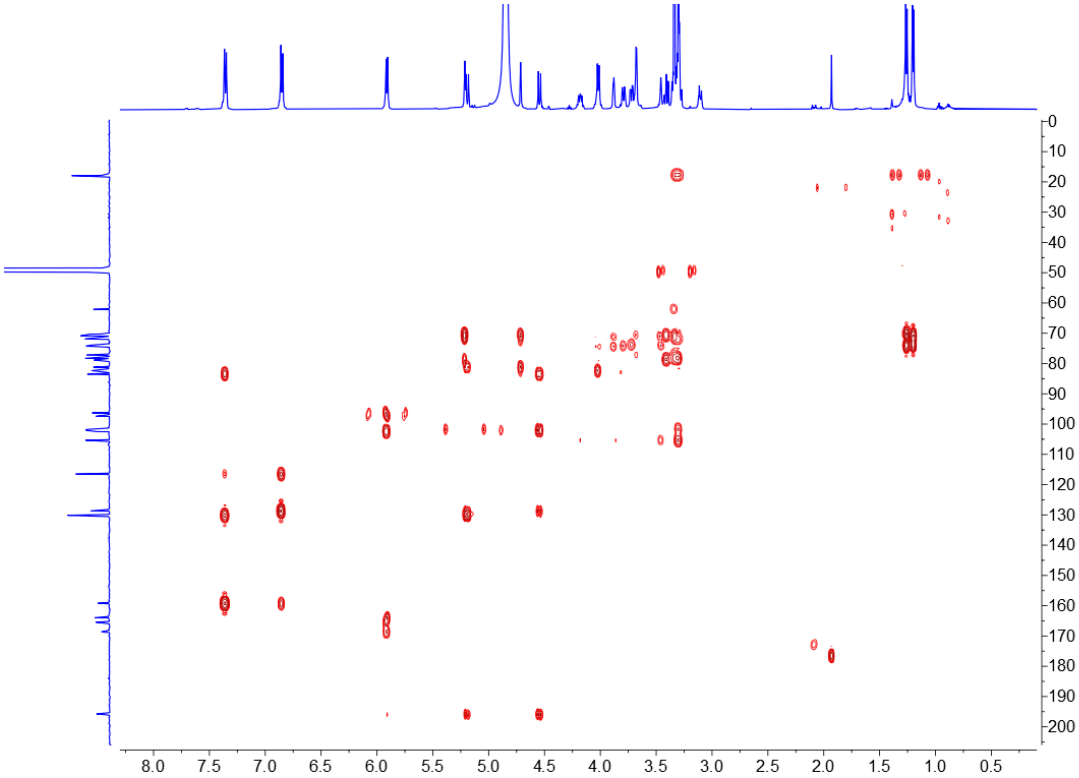

Figure S38. The HMBC spectrum of compound **4** (600/151 MHz, CD_3OD).

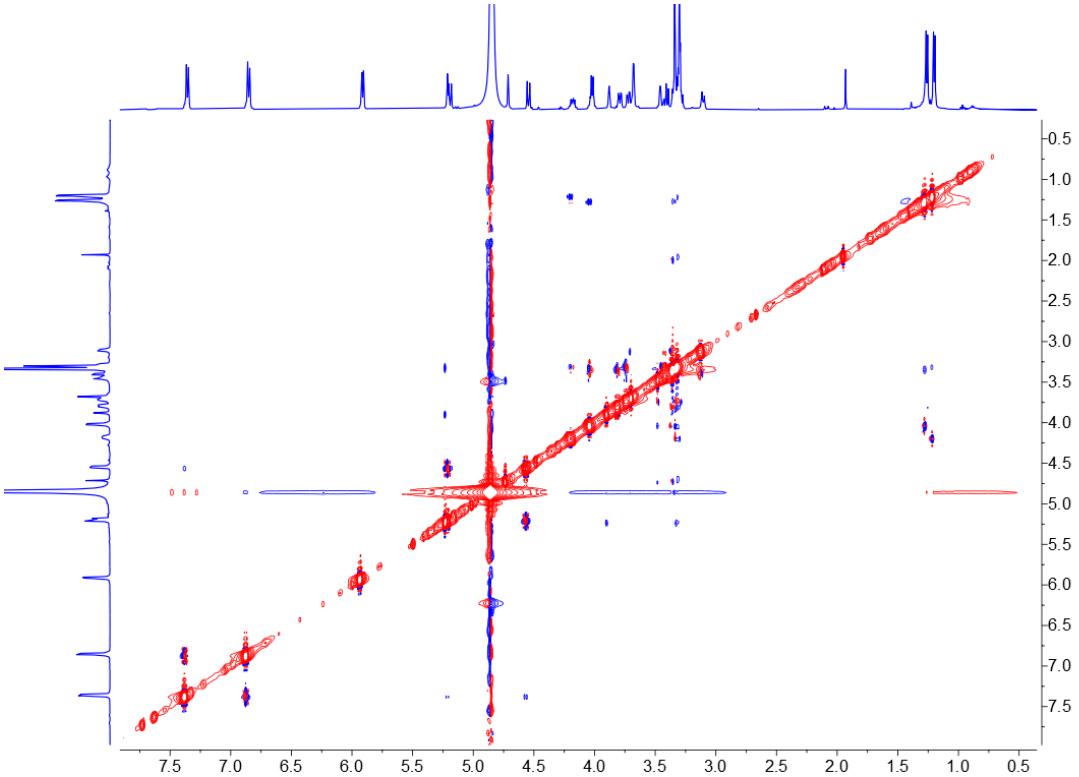

Figure S39. The NOESY spectrum of compound **4** (600 MHz, CD_3OD).

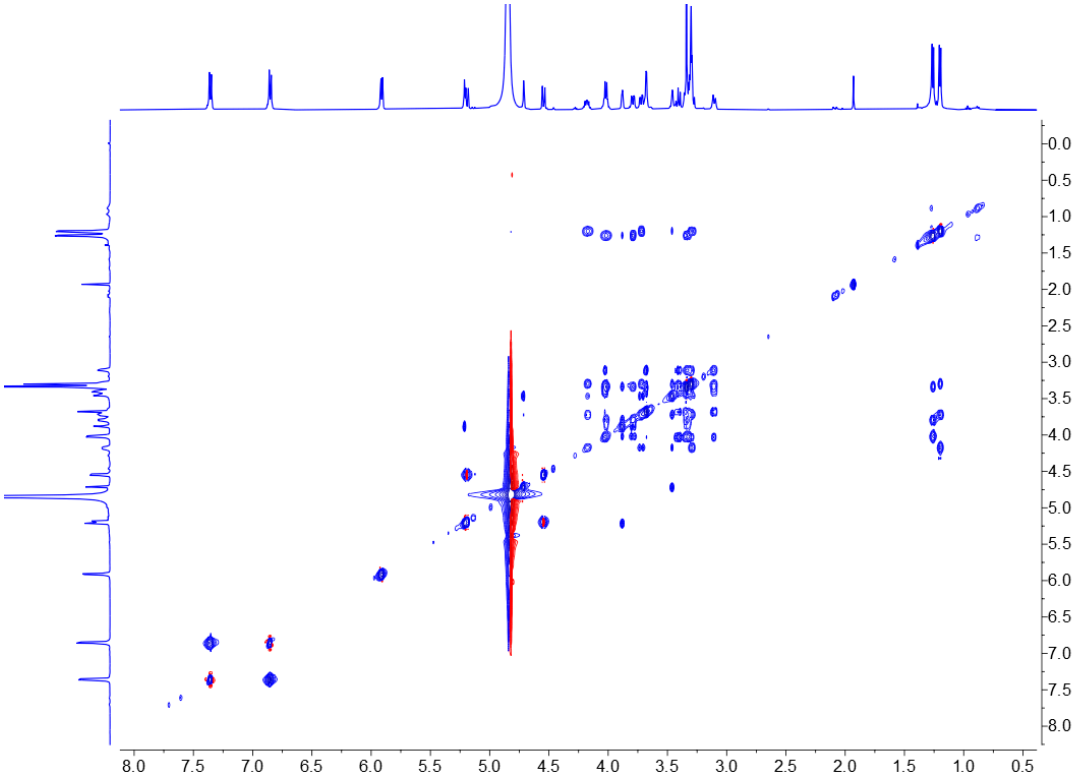

Figure S40. The TOCSY spectrum of compound **4** (600 MHz, CD_3OD).

5. Spectroscopic data for compound **5**

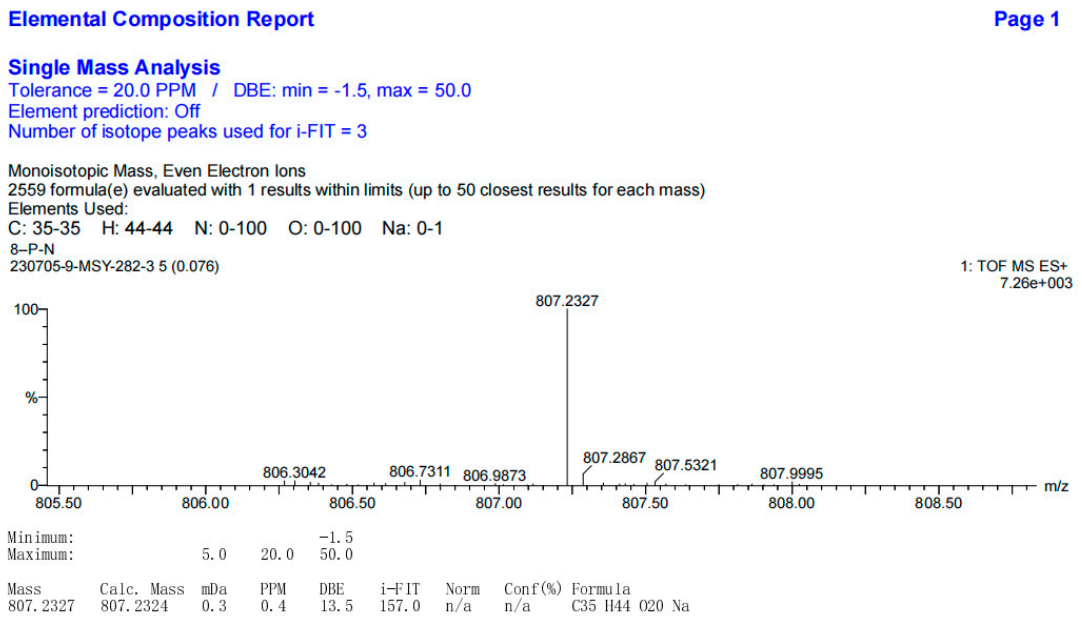

Figure S41. The HR-ESI-MS of compound **5**.

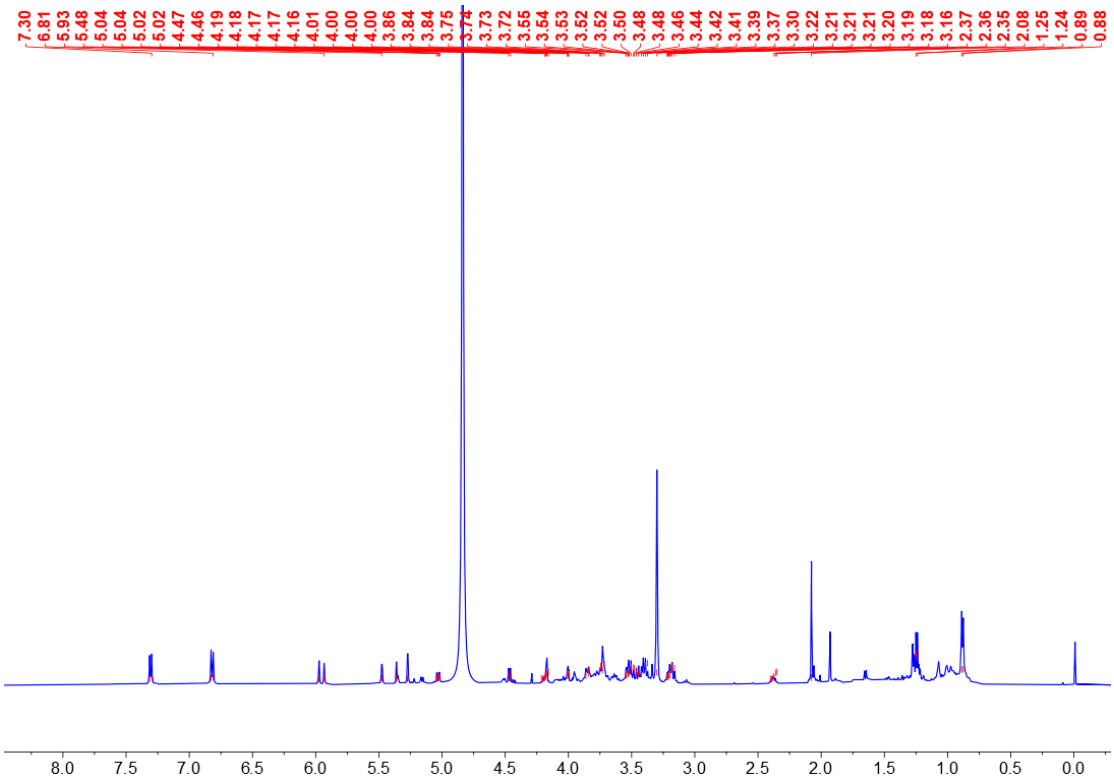

Figure S42. The ^{1}H NMR spectrum of compound **5** (600 MHz, CD_3OD).

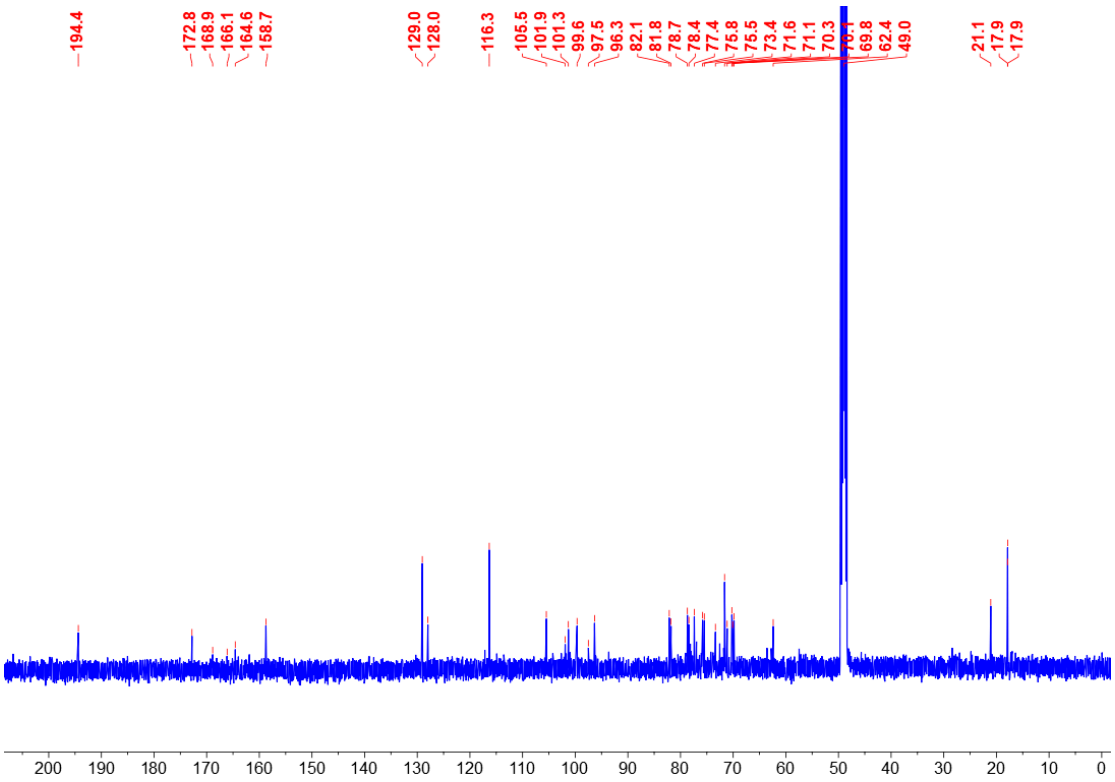

Figure S43. The ^{13}C NMR spectrum of compound **5** (151 MHz, CD_3OD).

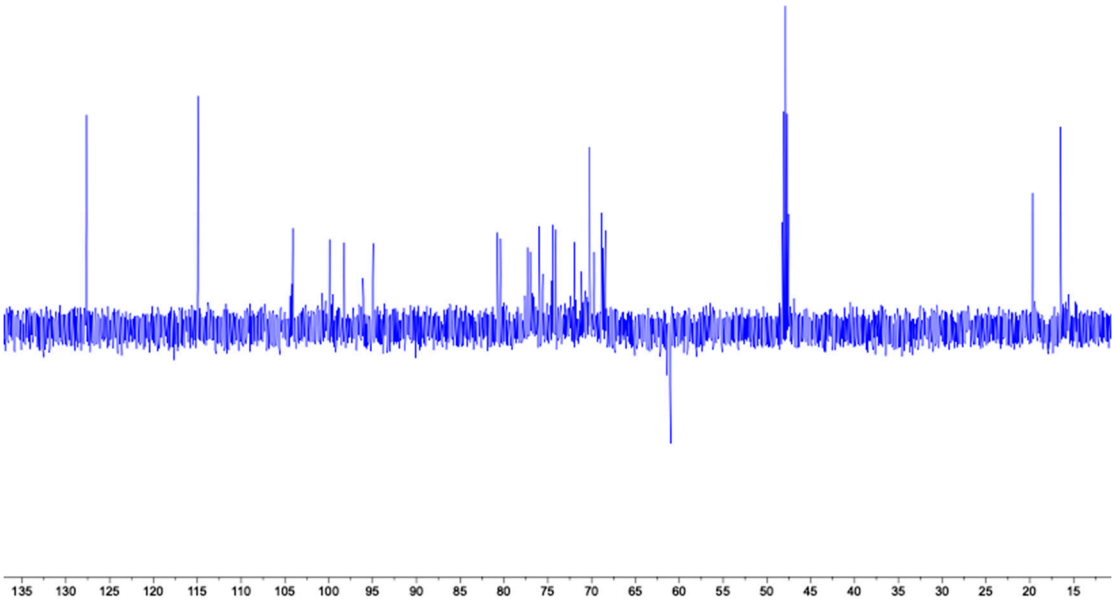

Figure S44. The DEPT 135 spectrum of compound **5** (151 MHz, CD_3OD).

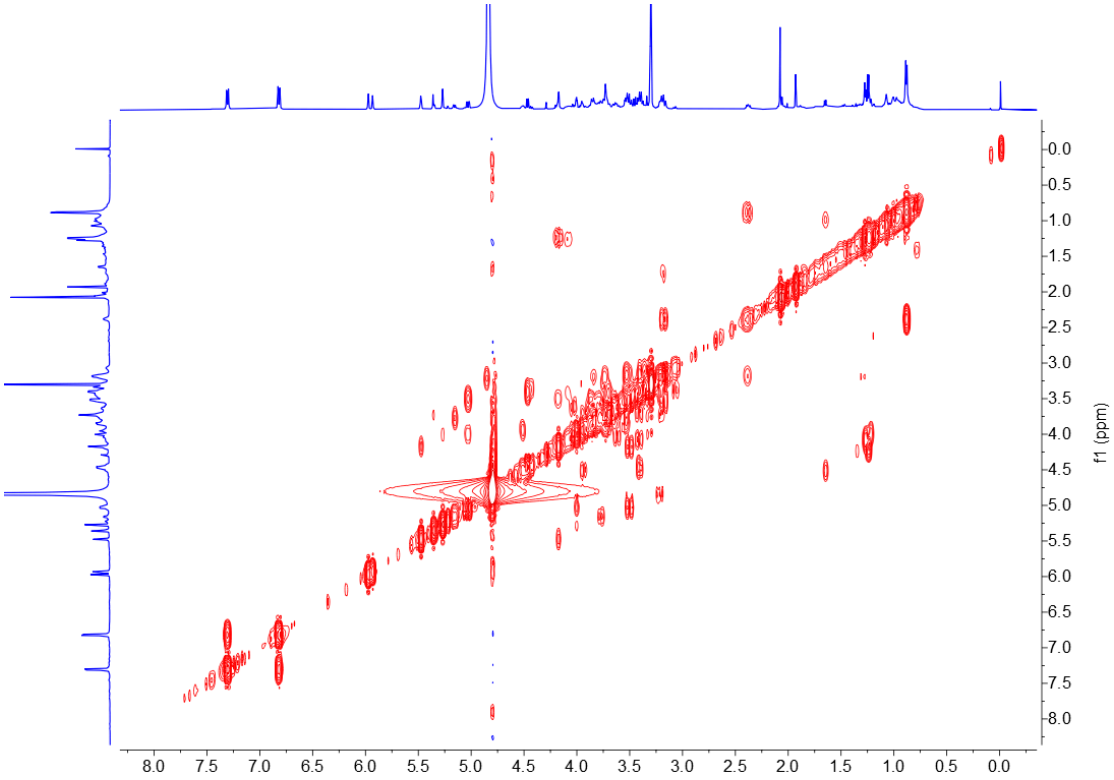

Figure S45. The ^{1}H-^{1}H COSY spectrum of compound **5** (600 MHz, CD_3OD).

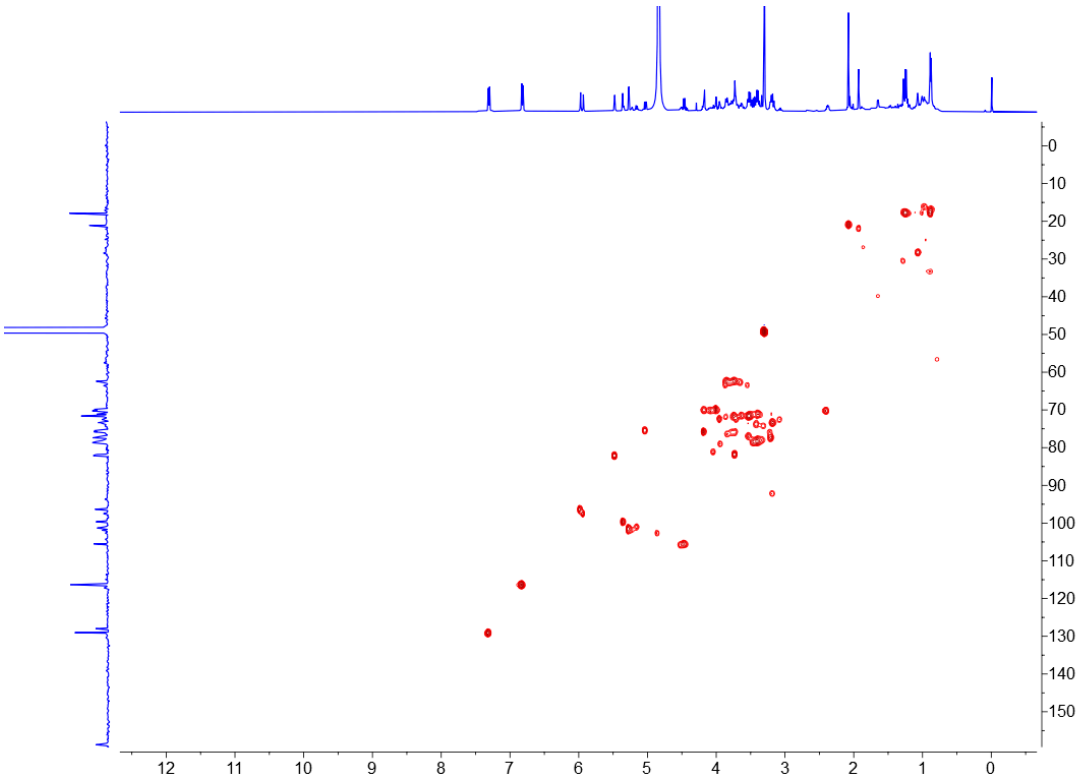

Figure S46. The HSQC spectrum of compound **5** (600/151 MHz, CD_3OD).

