

Supplementary material

Isolation, Structural Elucidation of Three New Triterpenoids from the Stems and Leaves of *Schisandra chinensis* (Turcz) Baill.

Feng Qiu, Han Liu, Huan Duan, Pian Chen, Shao-Juan Lu, Guang-Zhong Yang* and Xin-Xiang Lei *

School of Pharmaceutical Sciences, South-Central University for Nationalities, Wuhan 430074, China;

2016110449@mail.scuec.edu.cn (F.Q.); 2017110424@mail.scuec.edu.cn (H.L.);

2016110444@mail.scuec.edu.cn (H.D.); chenpian1104@126.com (P.C.); 201621154052@mail.scuec.edu.cn (S.L.)

* Correspondence: yanggz@mail.scuec.edu.cn (G.-Z.Y.); xxlei@mail.scuec.edu.cn (X.-X.L.);

Tel.: +86-27-67841196 (X.-X.L.)

Table of contents

Figure S1. ^1H -NMR (600 MHz, CD_3OD) spectrum of compound 1

Figure S2. ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound 1

Figure S3. DEPT 135° spectrum of compound 1

Figure S4. ^1H - ^1H COSY spectrum of compound 1

Figure S5. HSQC spectrum of compound 1

Figure S6. HMBC spectrum of compound 1

Figure S7. Key HMBC correlations and ^1H - ^1H COSY correlations of compound 1

Figure S8. X-ray SAINT drawing of compound 1

Figure S9. HR-ESI-MS spectrum of compound 1

Figure S10. IR spectrum of compound 1

Figure S11. ^1H -NMR (600 MHz, CD_3OD) spectrum of compound 2

Figure S12. ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound 2

Figure S13. DEPT 135° spectrum of compound 2

Figure S14. ^1H - ^1H COSY spectrum of compound 2

Figure S15. HSQC spectrum of compound 2

Figure S16. HMBC spectrum of compound 2

Figure S17. Key HMBC correlations and ^1H - ^1H COSY correlations of compound 2

Figure S18. HR-ESI-MS spectrum of compound 2