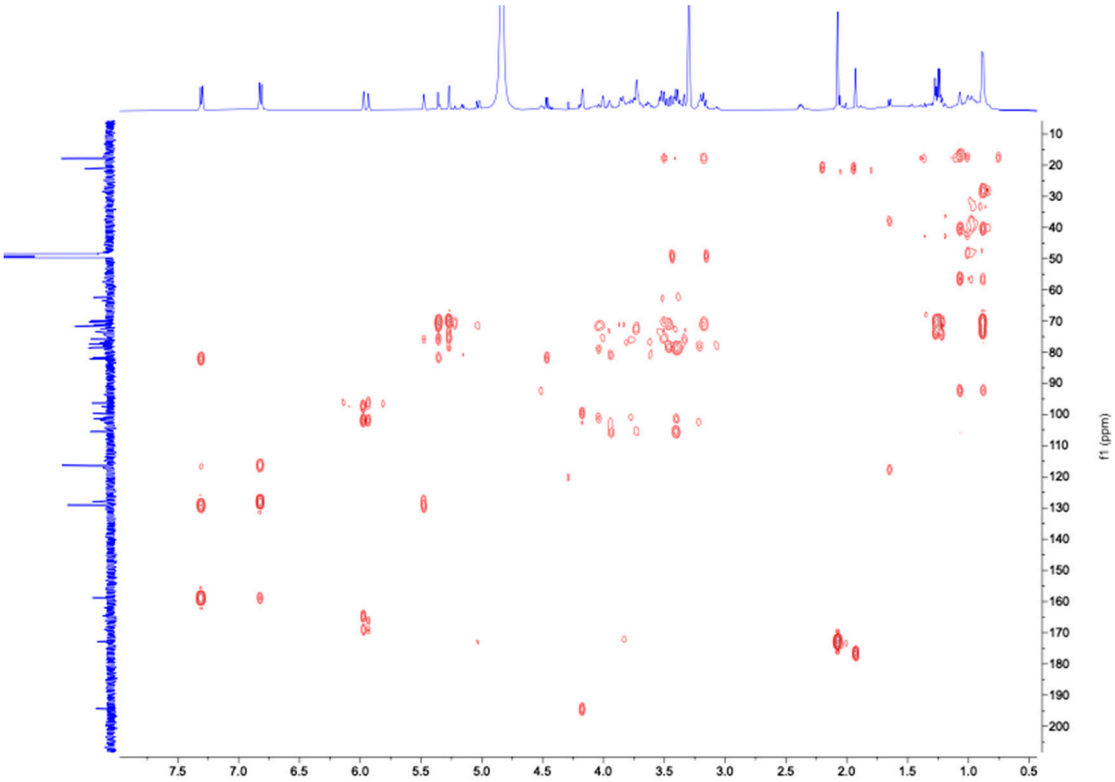

Figure S47. The HMBC spectrum of compound **5** (600/151 MHz, CD_3OD).

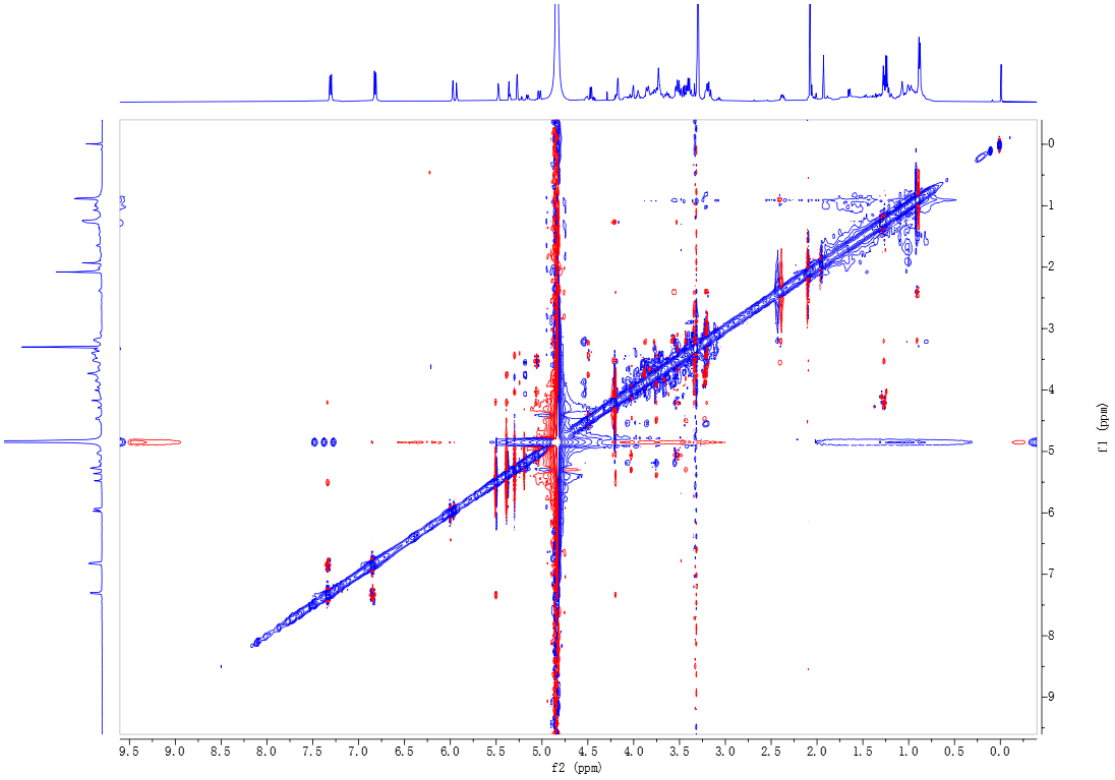

Figure S48. The NOESY spectrum of compound **5** (600 MHz, CD_3OD).

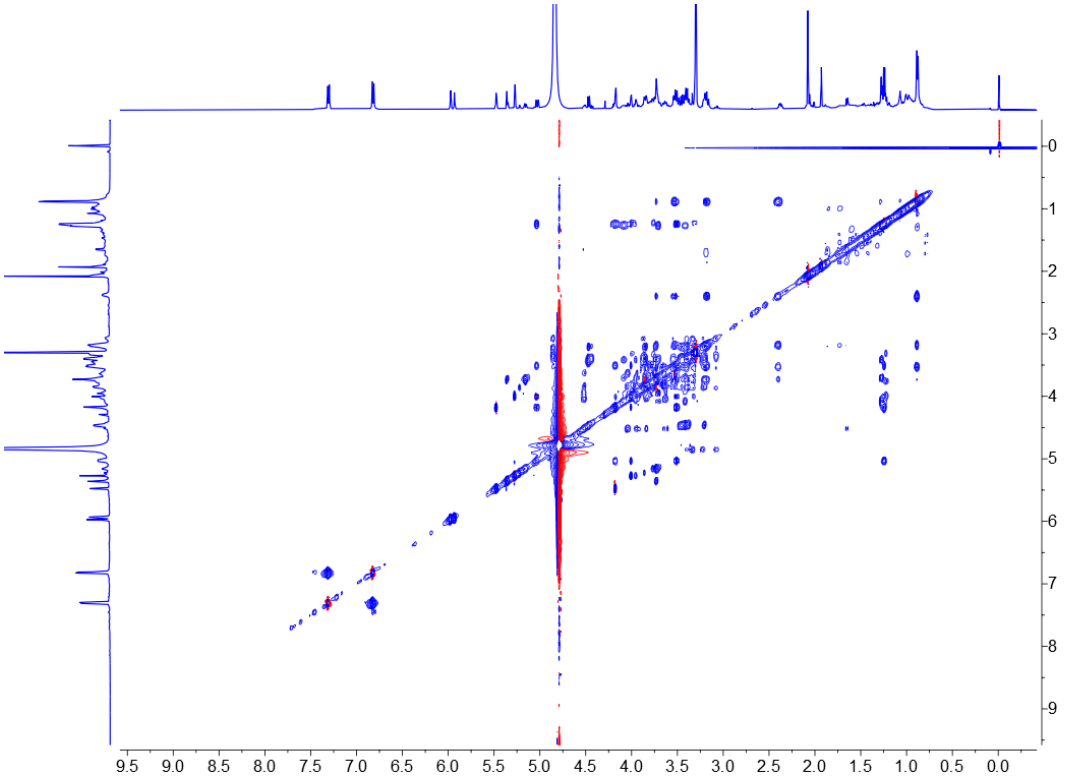

Figure S49. The TOCSY spectrum of compound **5** (600 MHz, CD_3OD).

6. Spectroscopic data for compound **6**

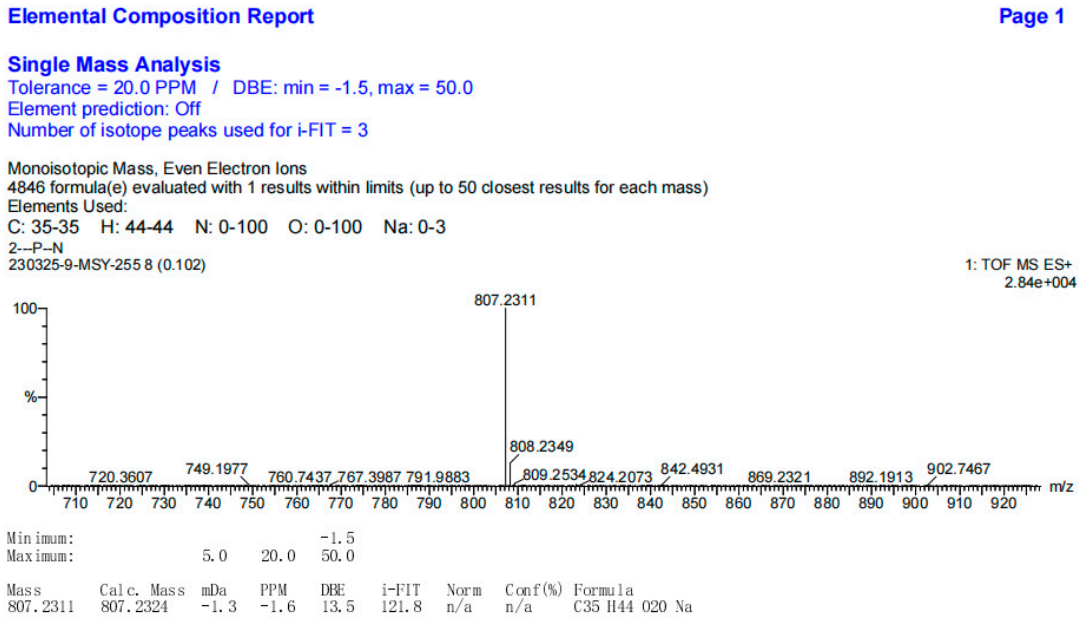

Figure S50. The HR-ESI-MS of compound **6**.

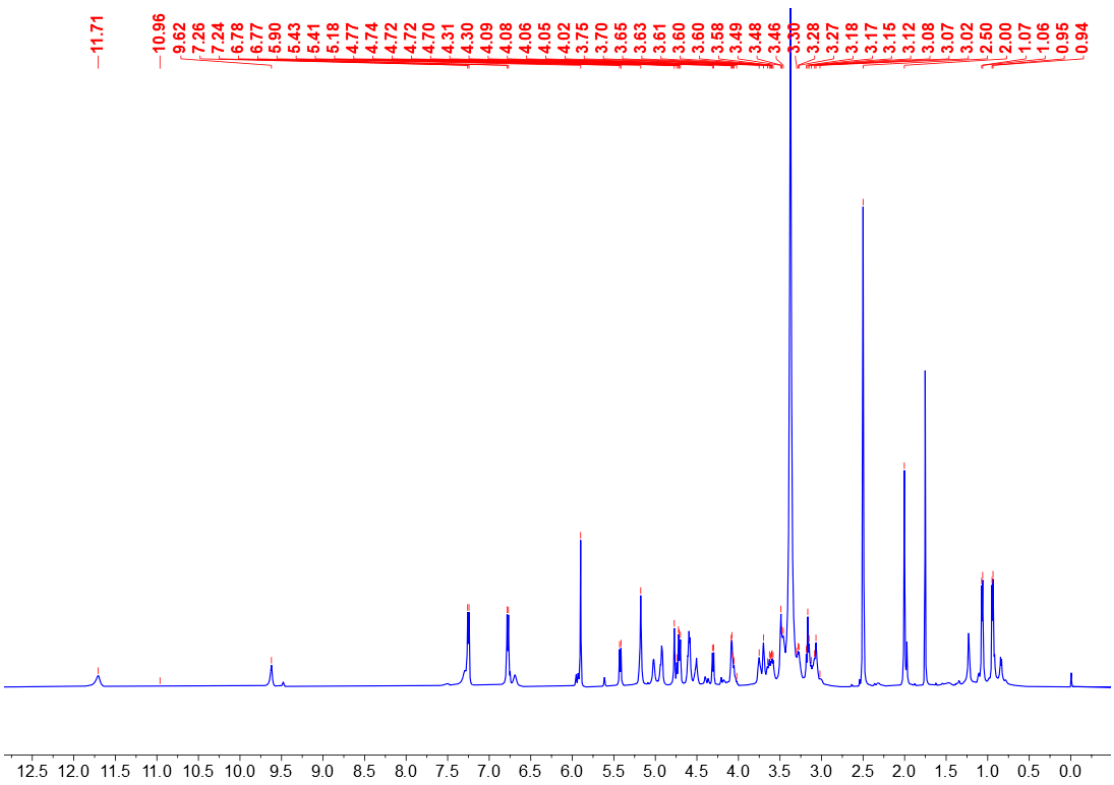

Figure S51. The ^{1}H NMR spectrum of compound **6** (600 MHz, DMSO-d_6).

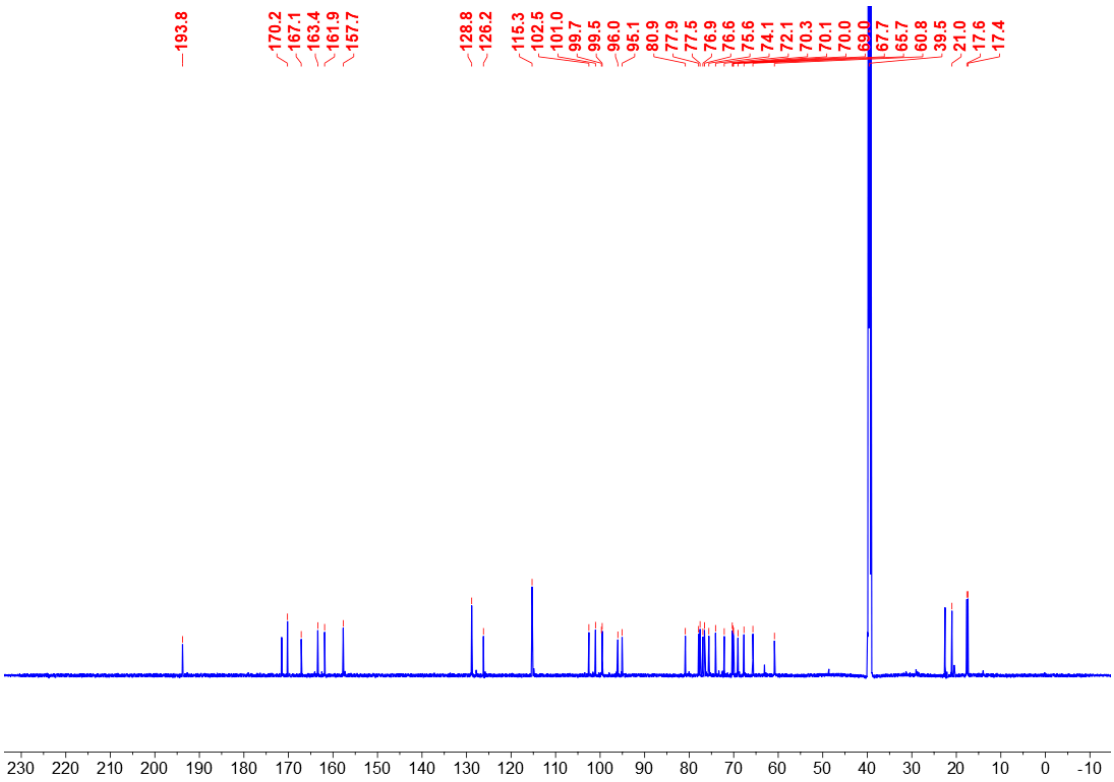

Figure S52. The ^{13}C NMR spectrum of compound **6** (151 MHz, DMSO-d_6).

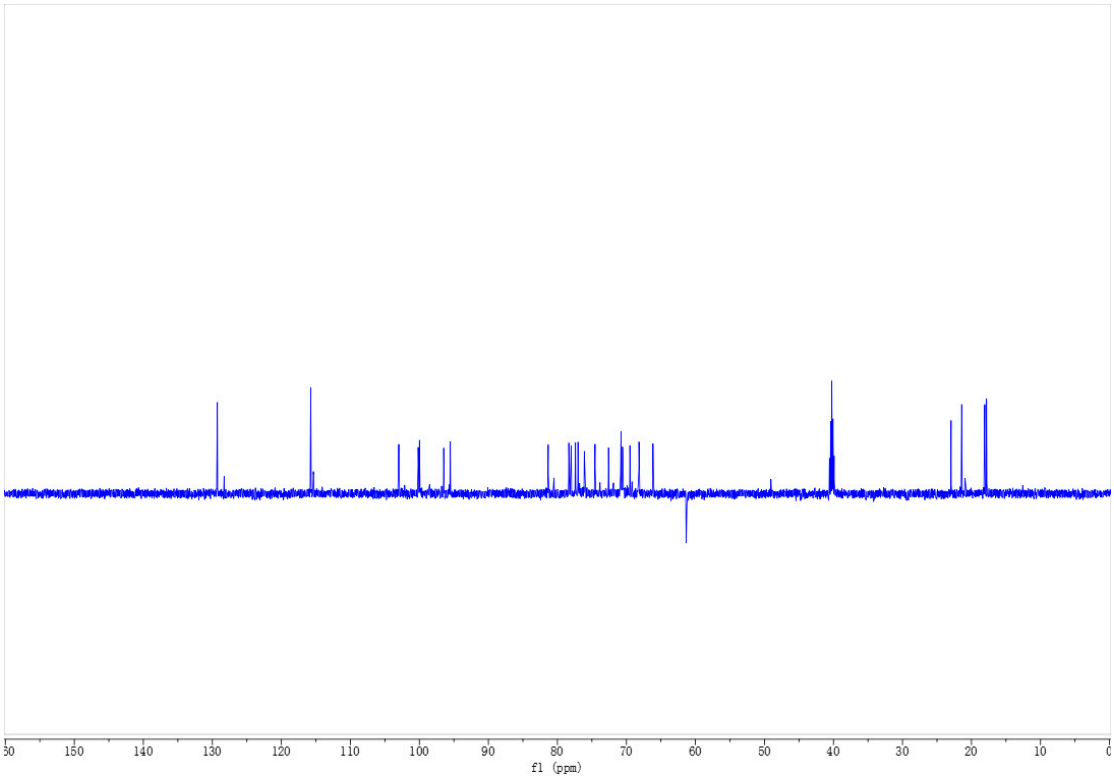

Figure S53. The DEPT 135 spectrum of compound **6** (151 MHz, DMSO-d_6).

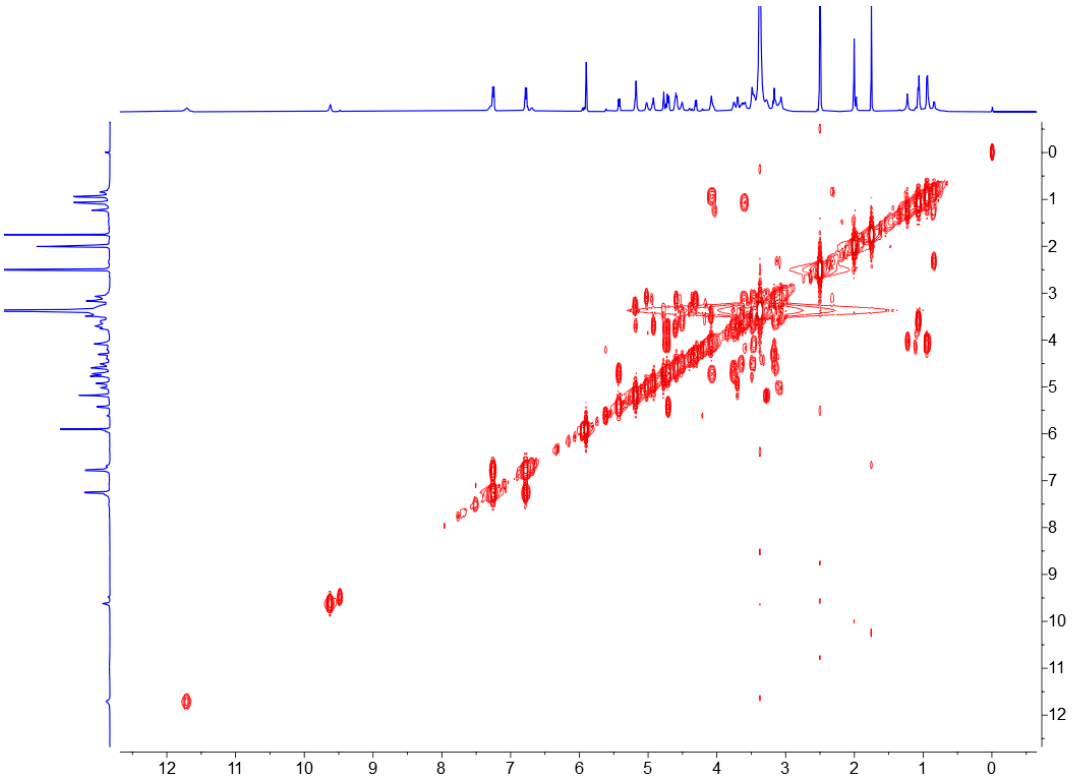

Figure S54. The ^{1}H-^{1}H COSY spectrum of compound **6** (600 MHz, DMSO-d_6).

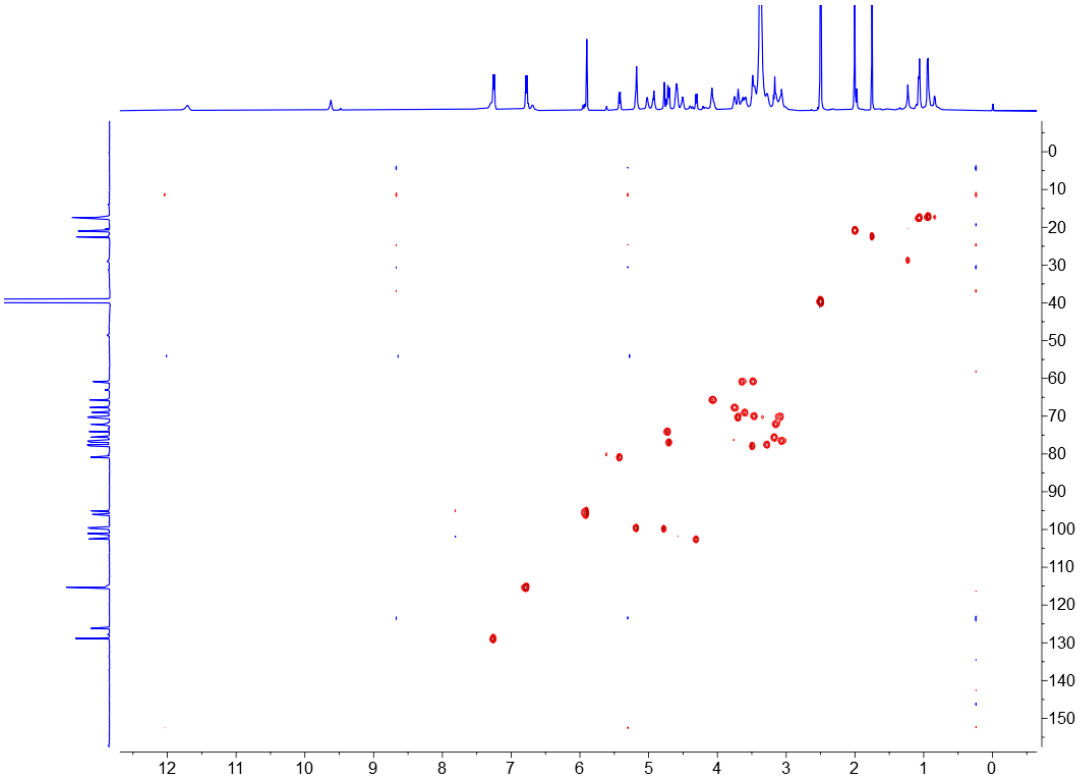

Figure S55. The HSQC spectrum of compound **6** (600/151 MHz, DMSO-d_6).