Figure S19. IR spectrum of compound **2**

Figure S20. ^1H -NMR (600 MHz, CD_3OD) spectrum of compound **3**

Figure S21. ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **3**

Figure S22. DEPT 135° spectrum of compound **3**

Figure S23. ^1H - ^1H COSY spectrum of compound **3**

Figure S24. HSQC spectrum of compound **3**

Figure S25. HMBC spectrum of compound **3**

Figure S26. HR-ESI-MS spectrum of compound **3**

Figure S27. IR spectrum of compound **3**

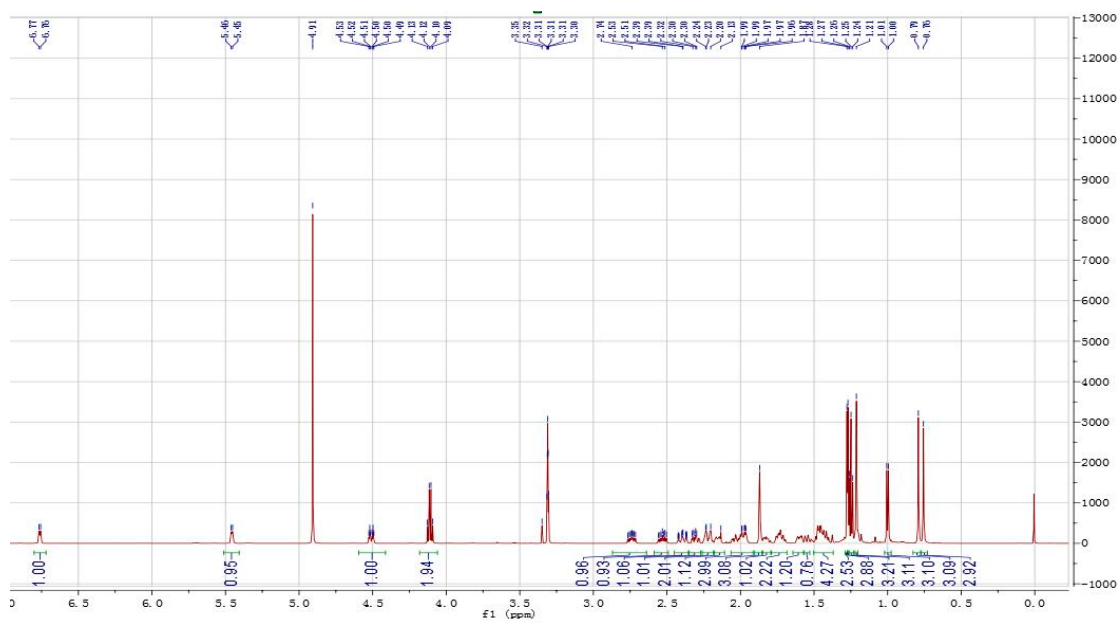


Figure S1. ^1H -NMR (600 MHz, CD_3OD) spectrum of compound **1**

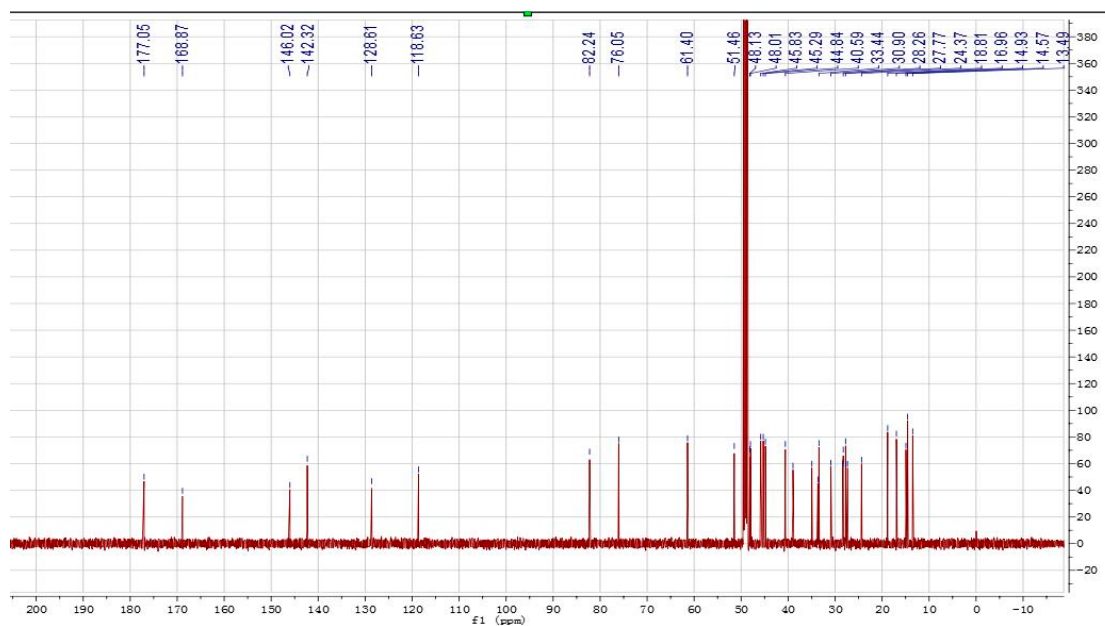
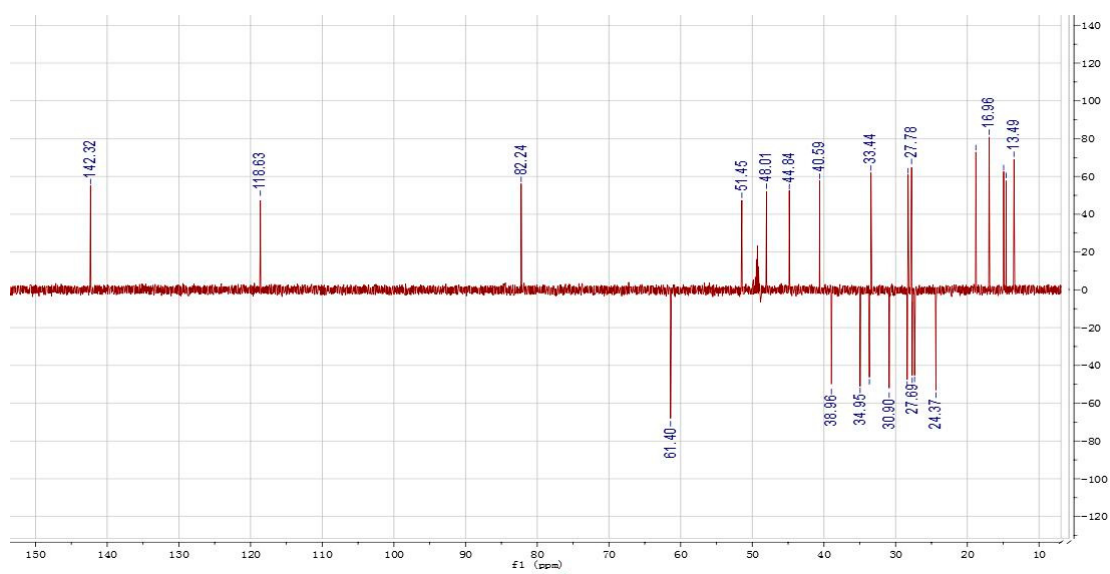
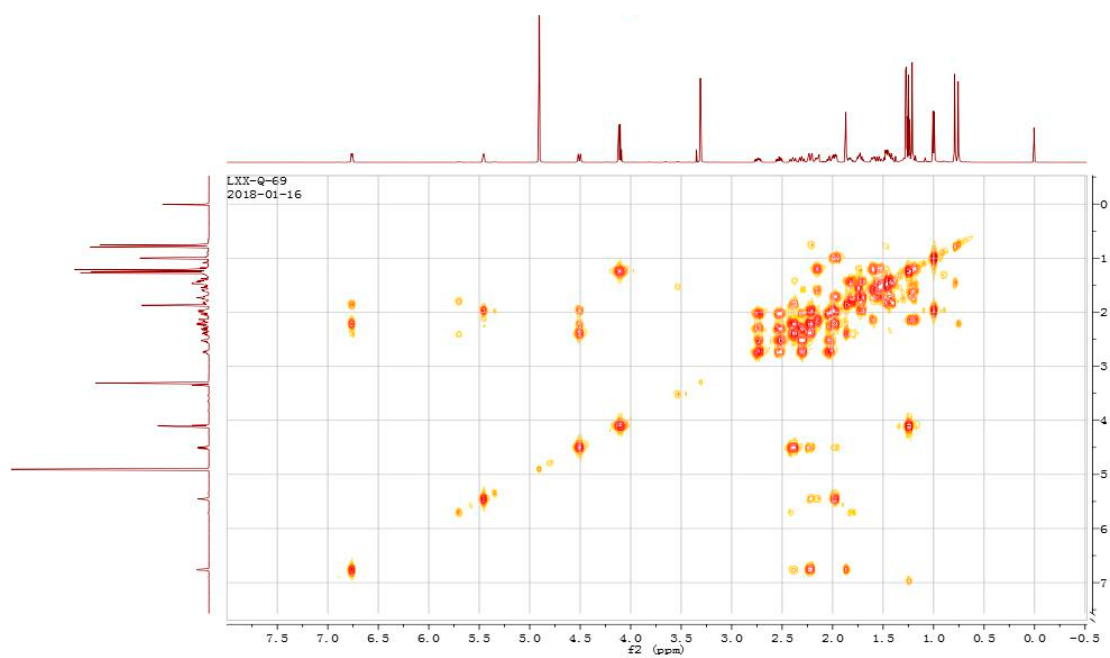
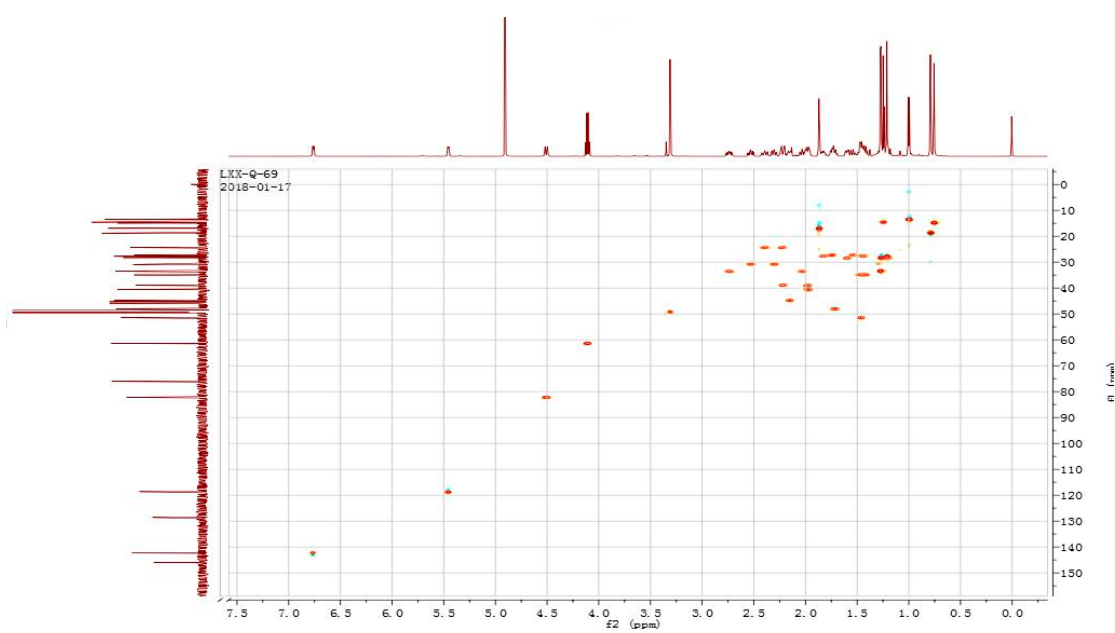
Figure S2. ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound 1