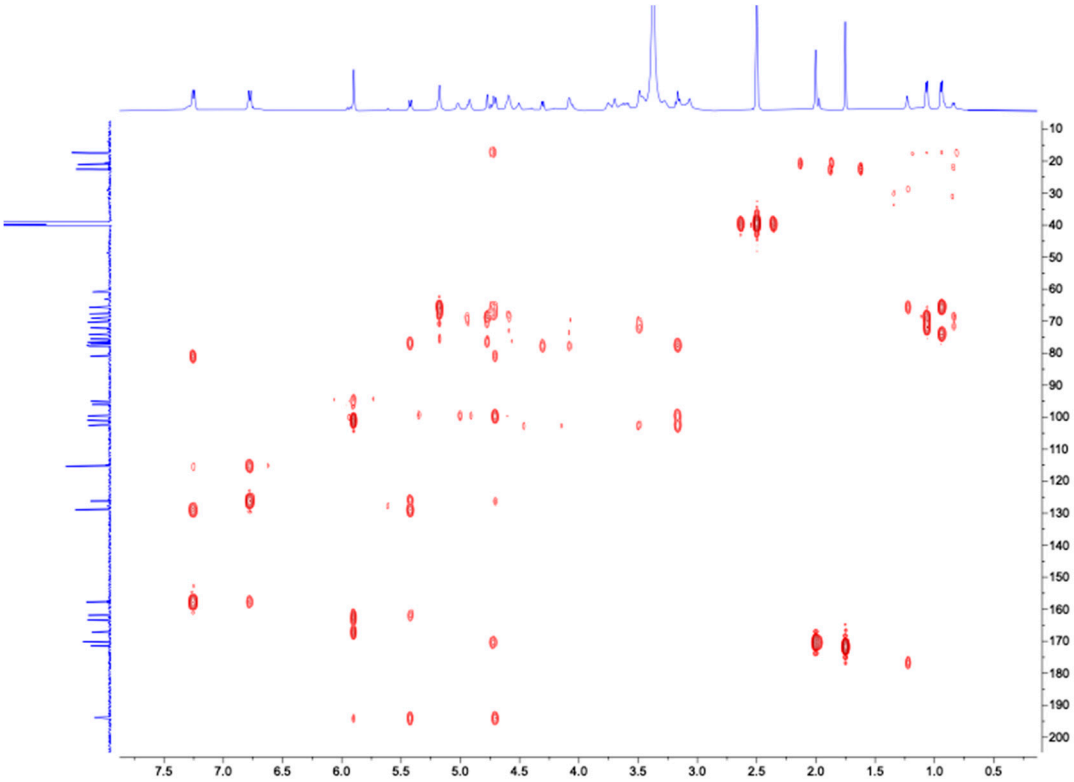

Figure S56. The HMBC spectrum of compound **6** (600/151 MHz, DMSO-d_6).

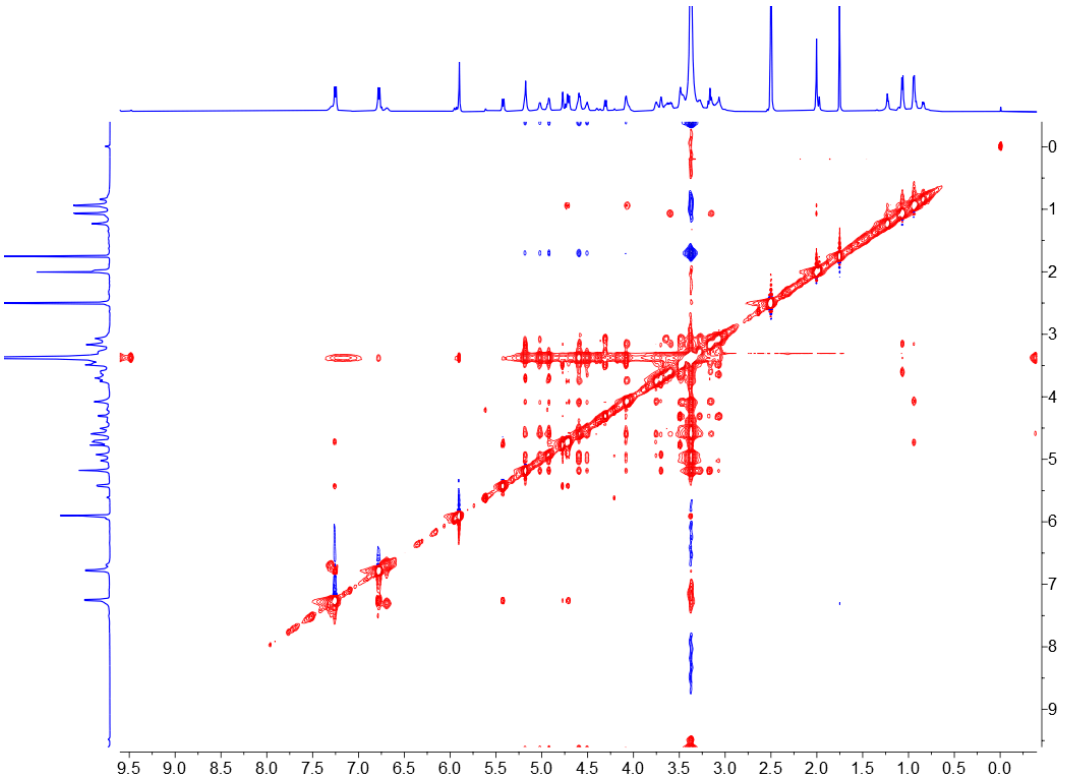

Figure S57. The NOESY spectrum of compound **6** (600 MHz, DMSO-d_6).

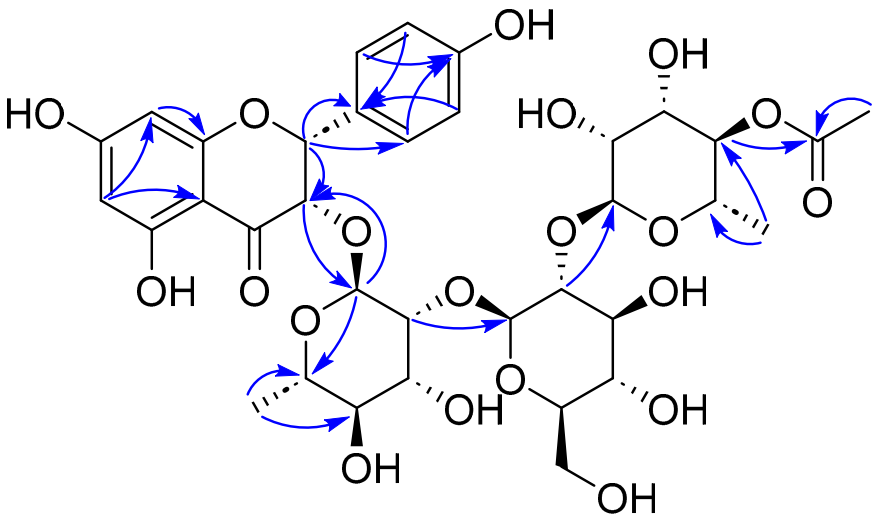

Figure S58. Key HMBC correlations of compound **6**.

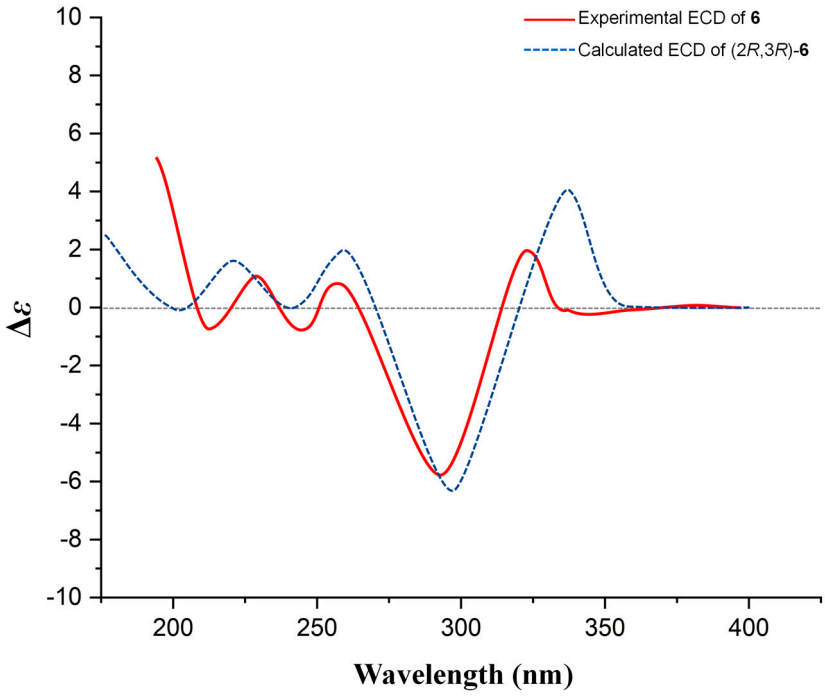

Figure S59. Experimental and calculated ECD spectra of compound **6**.

7. Spectroscopic data for compound **7**

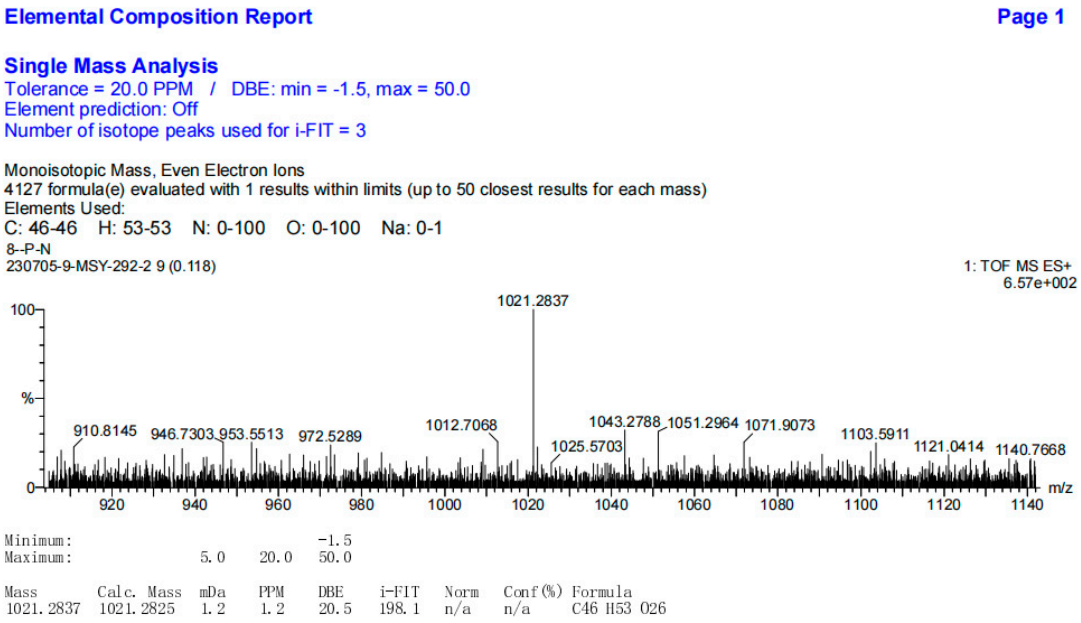

Figure S60. The HR-ESI-MS of compound **7**.

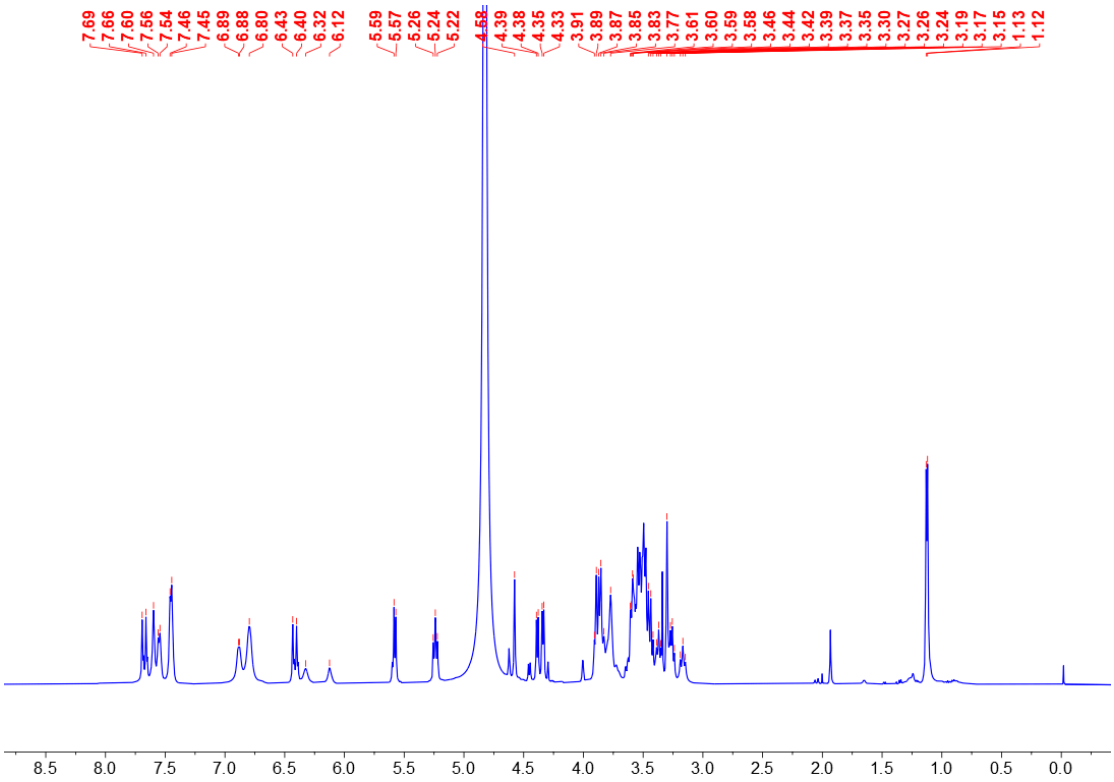

Figure S61. The ^{1}H NMR spectrum of compound **7** (600 MHz, CD_3OD).

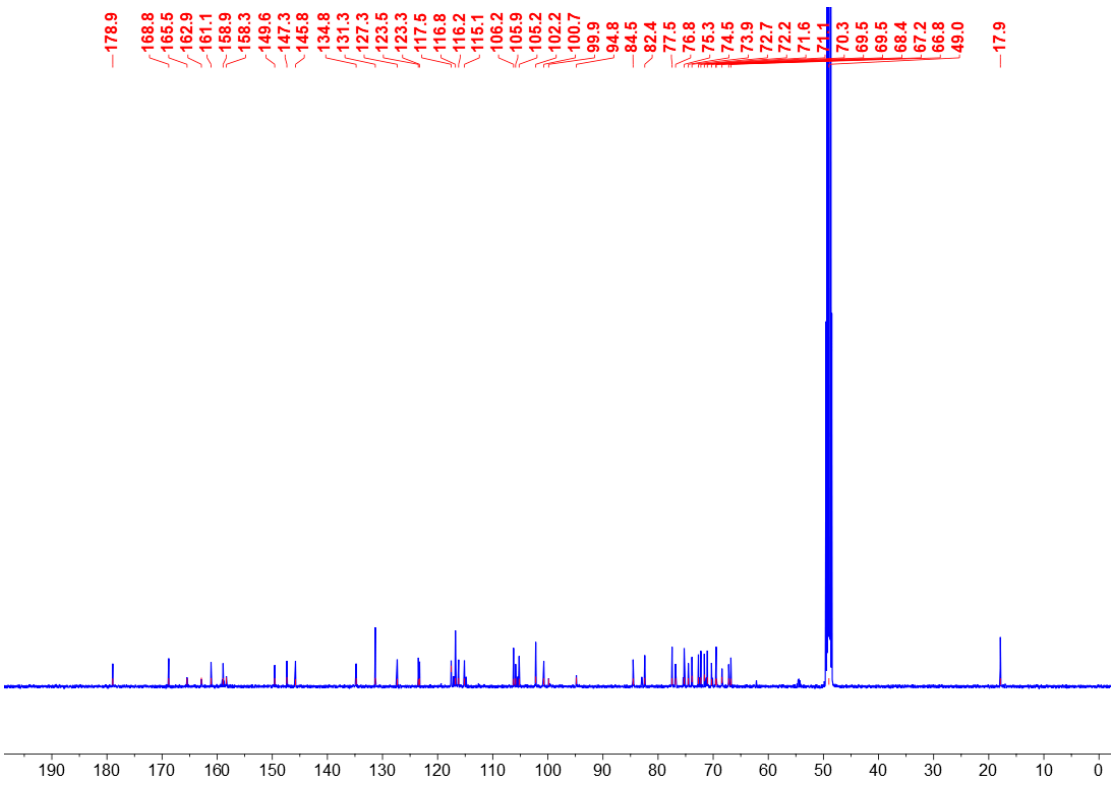

Figure S62. The ^{13}C NMR spectrum of compound **7** (151 MHz, CD_3OD).

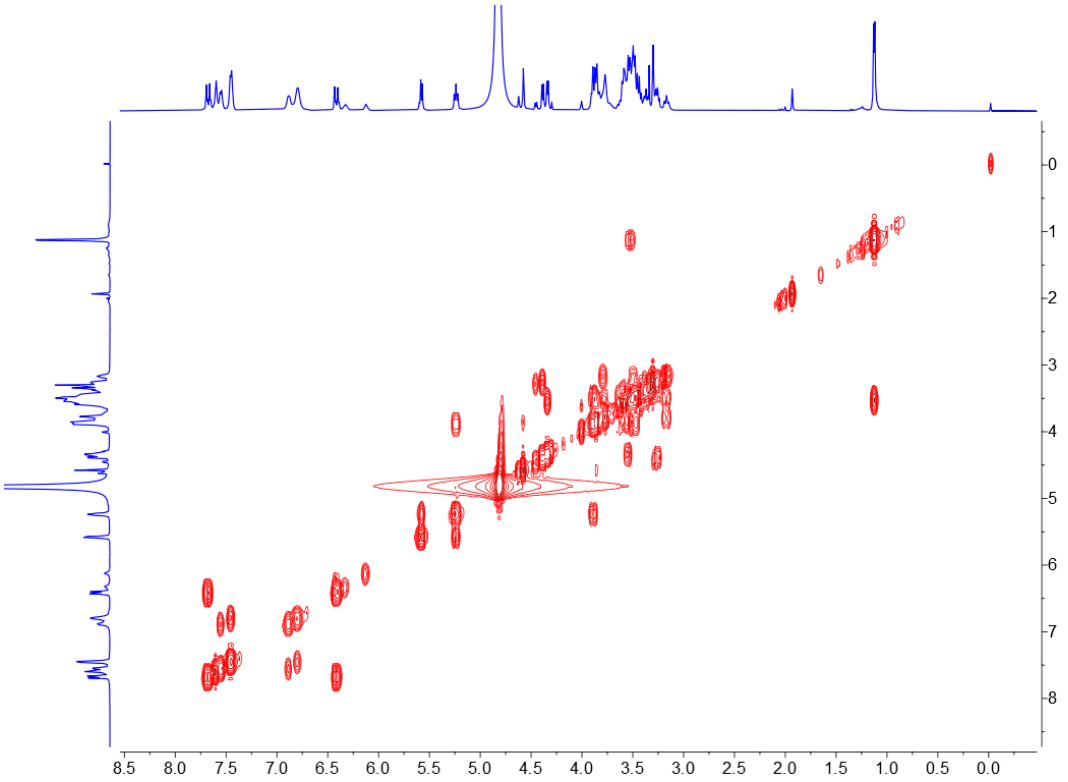

Figure S63. The ^{1}H-^{1}H COSY spectrum of compound **7** (600 MHz, CD_3OD).

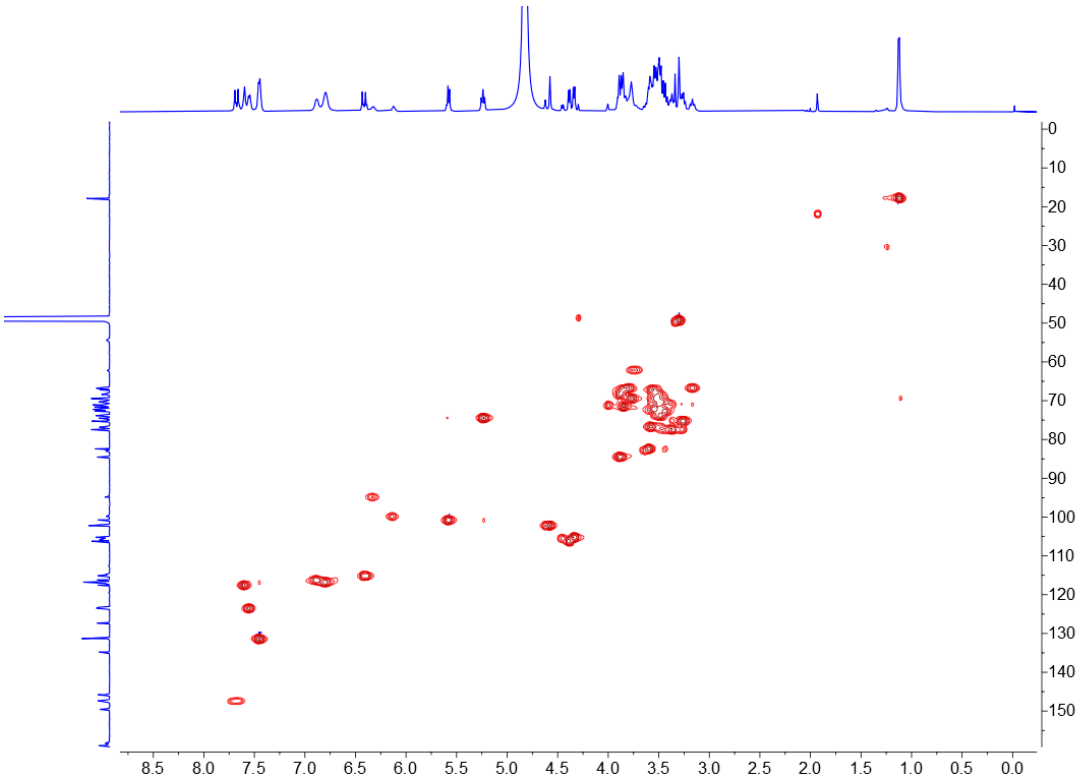

Figure S64. The HSQC spectrum of compound **7** (600/151 MHz, CD_3OD).

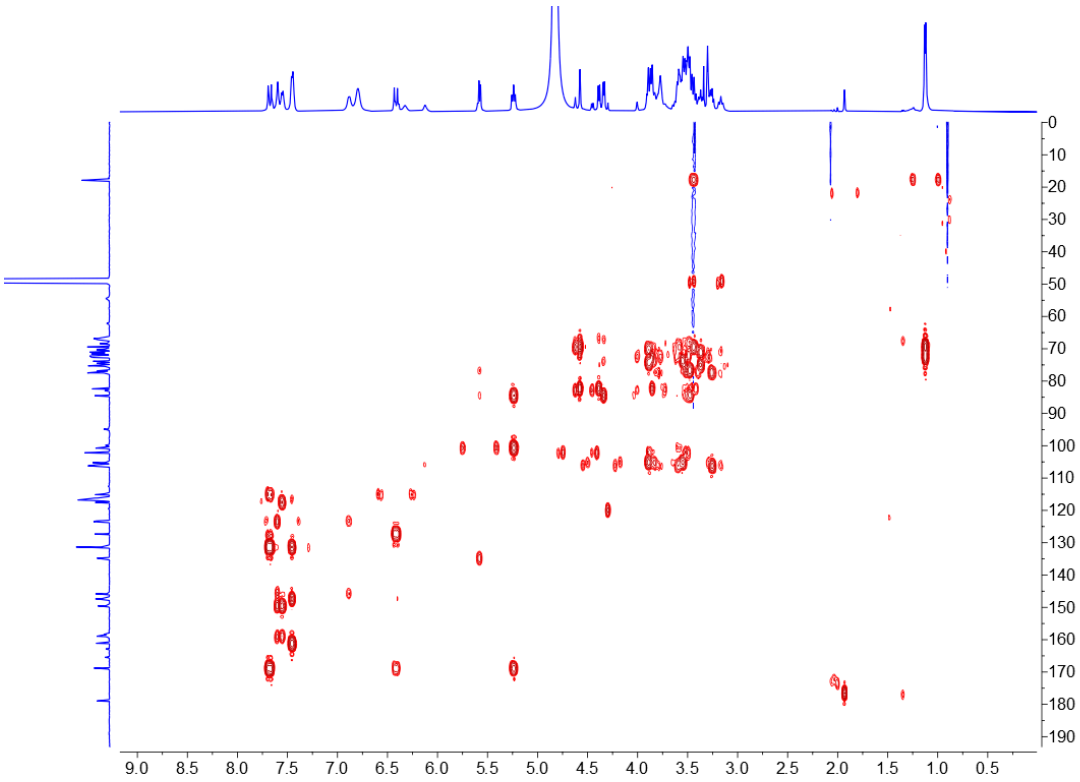

Figure S65. The HMBC spectrum of compound **7** (600/151 MHz, CD_3OD).

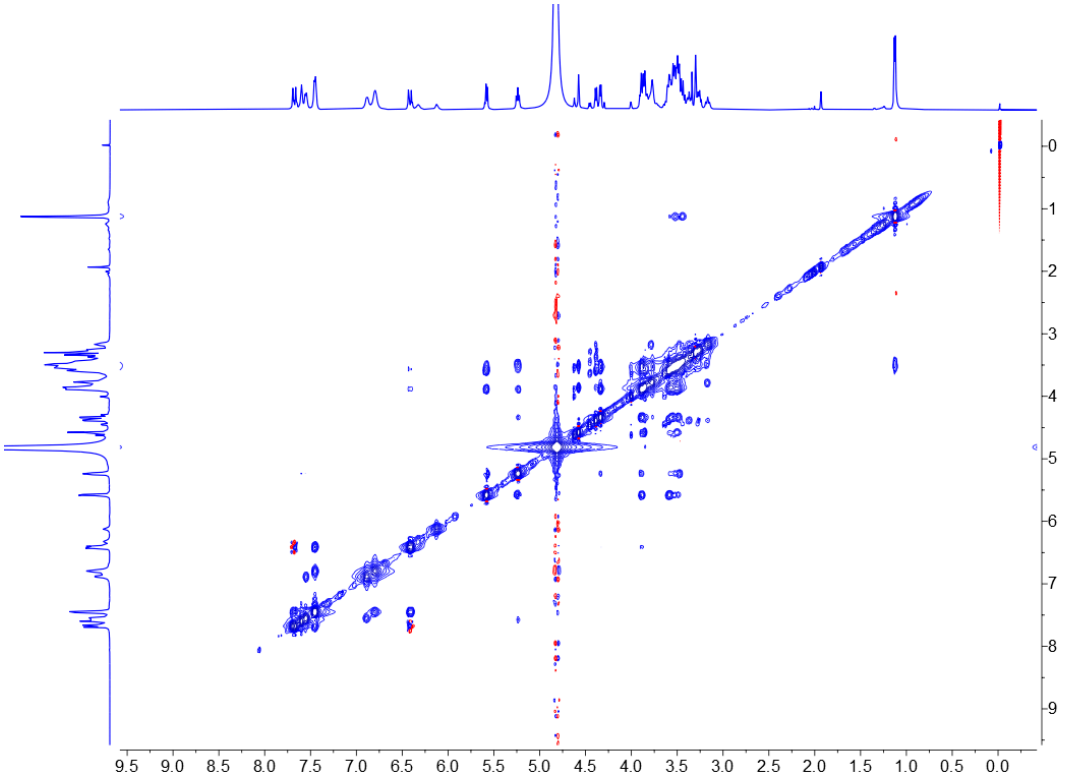

Figure S66. The NOESY spectrum of compound **7** (600 MHz, CD_3OD).

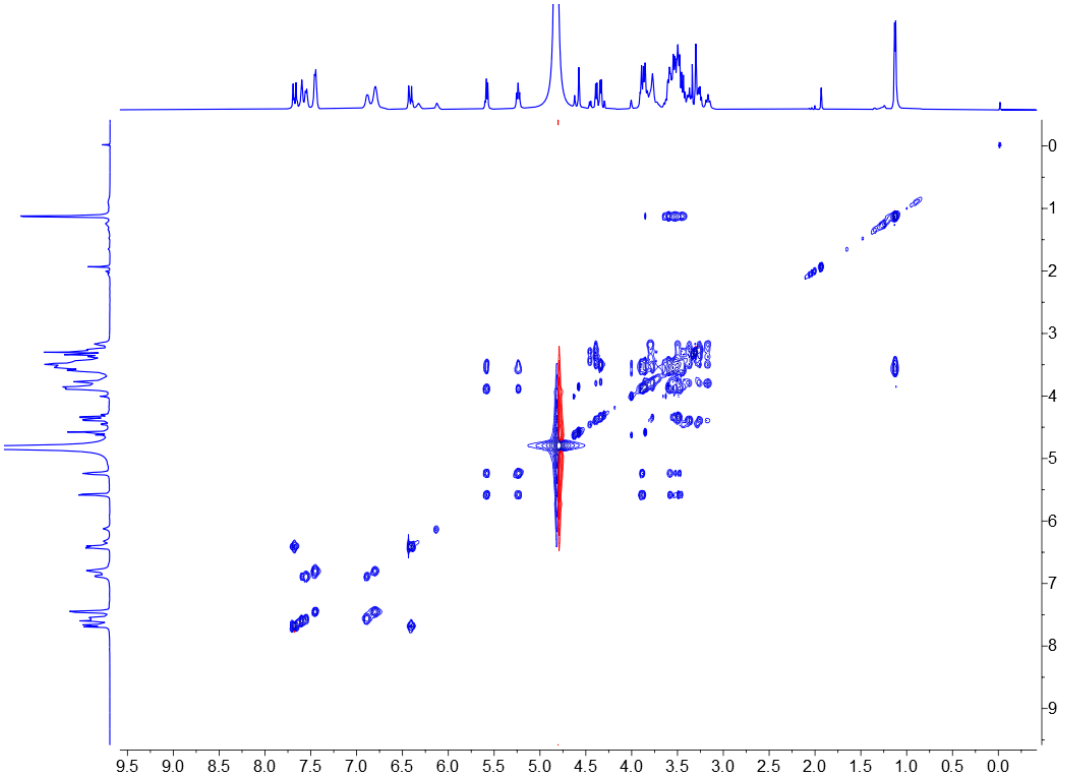

Figure S67. TheTOCSY spectrum of compound **7** (600 MHz, CD_3OD).

8. Spectroscopic data for compound **8**

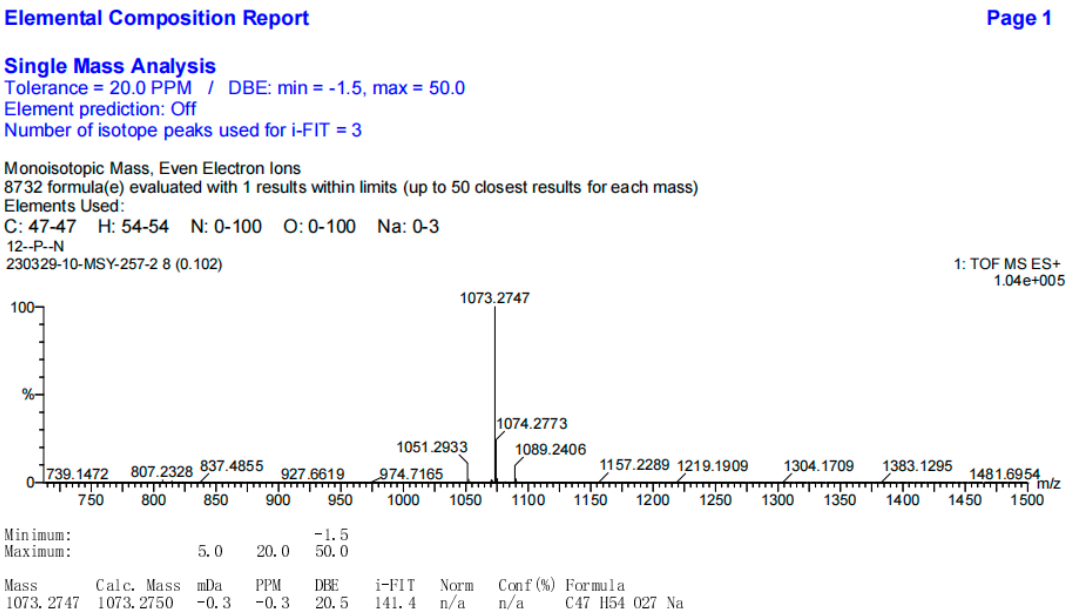

Figure S68. The HR-ESI-MS of compound **8**.

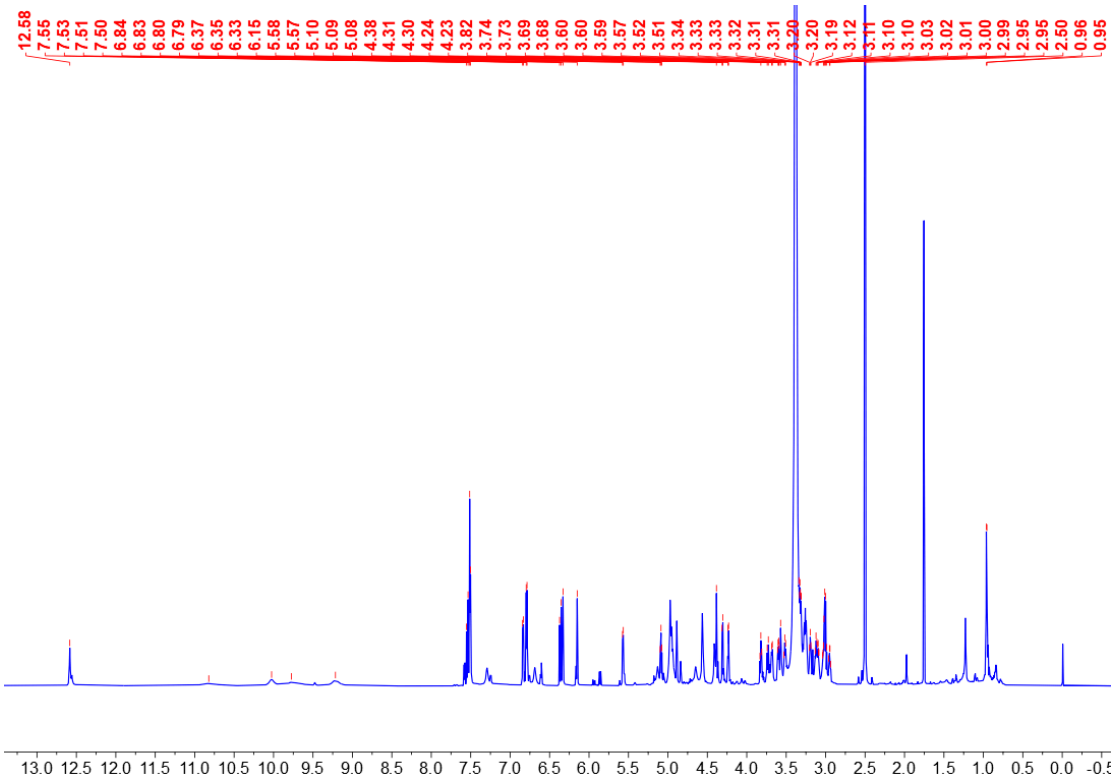

Figure S69. The ^{1}H NMR spectrum of compound **8** (600 MHz, DMSO-d_6).

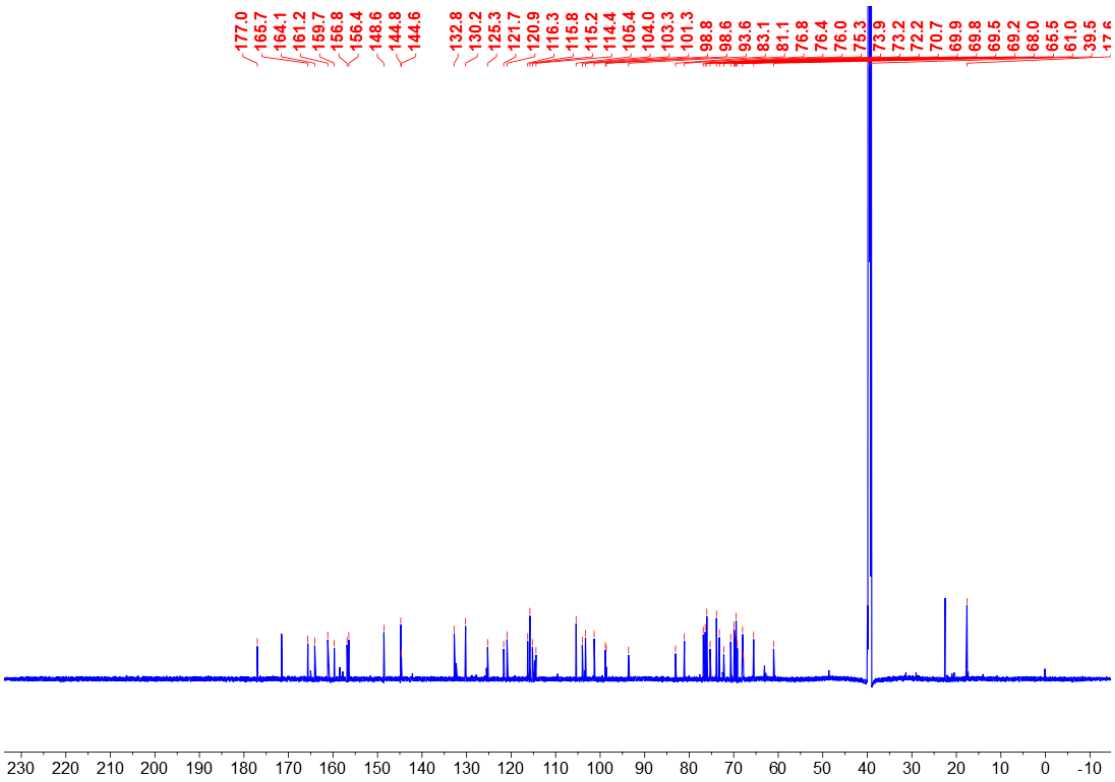

Figure S70. The ^{13}C NMR spectrum of compound **8** (151 MHz, DMSO-d_6).

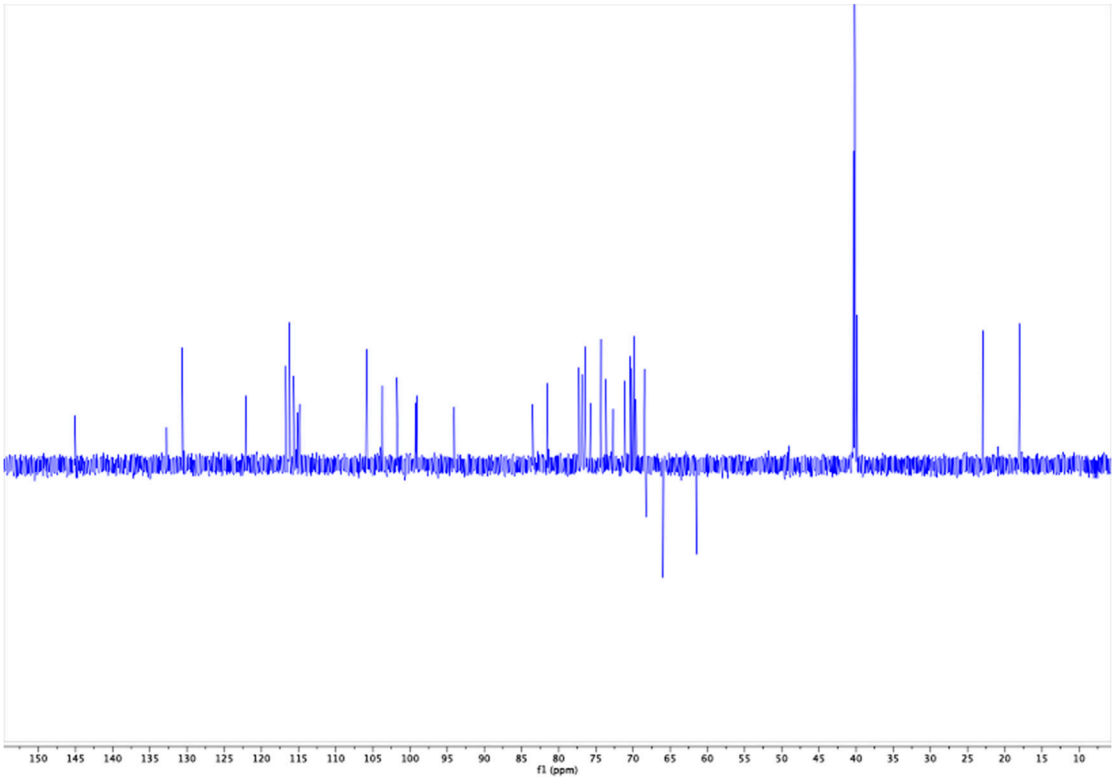

Figure S71. The DEPT135 spectrum of compound **8** (151 MHz, DMSO-d_6).

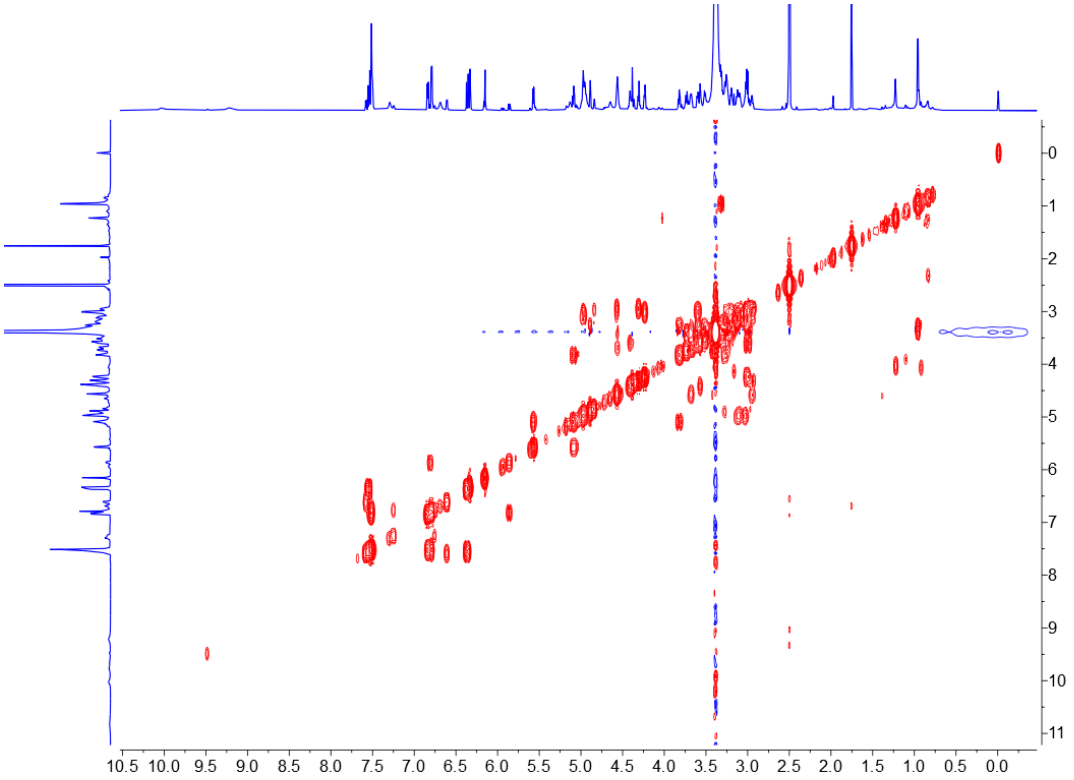

Figure S72. The ^{1}H-^{1}H COSY spectrum of compound **8** (600 MHz, DMSO-d_6).

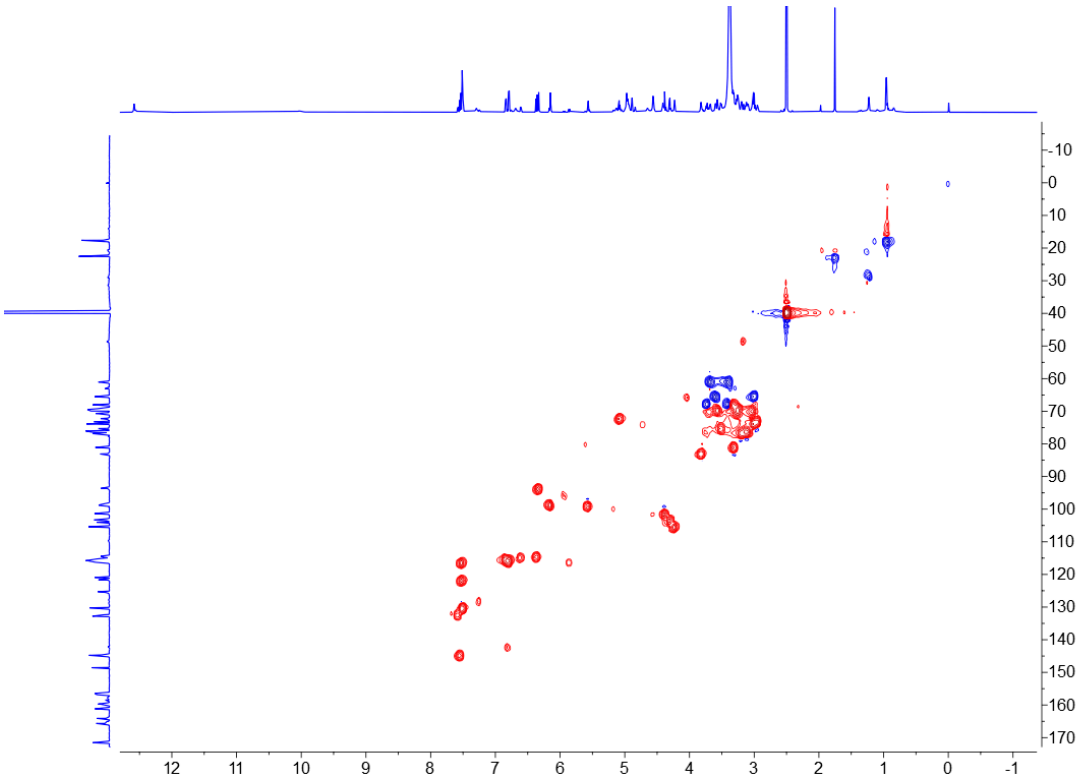

Figure S73. The HSQC spectrum of compound **8** (600/151 MHz, DMSO-d_6).

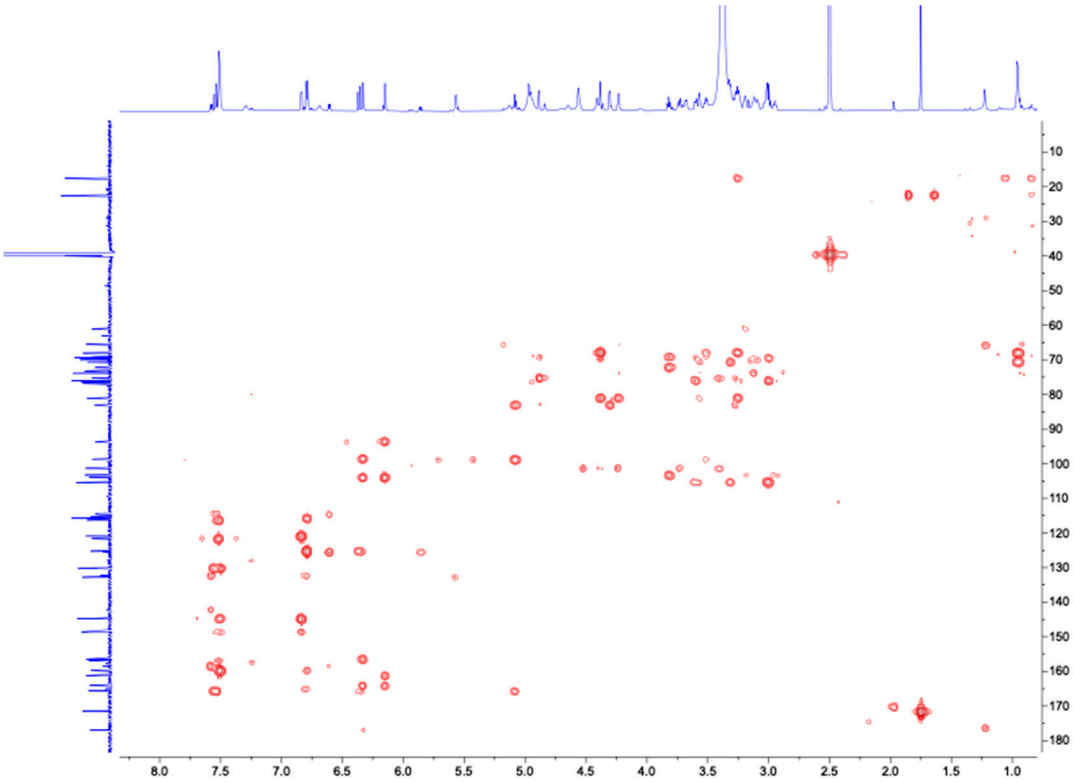

Figure S74. The HMBC spectrum of compound **8** (600/151 MHz, DMSO-d_6).

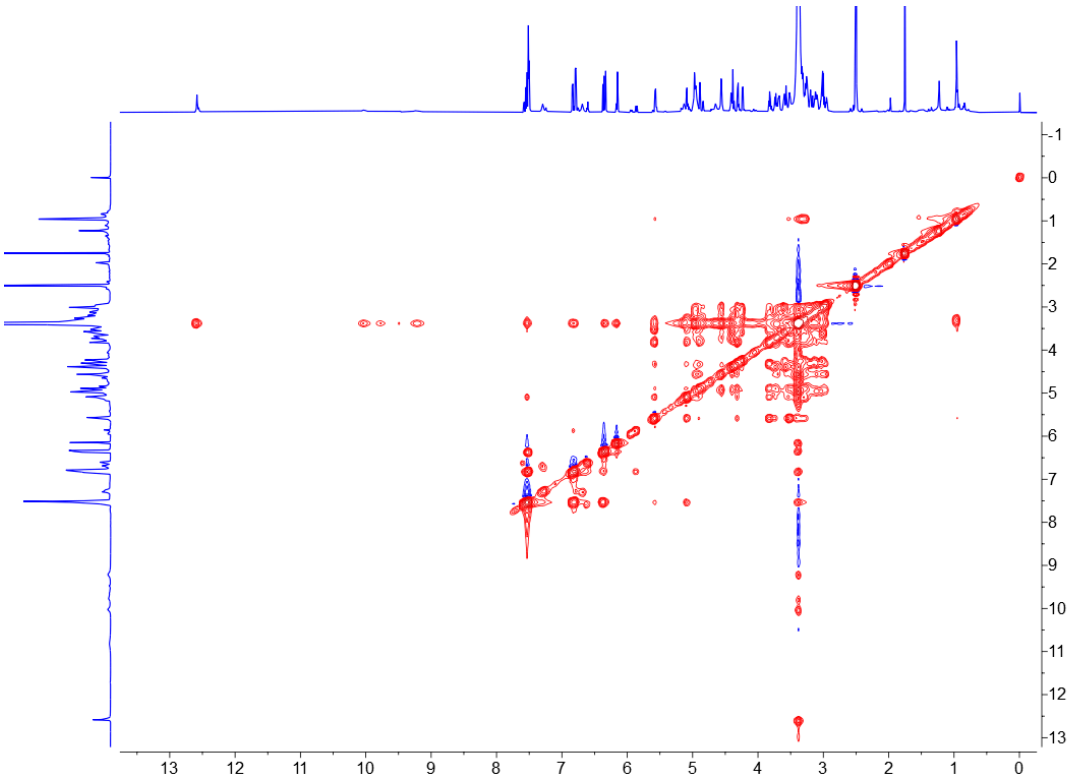

Figure S75. The NOESY spectrum of compound **8** (600 MHz, DMSO-d_6).