Figure S3. DEPT 135° spectrum of compound 1

Figure S4. ^1H - ^1H COSY spectrum of compound **1**Figure S5. HSQC spectrum of compound **1**

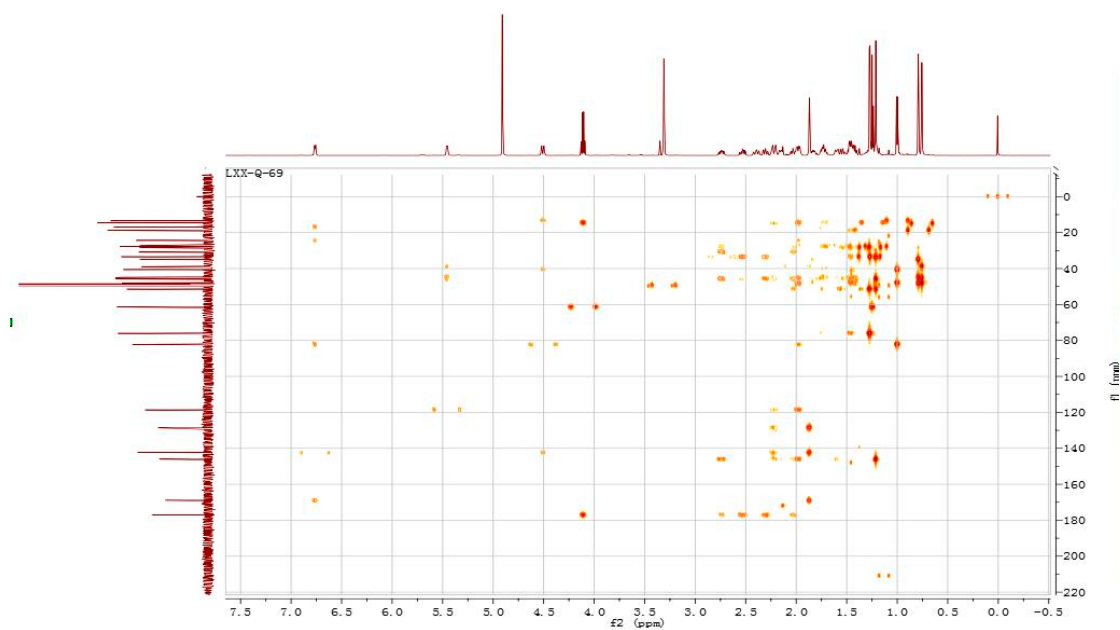
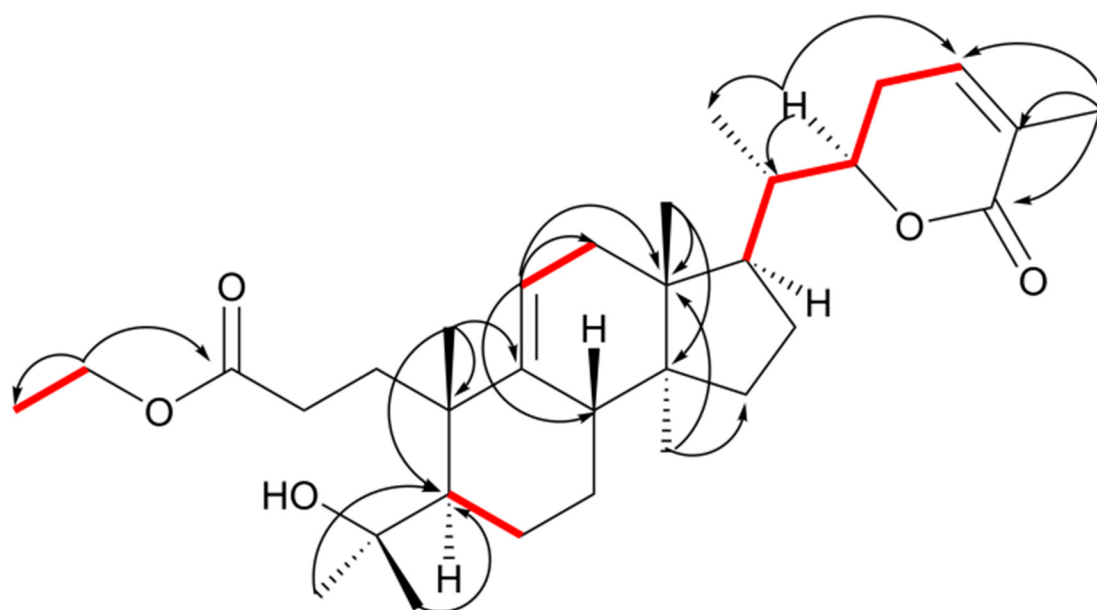


Figure S6. HMBC spectrum of compound 1

Figure S7. Key HMBC correlations and ^1H - ^1H COSY correlations of compound 1

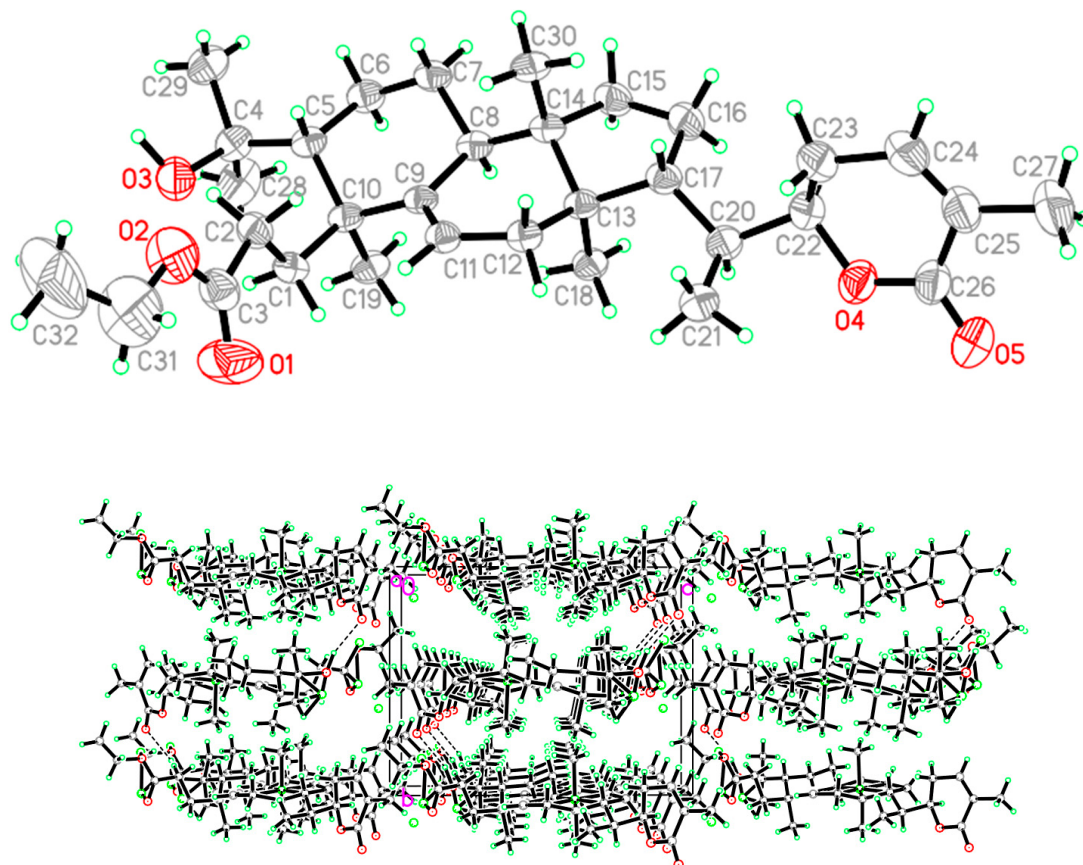