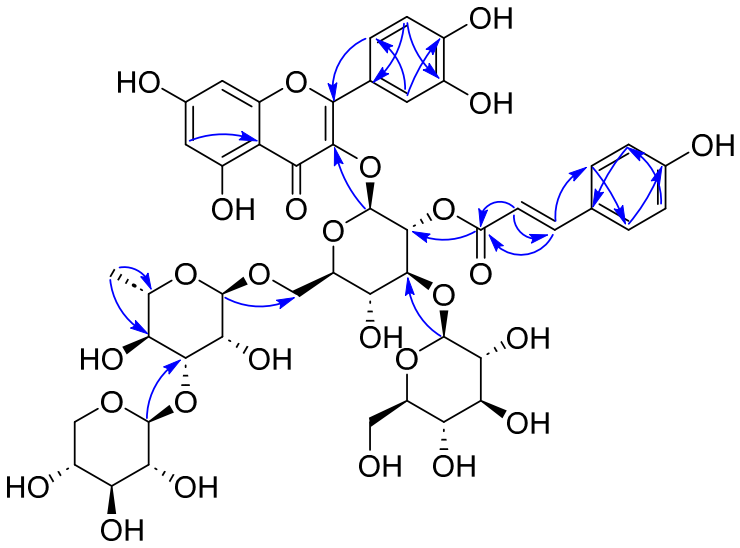

Figure S76. Key HMBC correlations of compound **8**.

9. Spectroscopic data for compound **9**

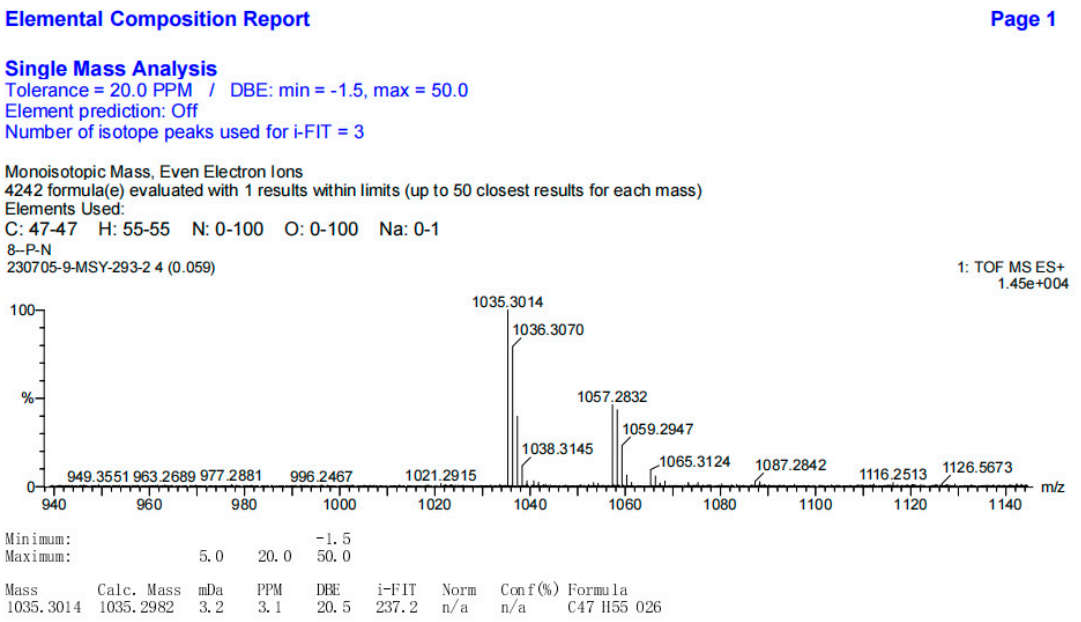

Figure S77. The HR-ESI-MS of compound **9**.

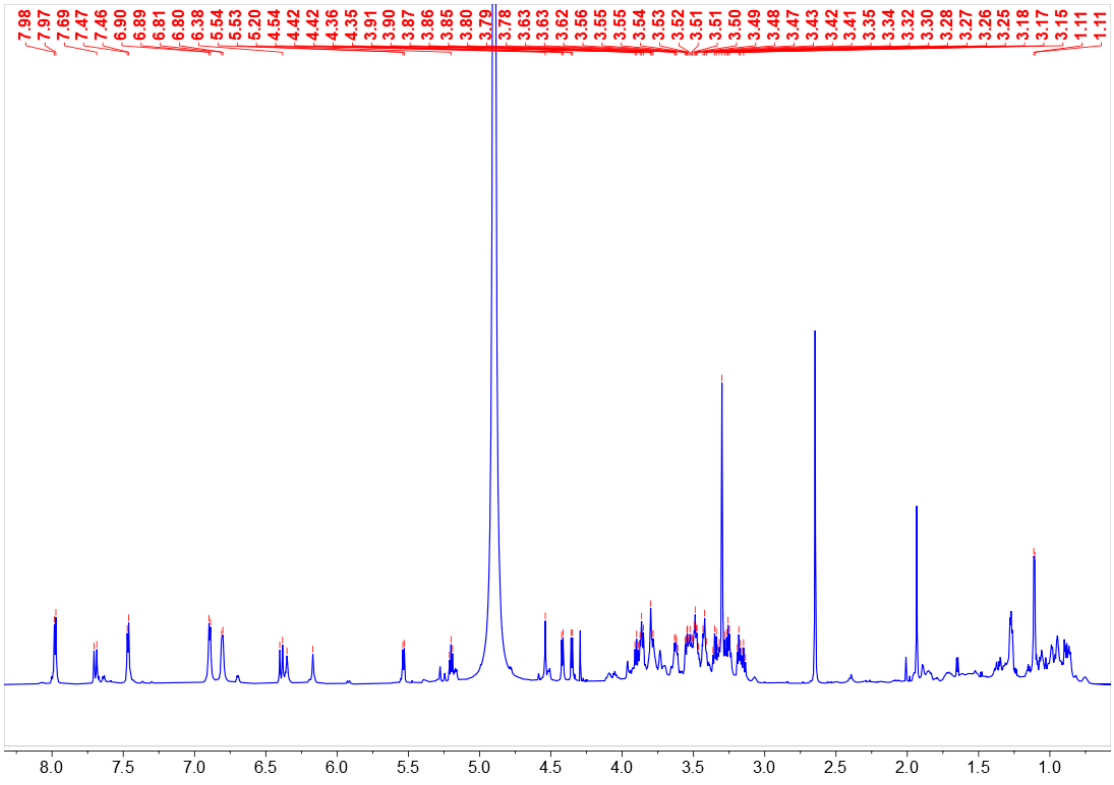

Figure S78. The ^{1}H NMR spectrum of compound **9** (600 MHz, CD_3OD).

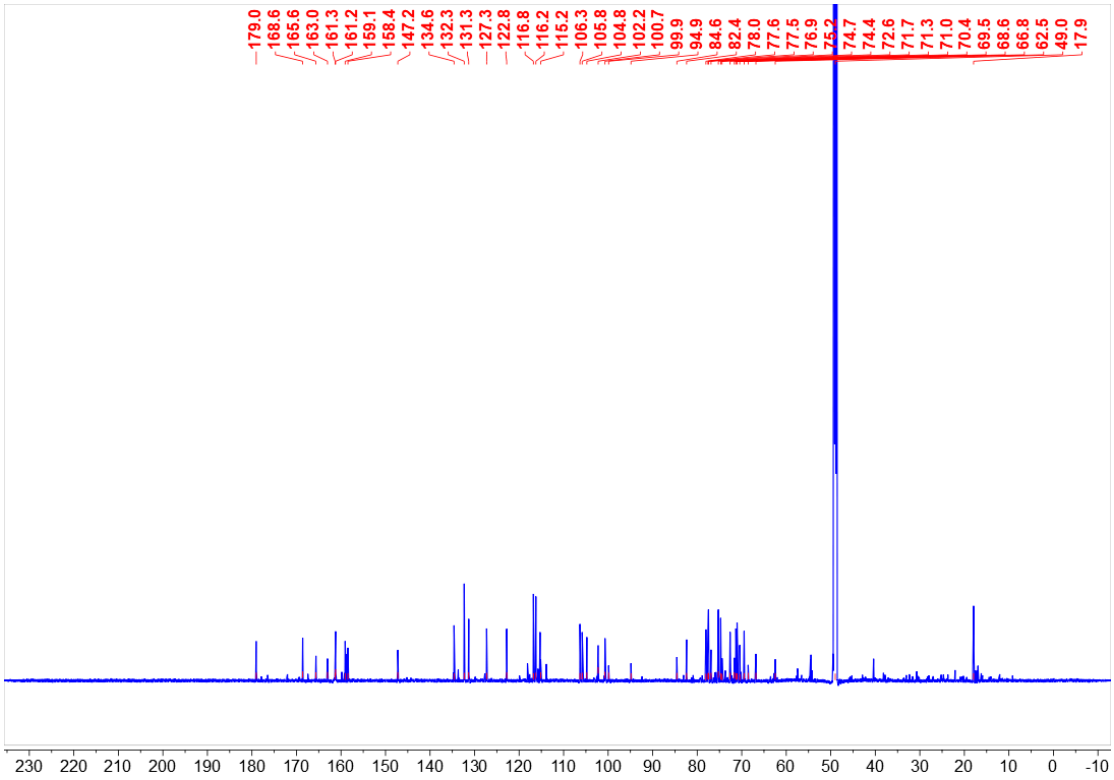

Figure S79. The ^{13}C NMR spectrum of compound **9** (151 MHz, CD_3OD).

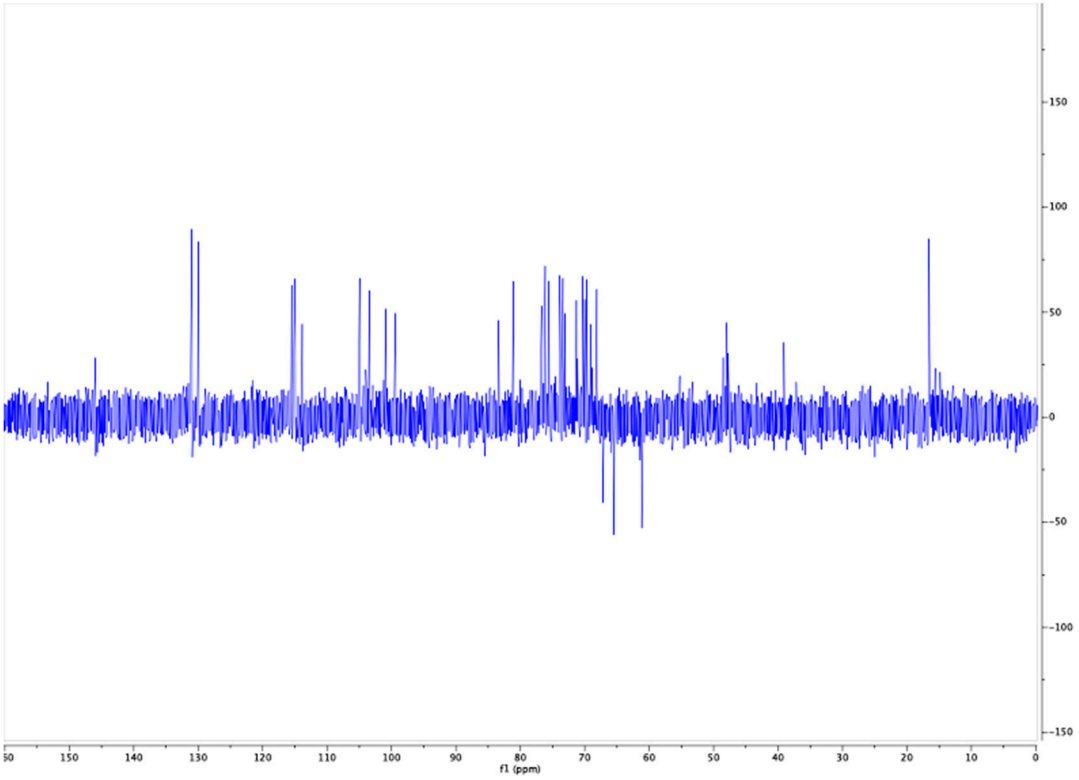

Figure S80. The DEPT135 spectrum of compound **9** (151 MHz, CD_3OD).

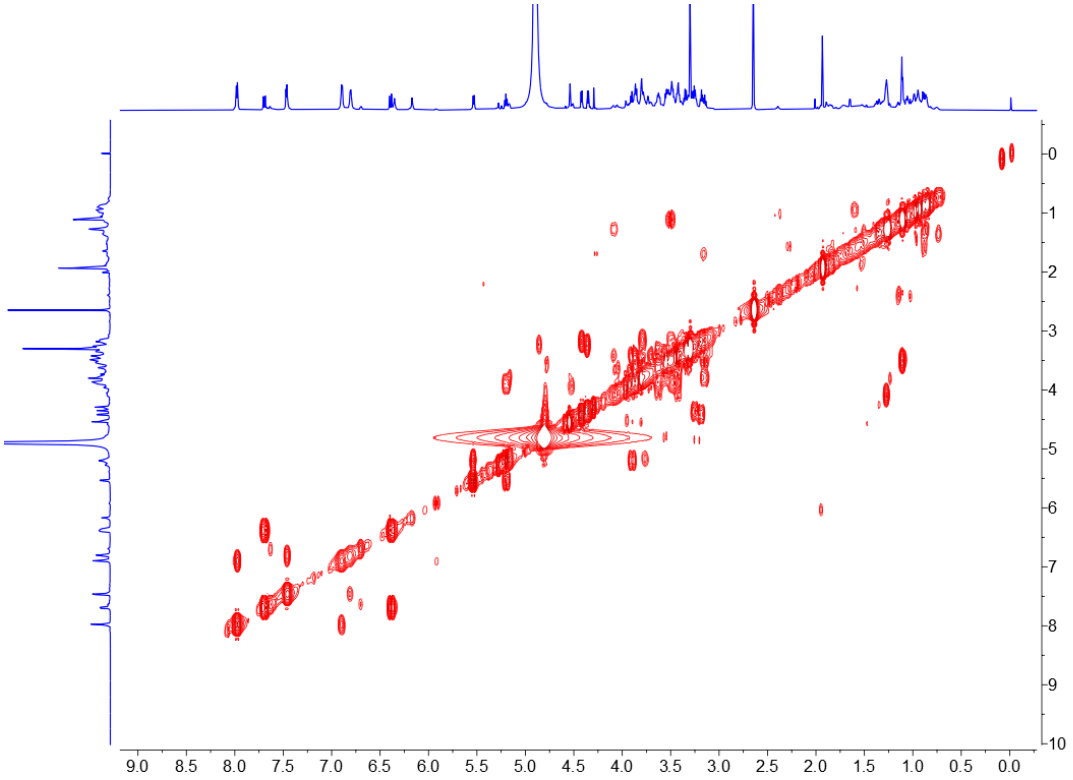

Figure S81. The ^{1}H-^{1}H COSY spectrum of compound **9** (600 MHz, CD_3OD).

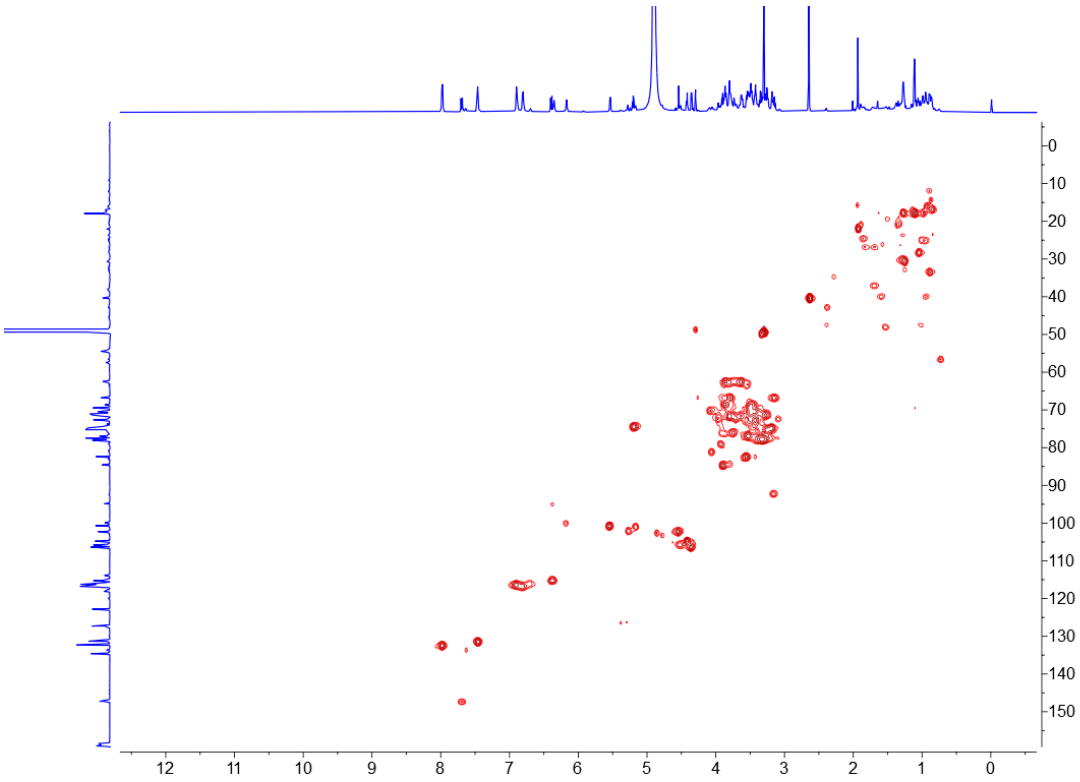

Figure S82. The HSQC spectrum of compound **9** (600/151 MHz, CD_3OD).

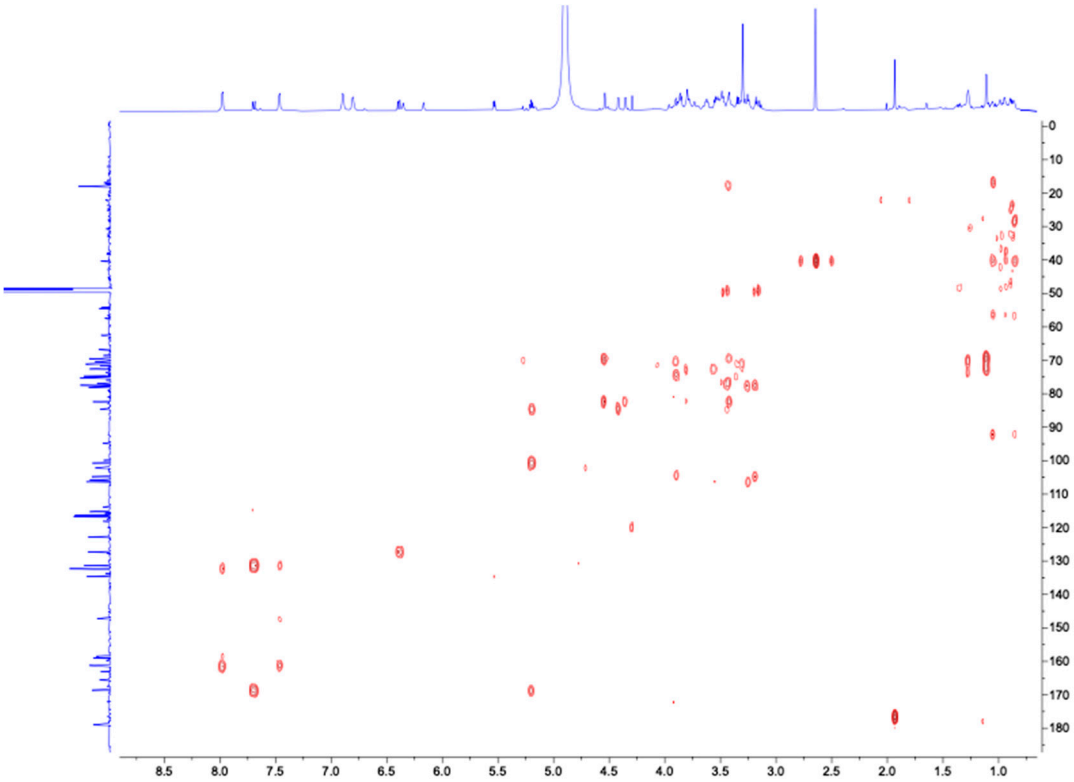

Figure S83. The HMBC spectrum of compound **9** (600/151 MHz, CD_3OD).

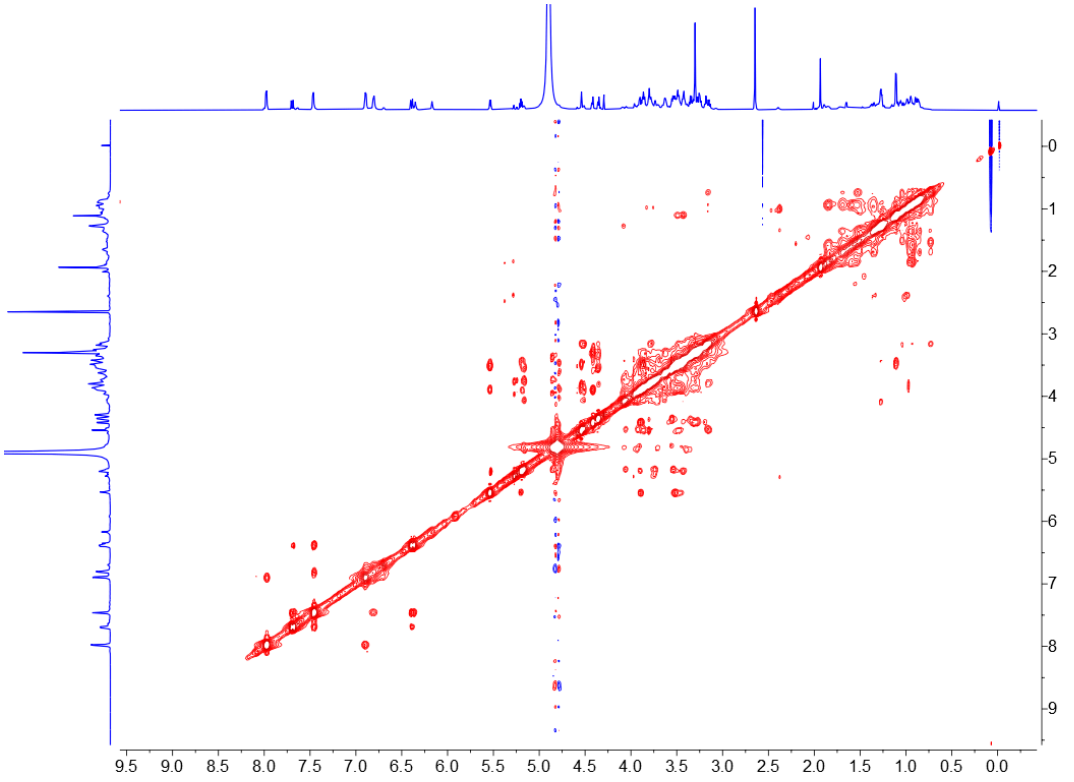

Figure S84. The NOESY spectrum of compound **9** (600 MHz, CD_3OD).