Figure S8. X-ray SAINT drawing of compound 1

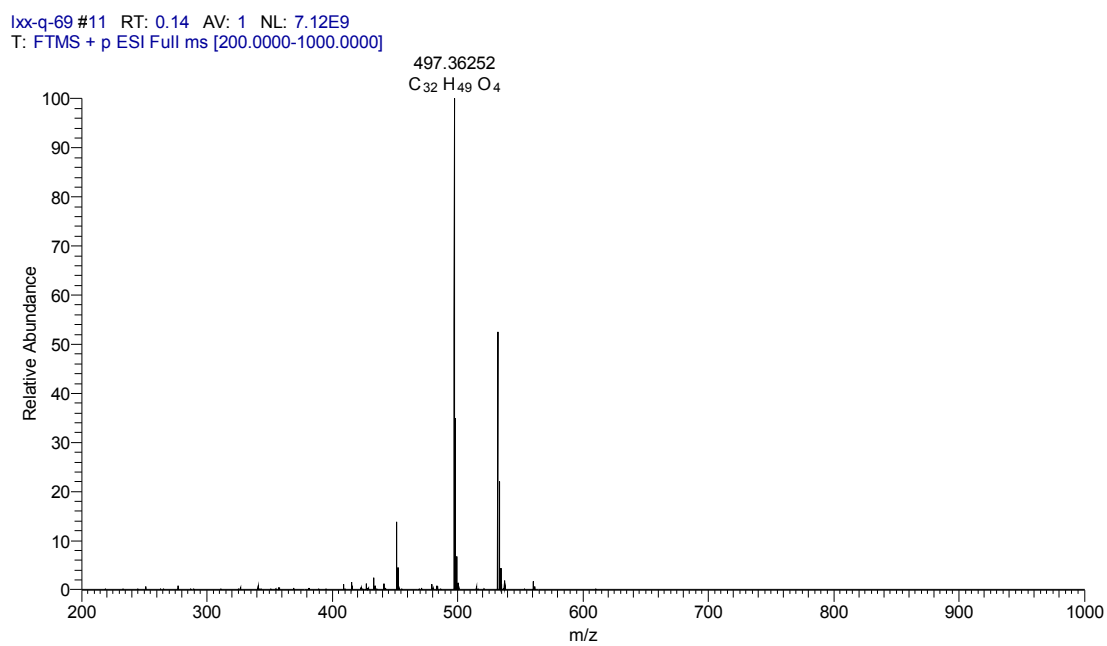


Figure S9. HR-ESI-MS spectrum of compound 1

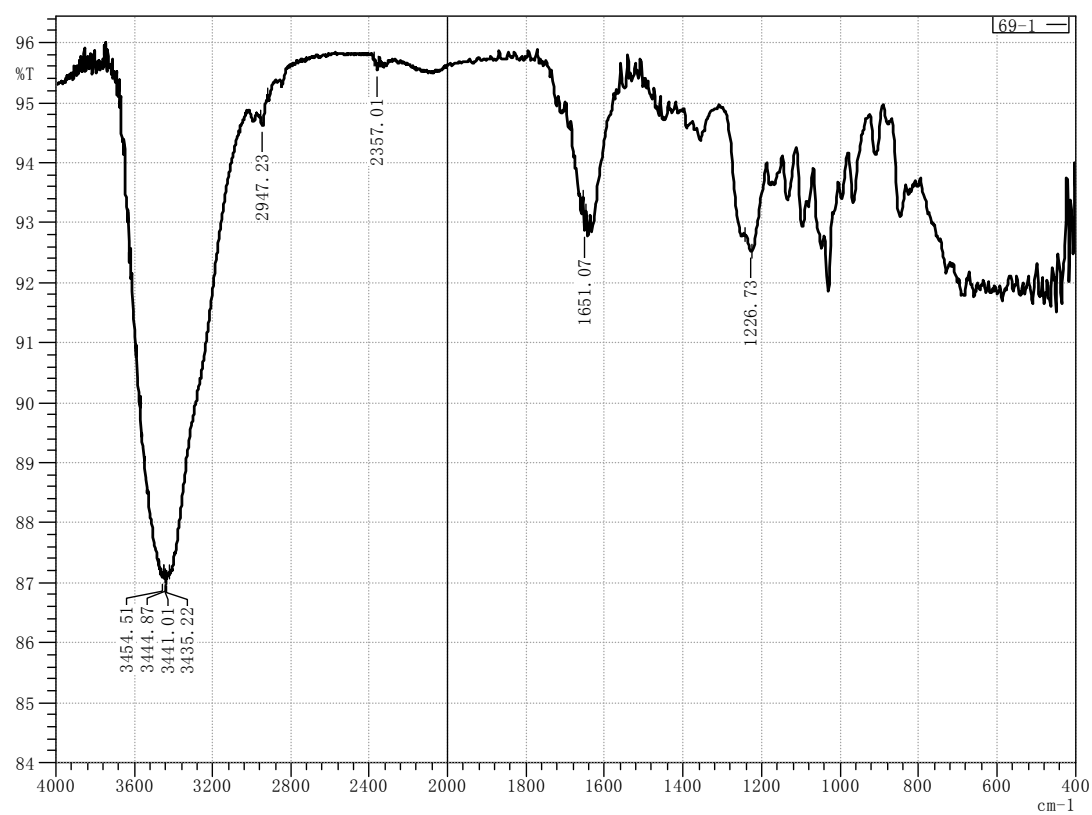