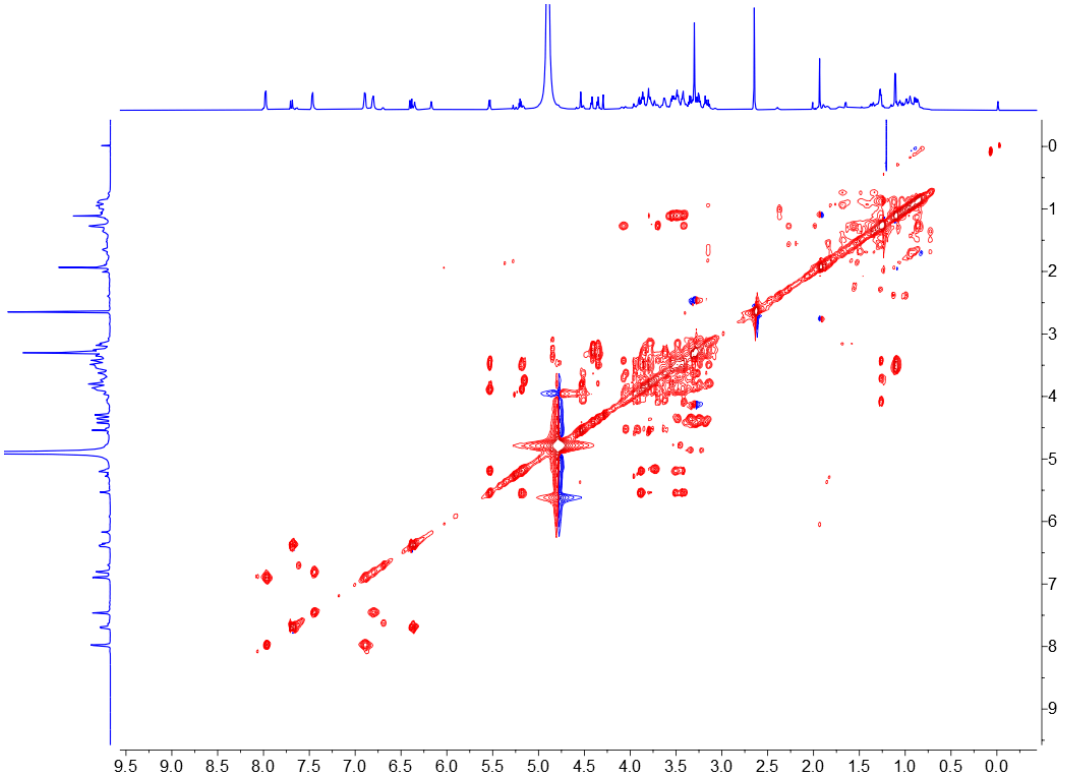

Figure S85. The TOCSY spectrum of compound **9** (600 MHz, CD_3OD).

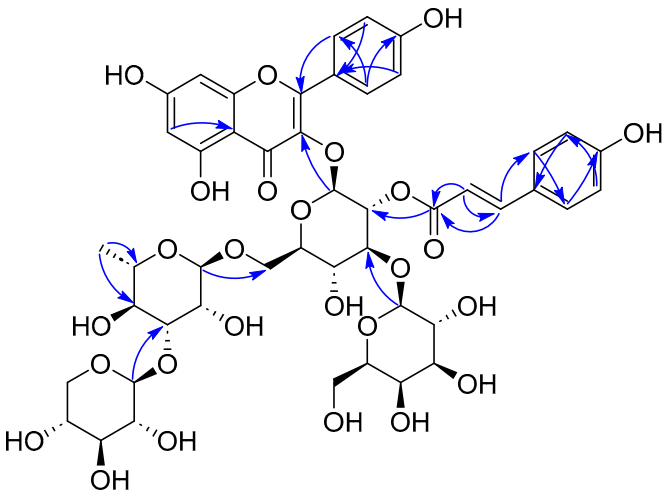

Figure S86. Key HMBC correlations of compound **9**.

10. Spectroscopic data for compound **10**

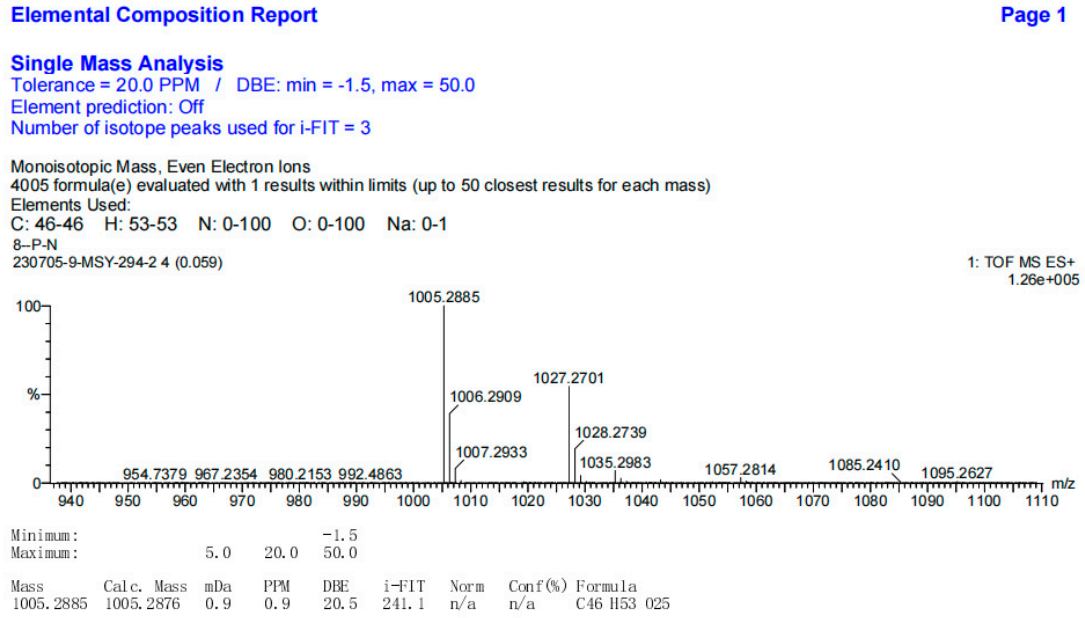

Figure S87. The HR-ESI-MS of compound **10**.

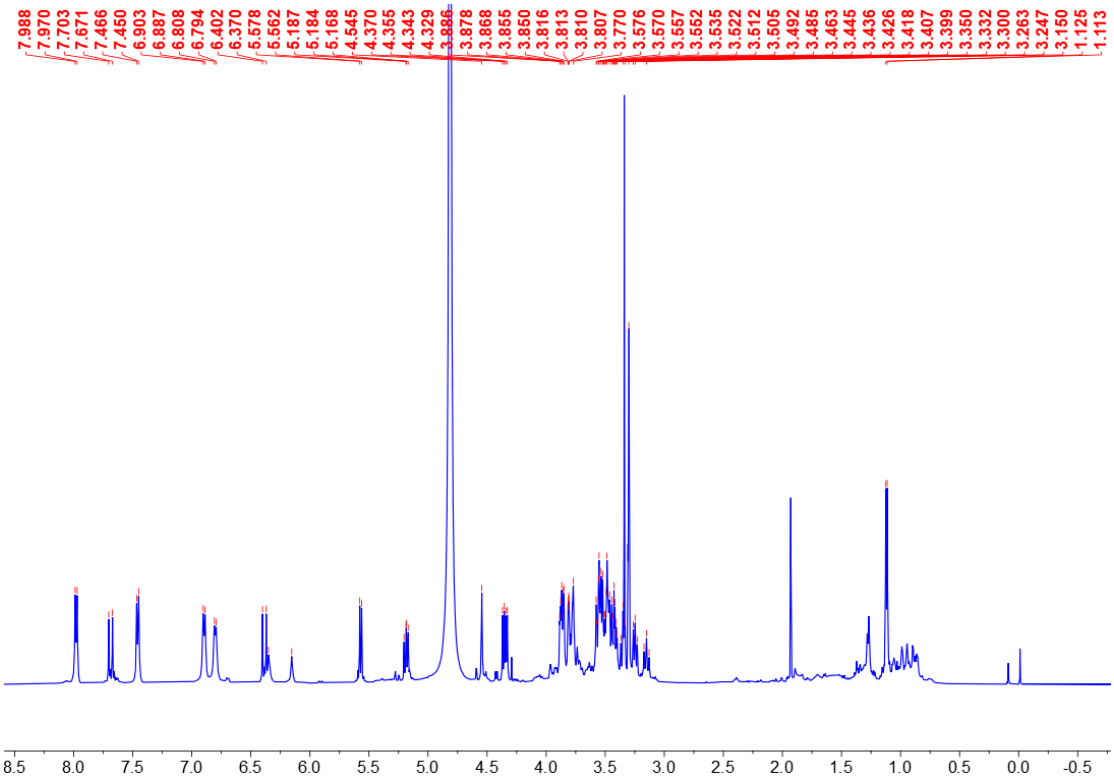

Figure S88. The ^{1}H NMR spectrum of compound **10** (600 MHz, CD_3OD).

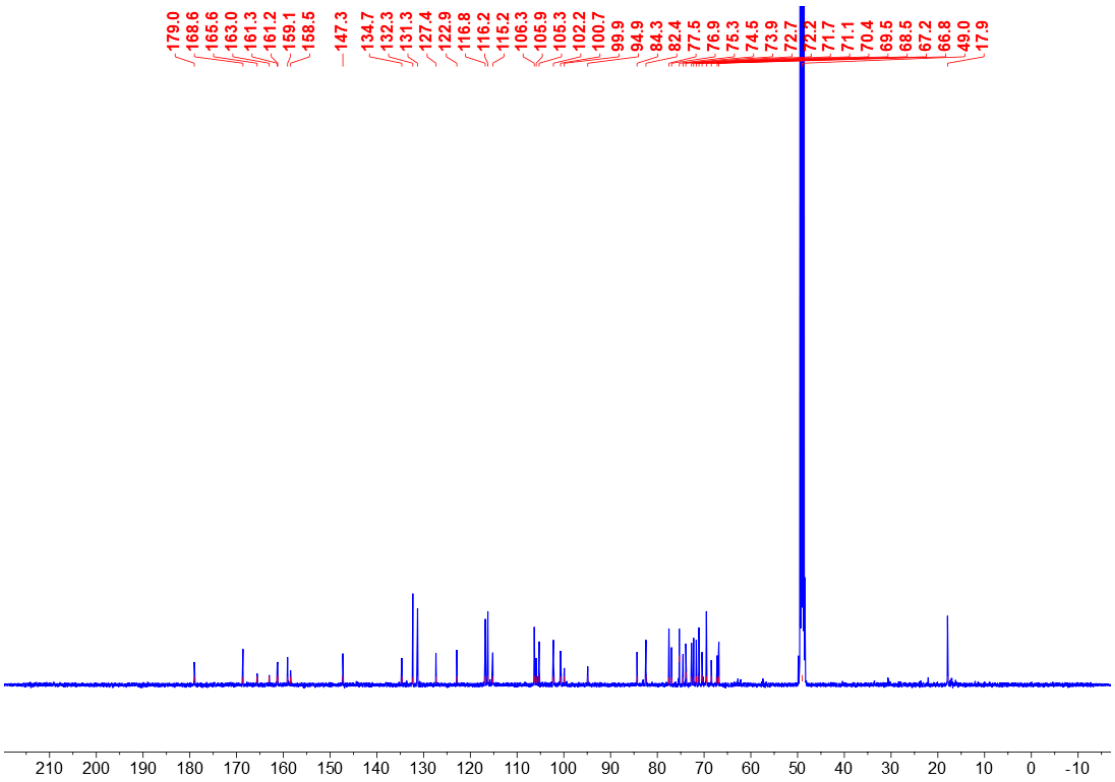

Figure S89. The ^{13}C NMR spectrum of compound **10** (151 MHz, CD_3OD).

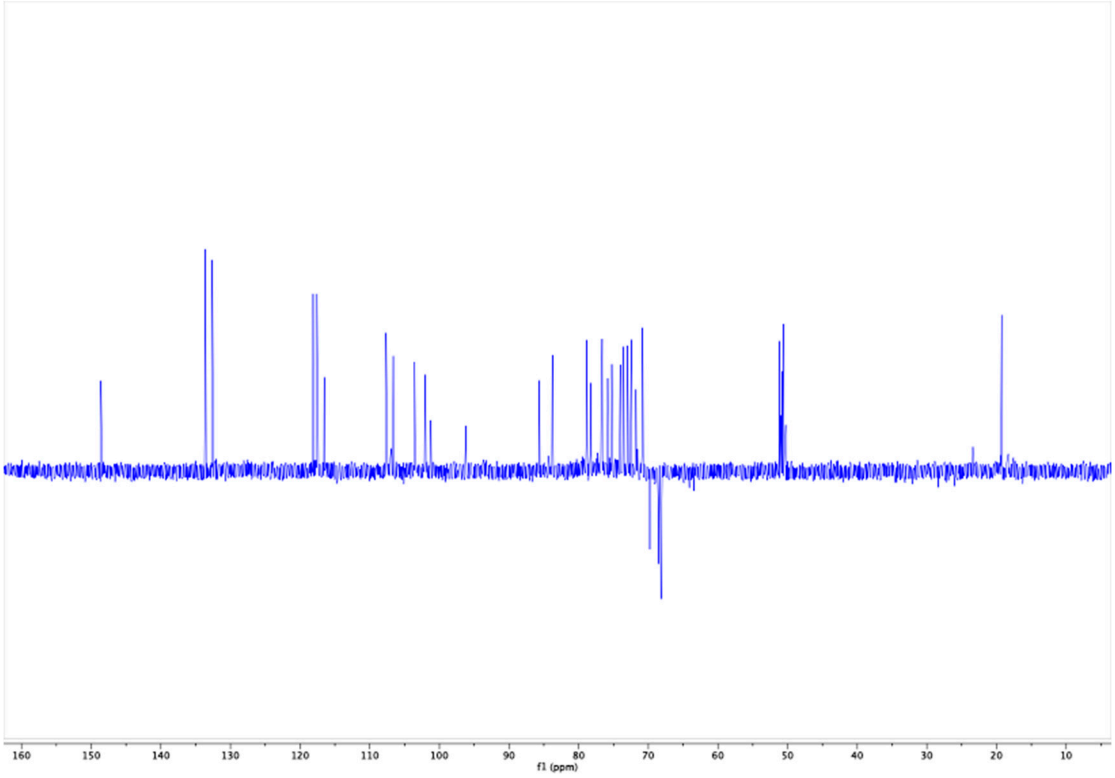

Figure S90. The DEPT135 spectrum of compound **10** (151 MHz, CD_3OD).

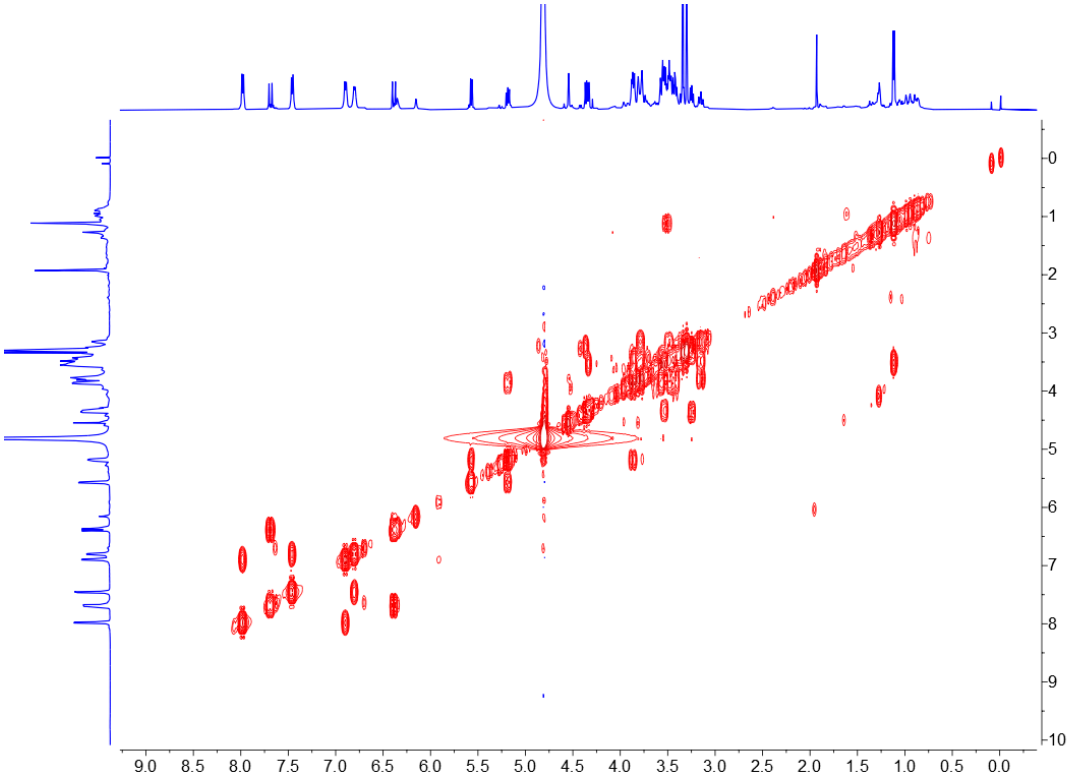

Figure S91. The ^{1}H-^{1}H COSY spectrum of compound **10** (600 MHz, CD_3OD).

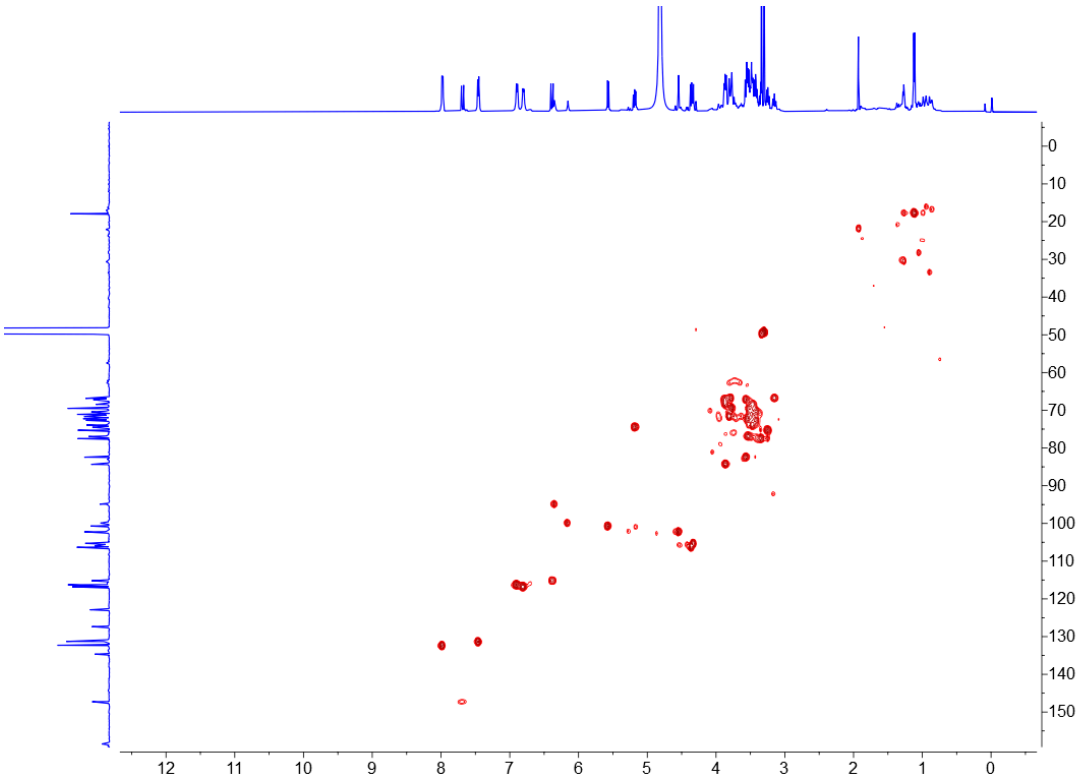

Figure S92. The HSQC spectrum of compound **10** (600/151 MHz, CD_3OD).

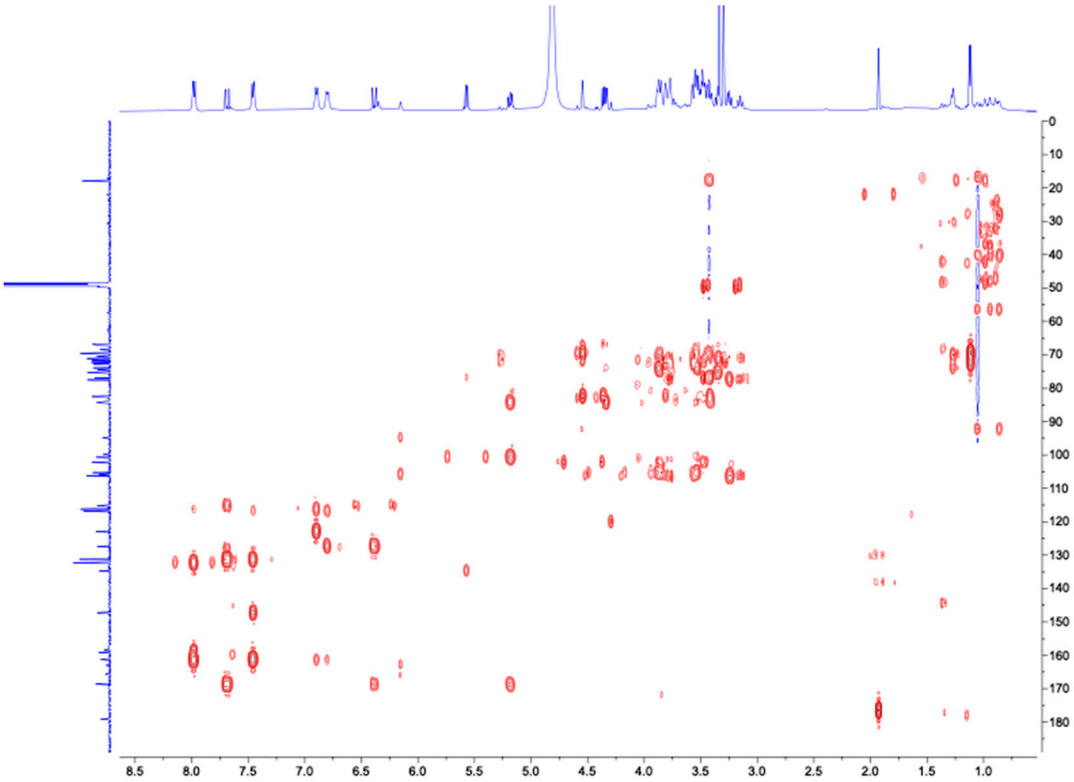

Figure S93. The HMBC spectrum of compound **10** (600/151 MHz, CD_3OD).

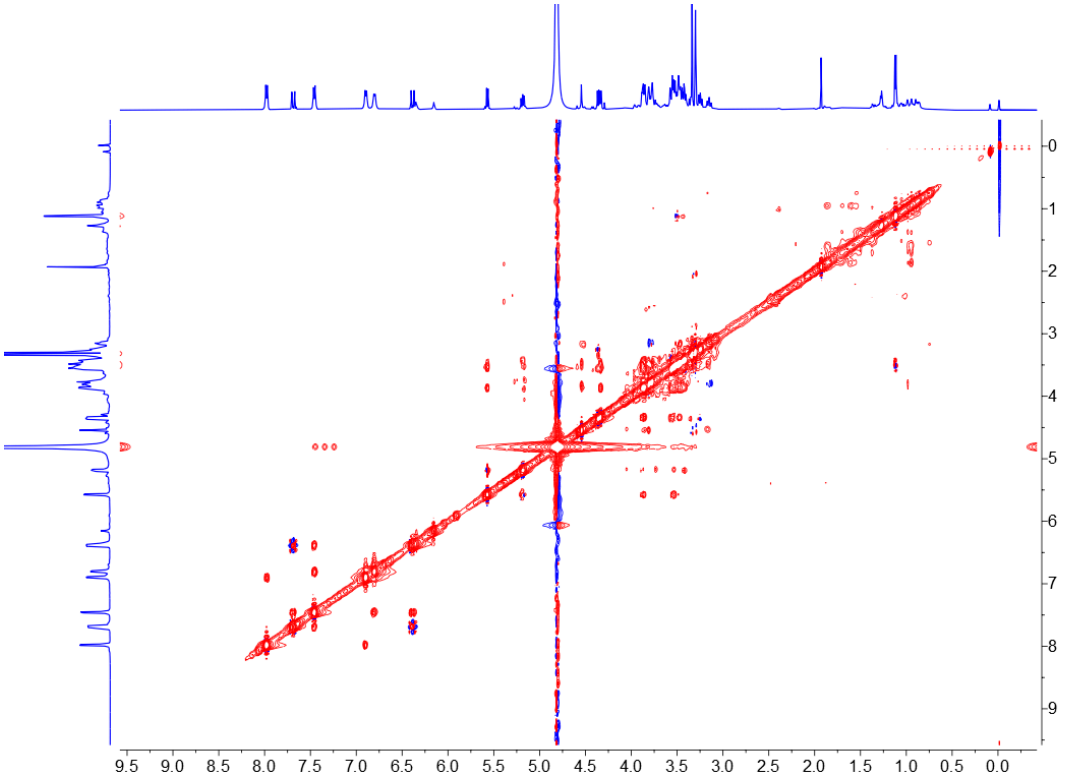

Figure S94. The NOESY spectrum of compound **10** (600 MHz, CD_3OD).

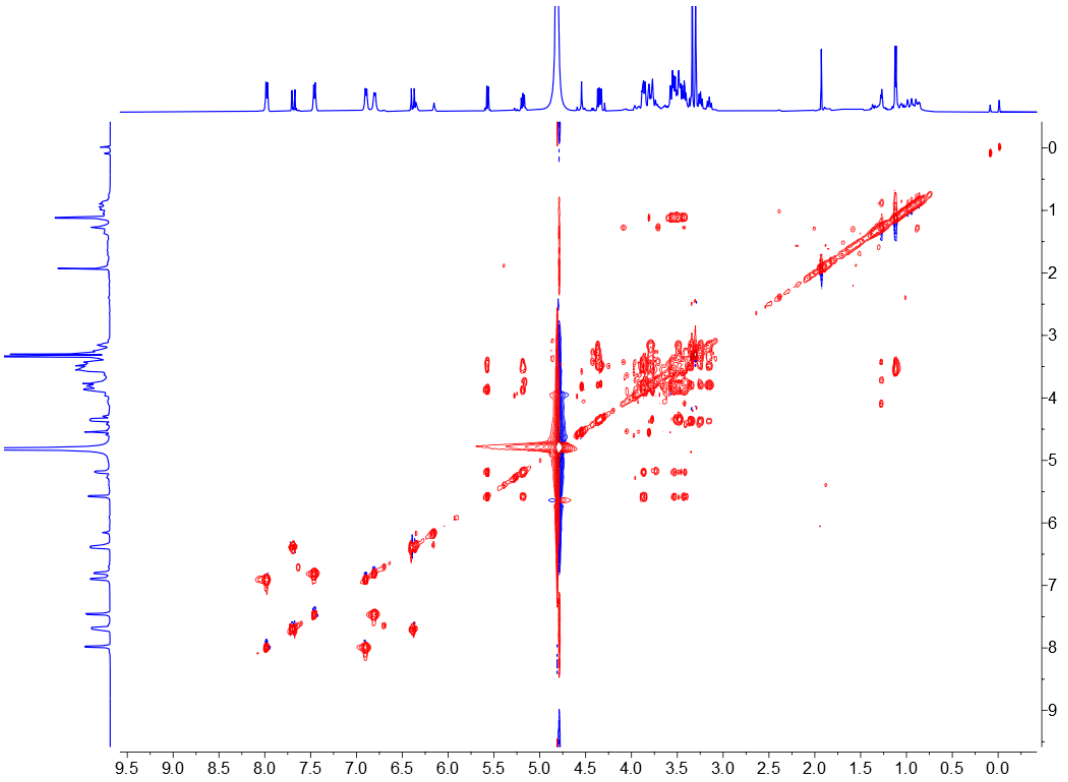

Figure S95. The TOCSY spectrum of compound **10** (600 MHz, CD_3OD).

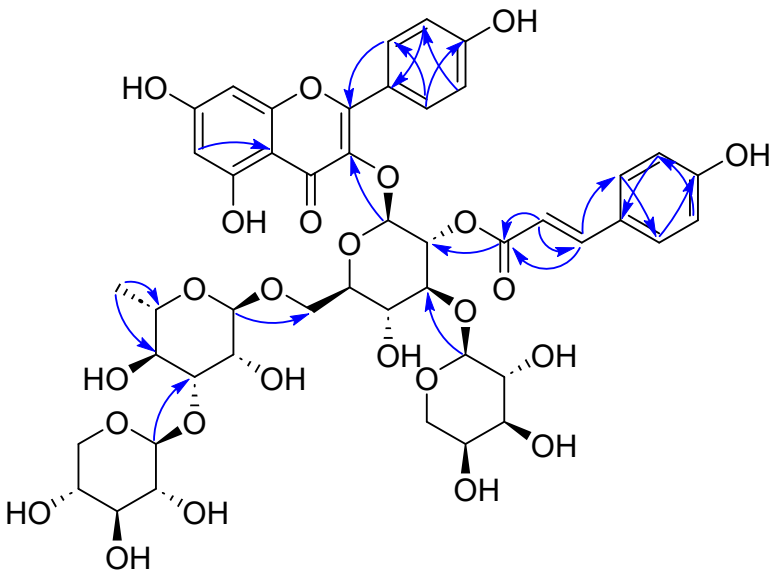

Figure S96. Key HMBC correlations of compound **10**.

11. ^{1}H and ^{13}C NMR spectroscopic data for compound **11**−**15**

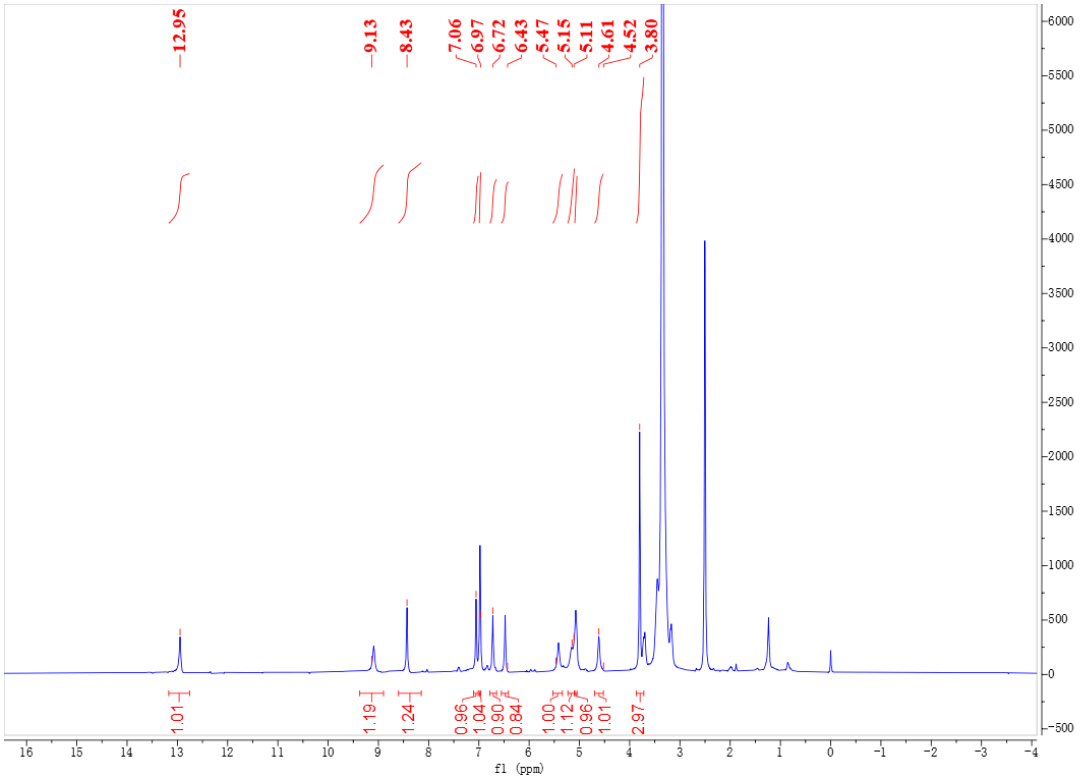

Figure S97. The ^{1}H NMR spectrum of compound **11** (600 MHz, DMSO-d_6).

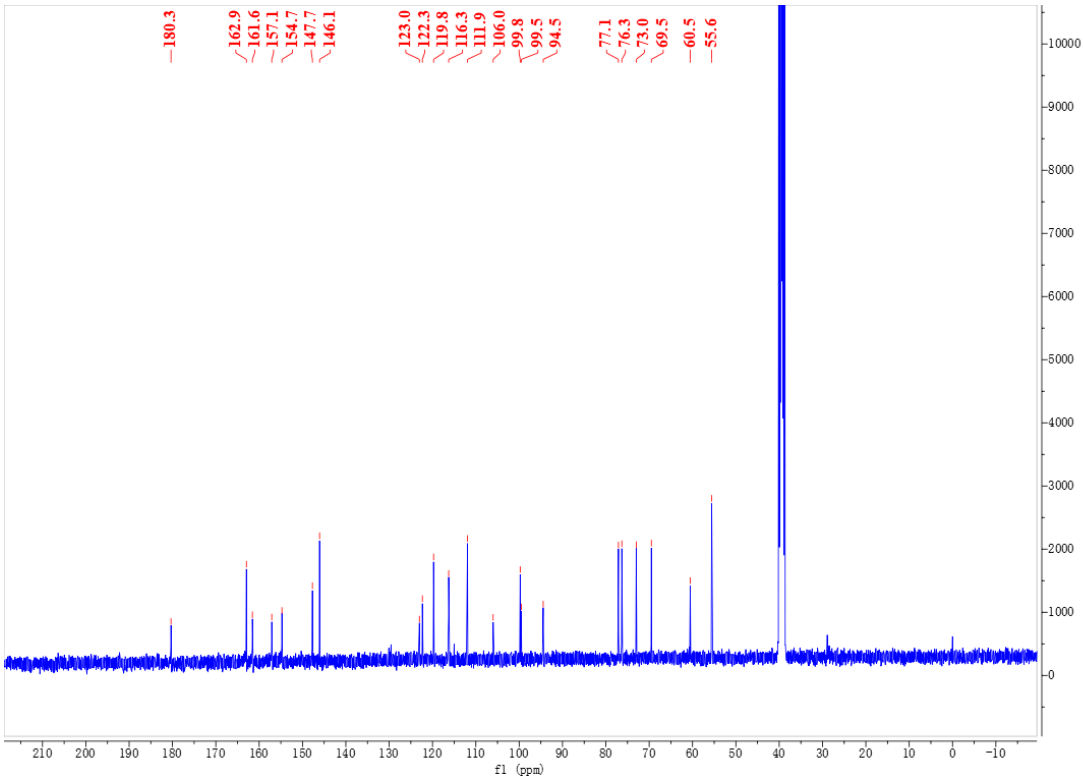

Figure S98. The ^{13}C NMR spectrum of compound **11** (151 MHz, DMSO-d_6).

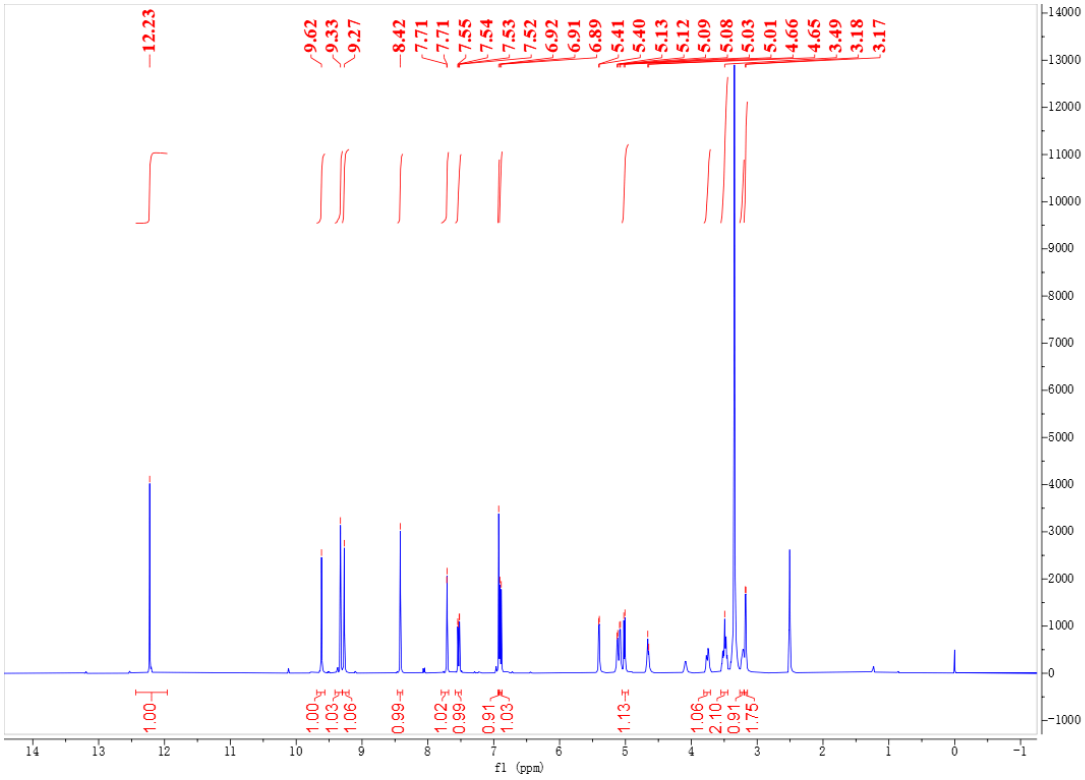

Figure S99. The ^{1}H NMR spectrum of compound **12** (600 MHz, DMSO-d_6).

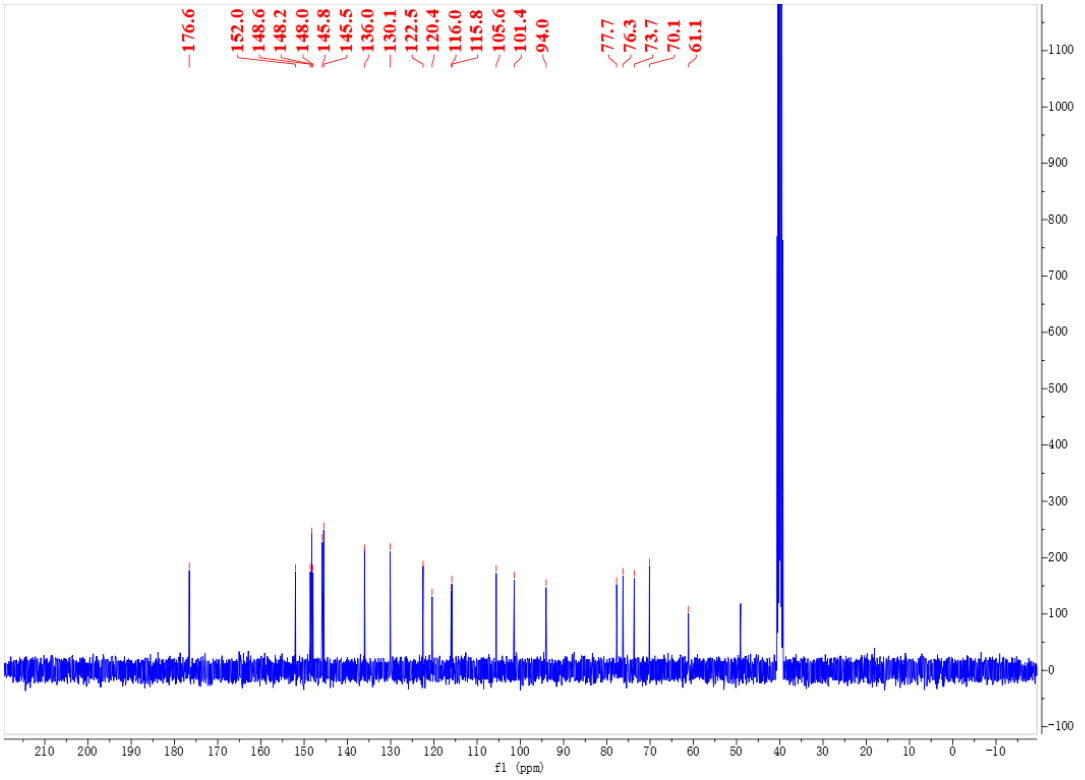

Figure S100. The ^{13}C NMR spectrum of compound **12** (151 MHz, DMSO-d_6).

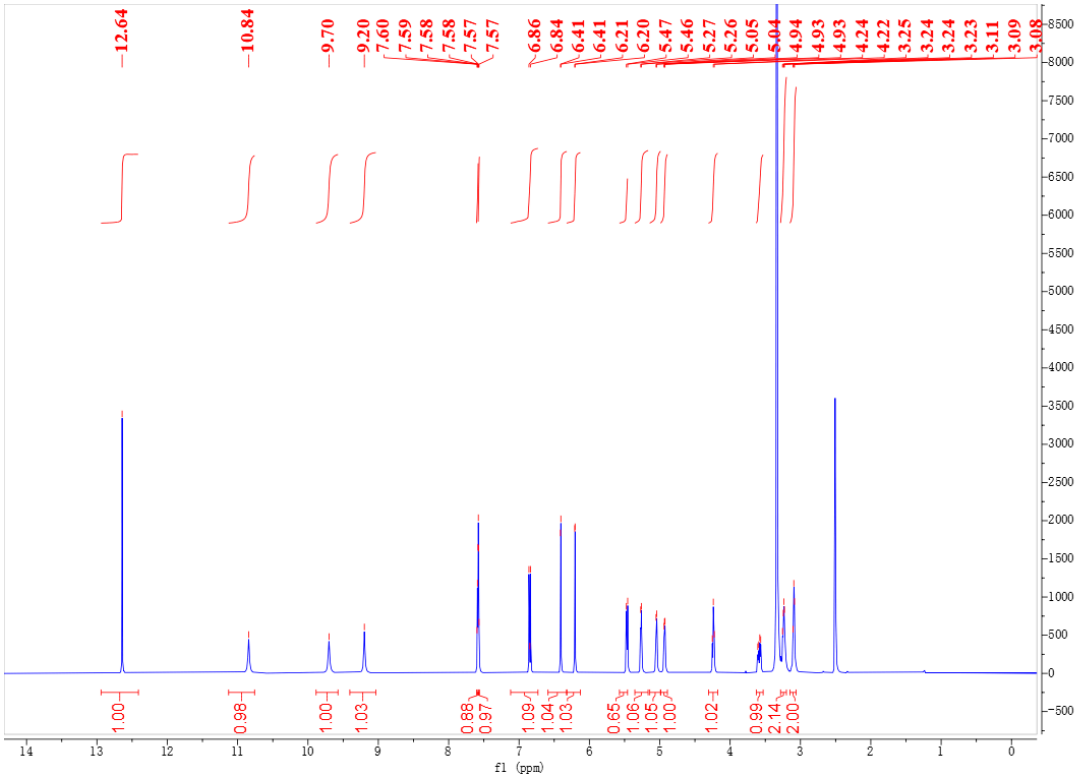

Figure S101. The ^{1}H NMR spectrum of compound **13** (600 MHz, DMSO-d_6).

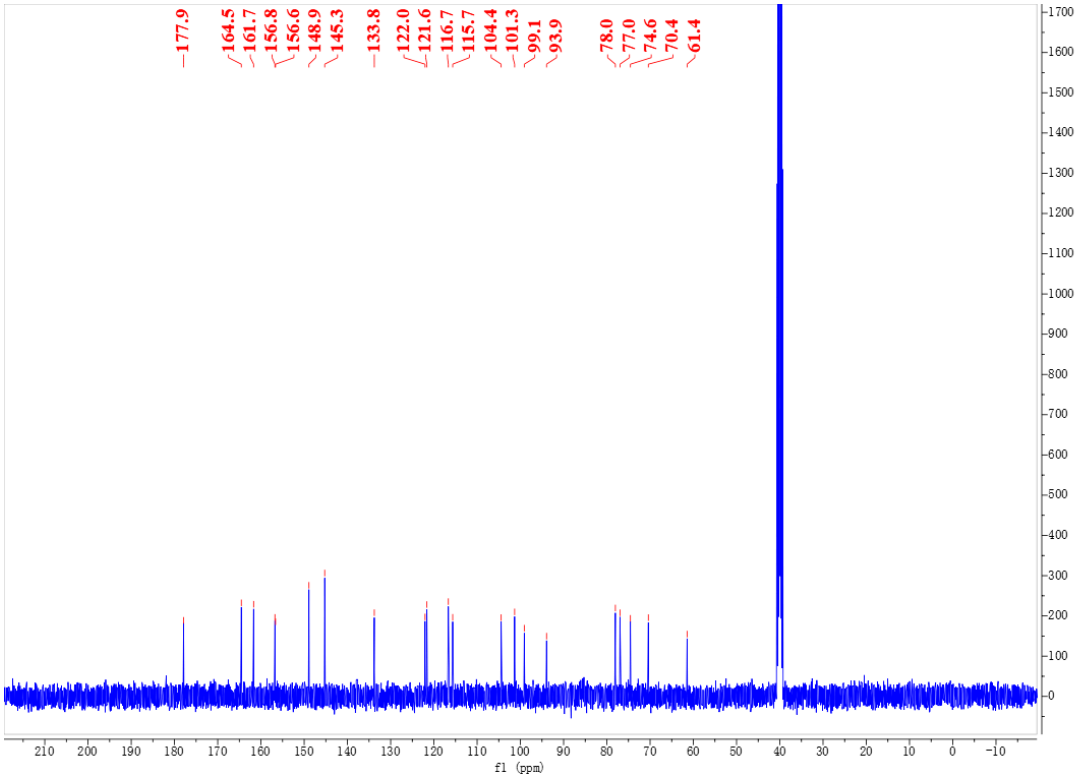

Figure S102. The ^{13}C NMR spectrum of compound **13** (151 MHz, DMSO-d_6).

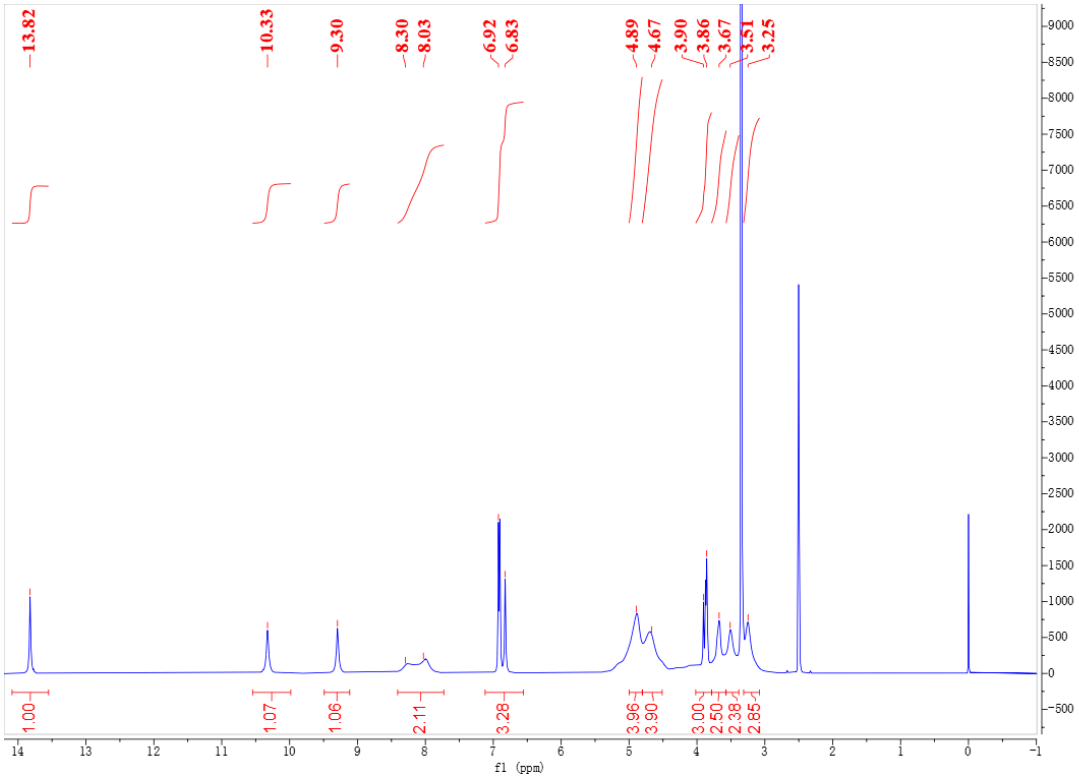

Figure S103. The ^{1}H NMR spectrum of compound **14** (600 MHz, DMSO-d_6).

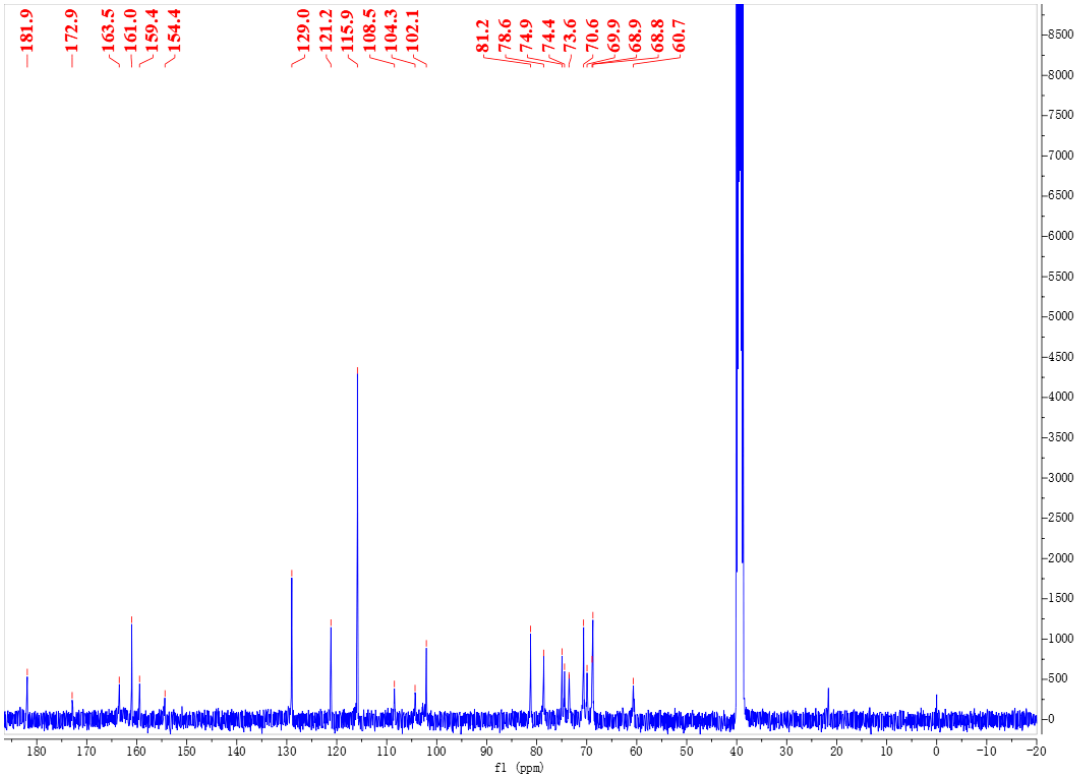

Figure S104. The ^{13}C NMR spectrum of compound **14** (151 MHz, DMSO-d_6).

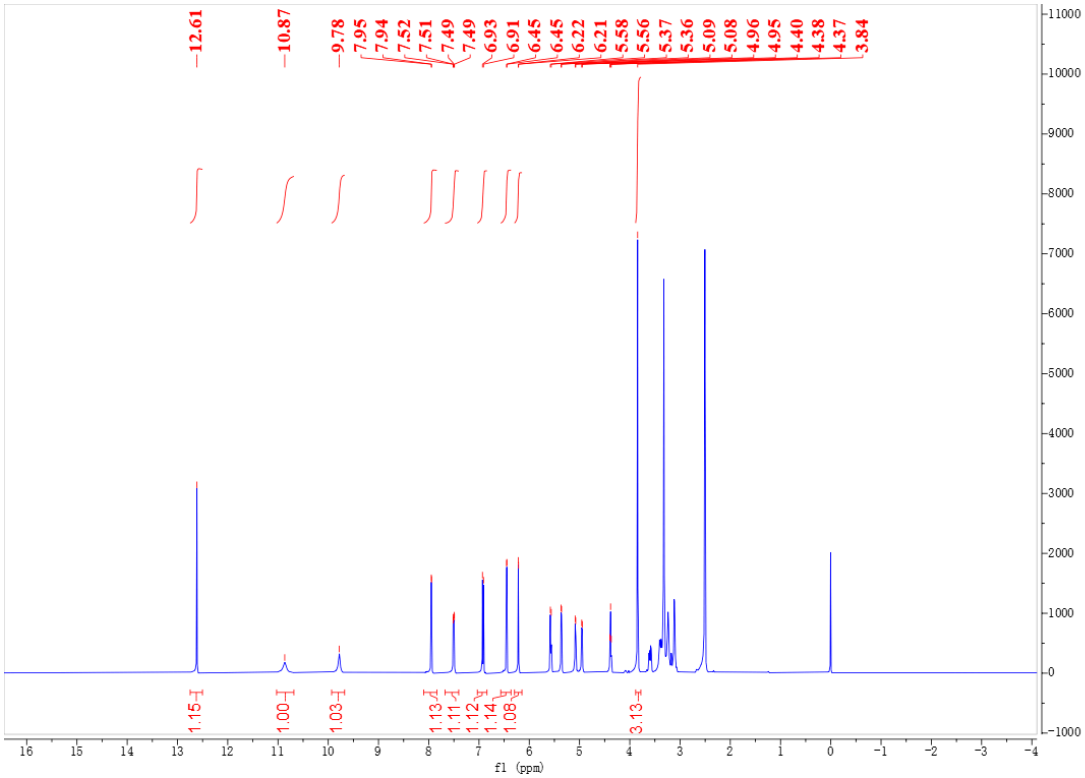

Figure S105. The ^{1}H NMR spectrum of compound **15** (600 MHz, DMSO-d_6).

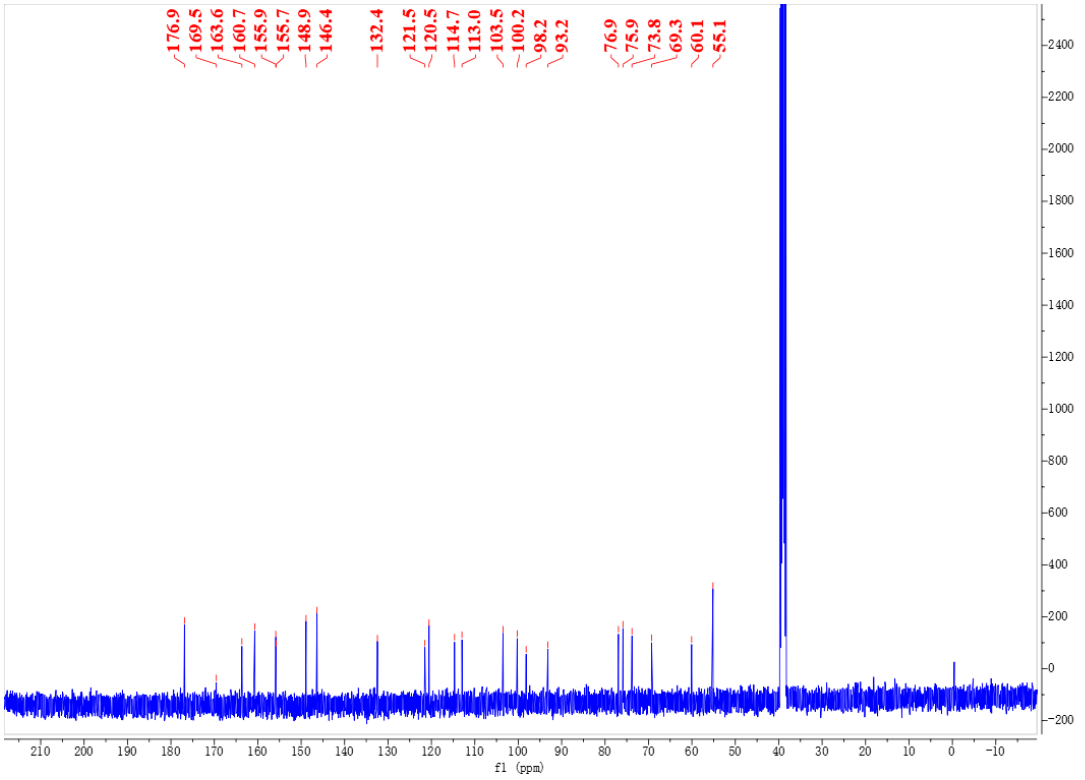

Figure S106. The ^{13}C NMR spectrum of compound **15** (151 MHz, DMSO-d_6).

12. Molecular docking results of compounds **1**−**7** and **9**−**10** with α-Glycosidase.

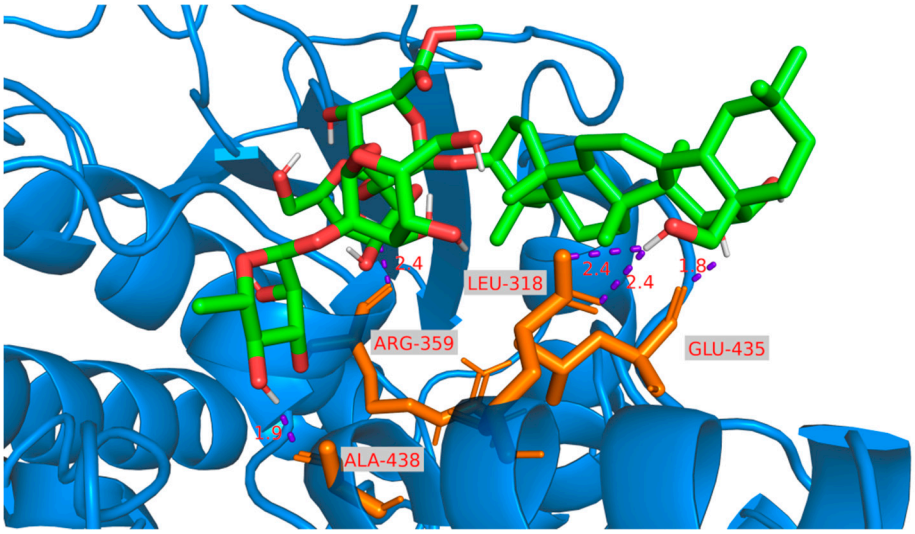

Figure S107. Molecular docking of compound **1**.

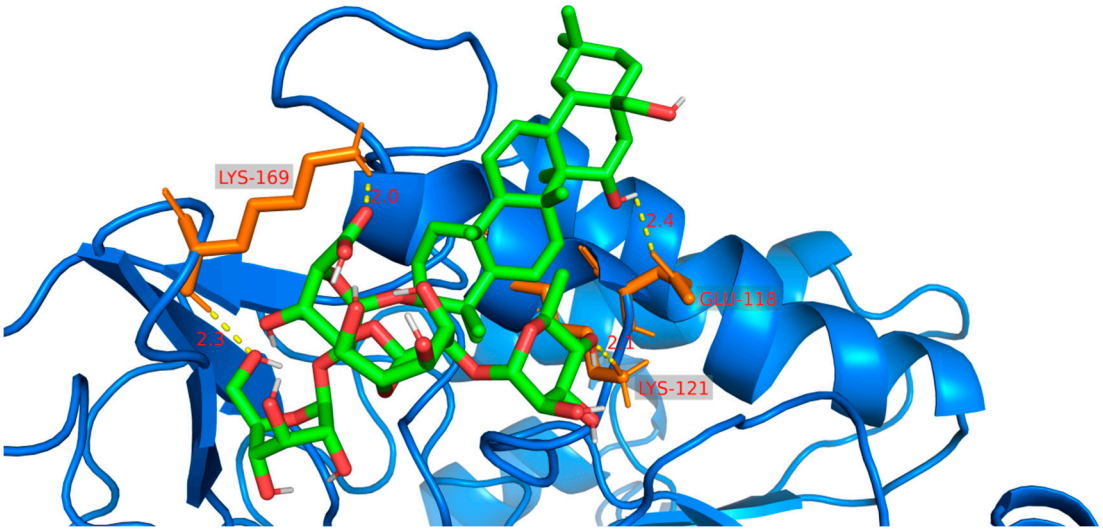

Figure S108. Molecular docking of compound **2**.

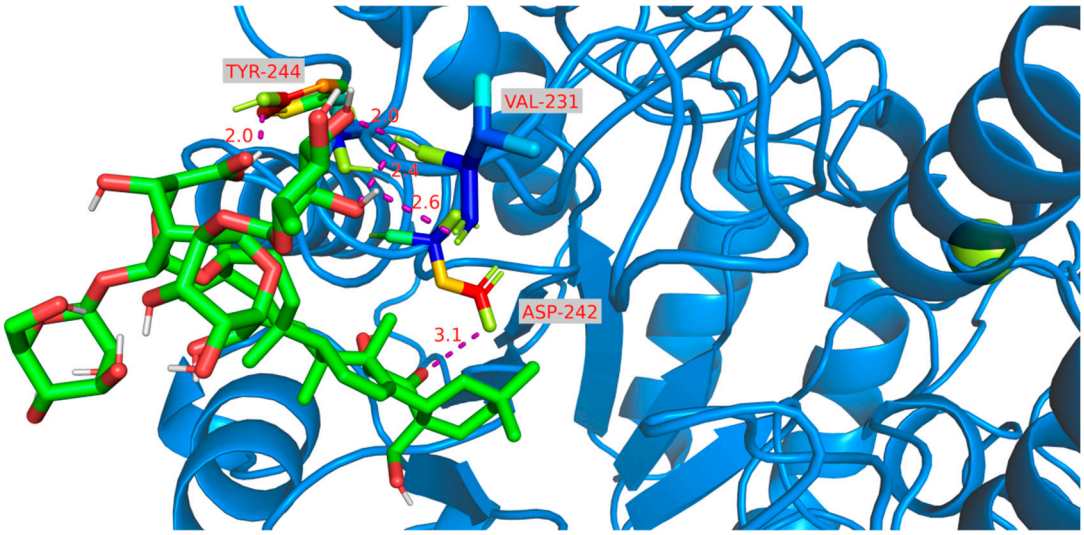

Figure S109. Molecular docking of compound **3**.

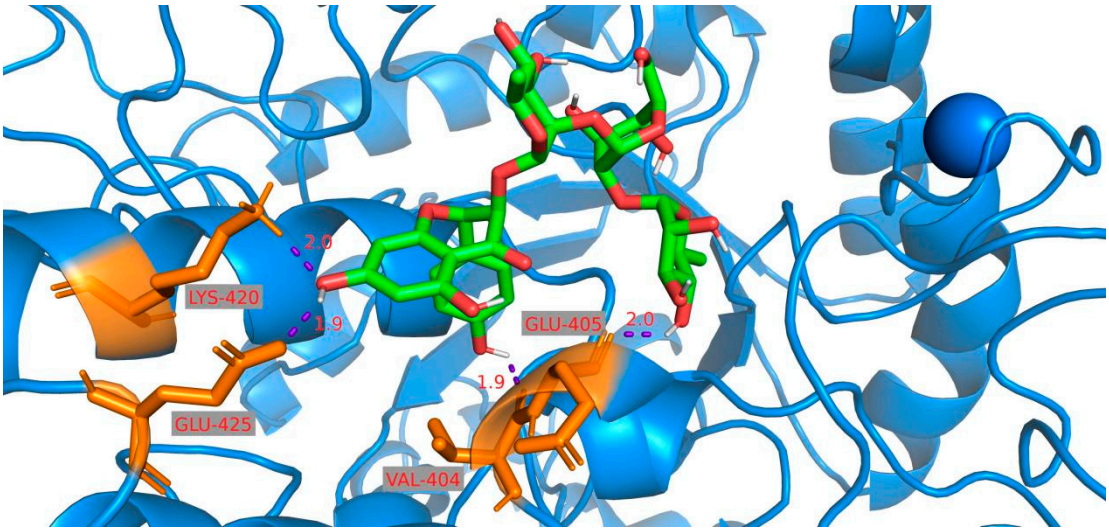

Figure S110. Molecular docking of compound **4**.

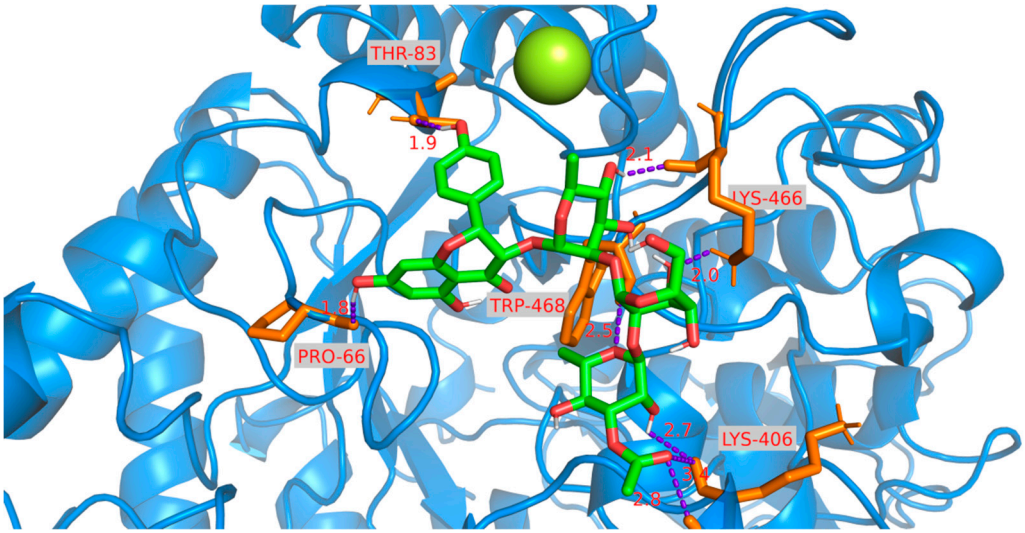

Figure S111. Molecular docking of compound **5**.

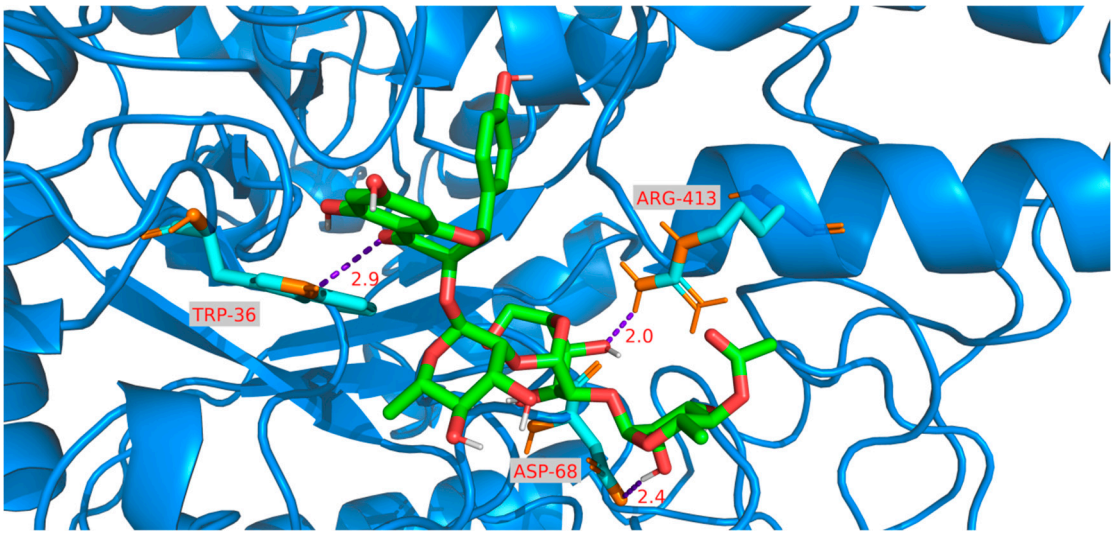

Figure S112. Molecular docking of compound **6**.

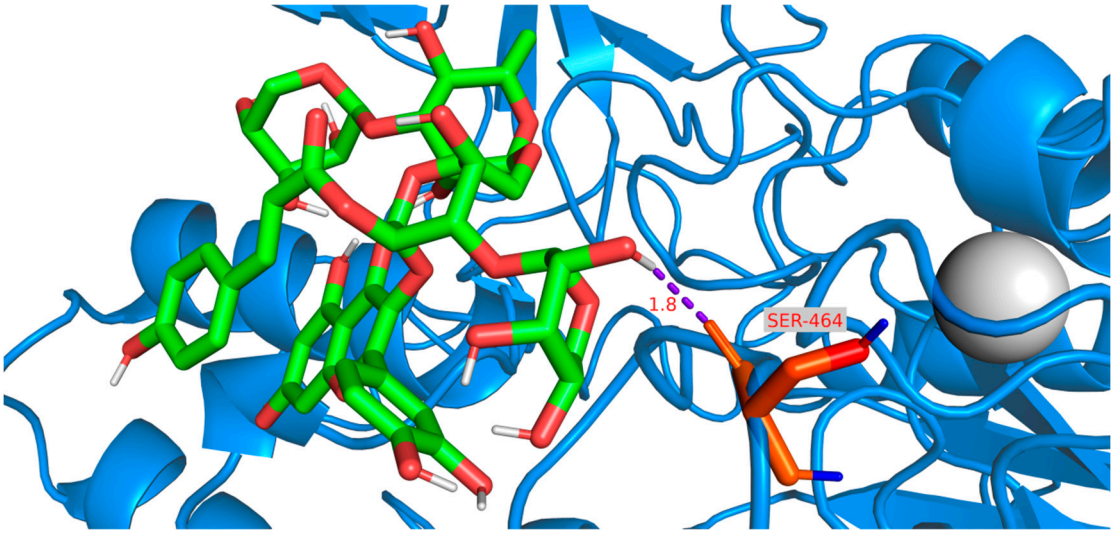

Figure S113. Molecular docking of compound **7**.

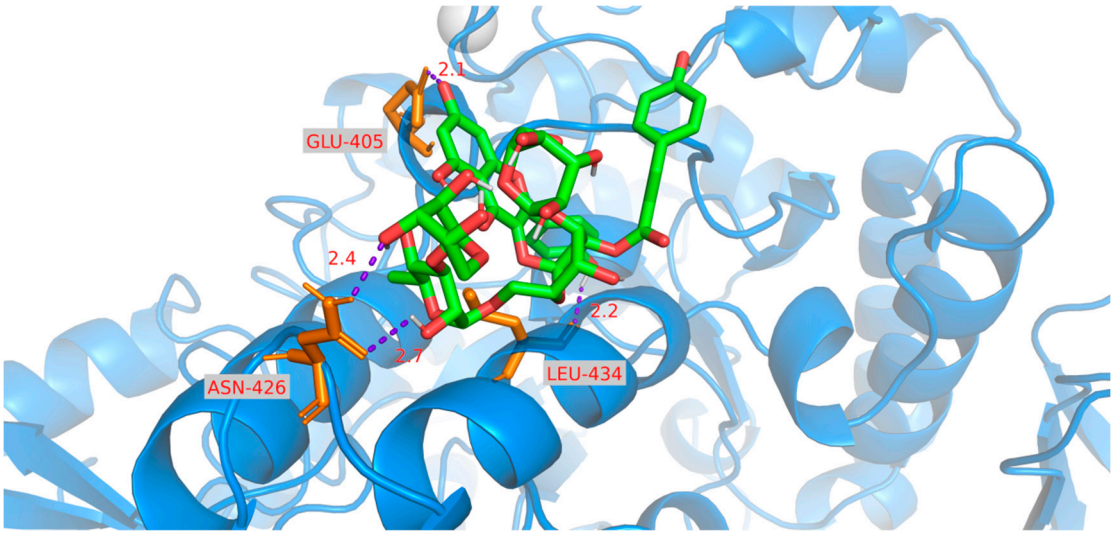

Figure S114. Molecular docking of compound **9**.

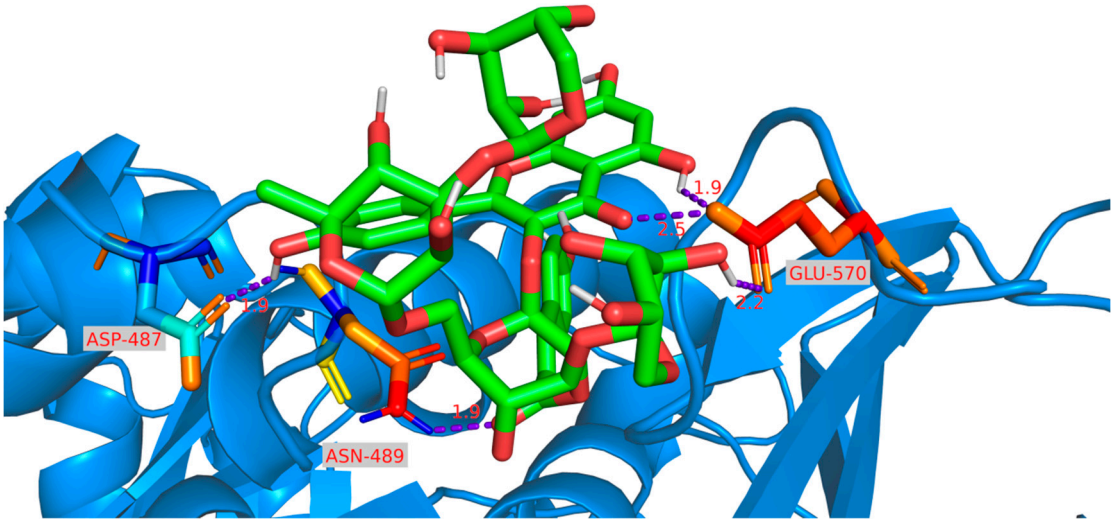

Figure S115. Molecular docking of compound **10**.

Table S1 Molecular docking results of compounds **1–10** with α-glucosidase

Compounds	Binding energy (kcal/mol)	Number of hydrogen bonds	H-bond length	Amino acid residue
1	-0.93	5	1.8、1.9、2.4、2.4、2.4	LEU-318、ALA-438、ARG-359、GLU-435
2	-0.68	4	2.0、2.1、2.3、2.4	LYS-169、LYS-121、GLU-118
3	-1.21	5	2.0、2.0、2.4、2.6、3.1	TYR-244、VAL-231、ASP-242
4	-2.32	4	1.9、1.9、2.0、2.0	GLU-425、VAL-404、LYS-420、GLU-405
5	-3.17	8	1.8、1.9、2.0、2.1、2.5、2.7、2.8、3.4	PRO-66、THR-83、LYS-466、TRP-468、LYS-406、GLU-405
6	-2.44	3	2.0、2.4、2.9	ARG-413、ASP-68、TRP-36
7	-1.52	1	1.8	SER-464
8	-5.48	5	2.9、2.9、3.1、3.2、3.5	ASP-307、PRO-320、GLU-322、THR-310
9	-2.68	4	2.1、2.2、24、2.7	GLU-405、LEU-434、ASN-426
10	-2.04	5	1.9、1.9、1.9、2.2、2.5	ASP-487、ASN-489、GLU-570