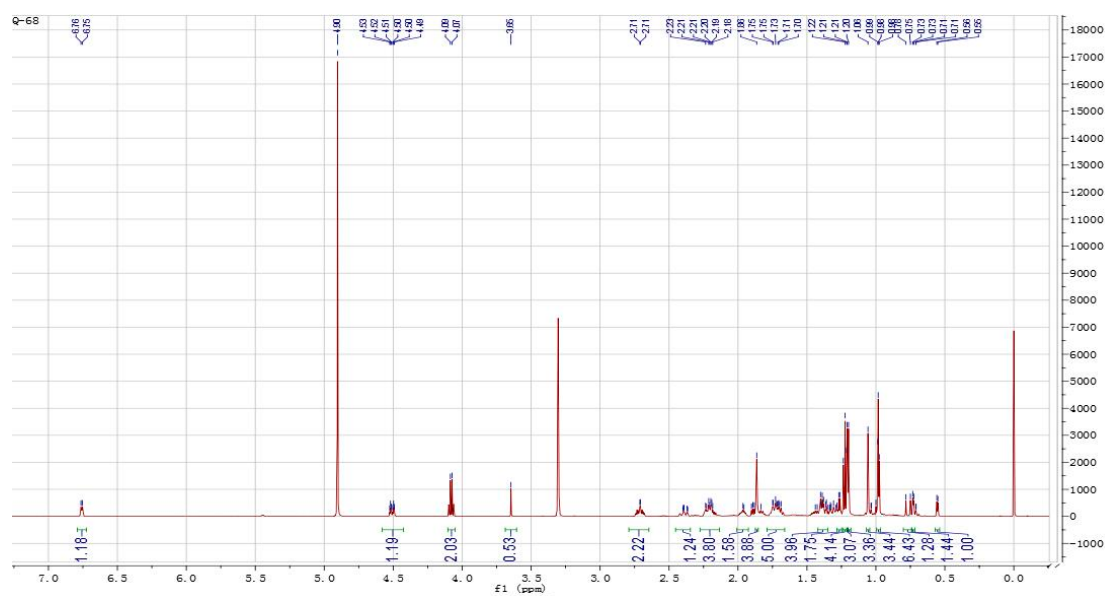


Figure S10. IR spectrum of compound 1

Figure S11. ¹H-NMR (600 MHz, CD₃OD) spectrum of compound 2

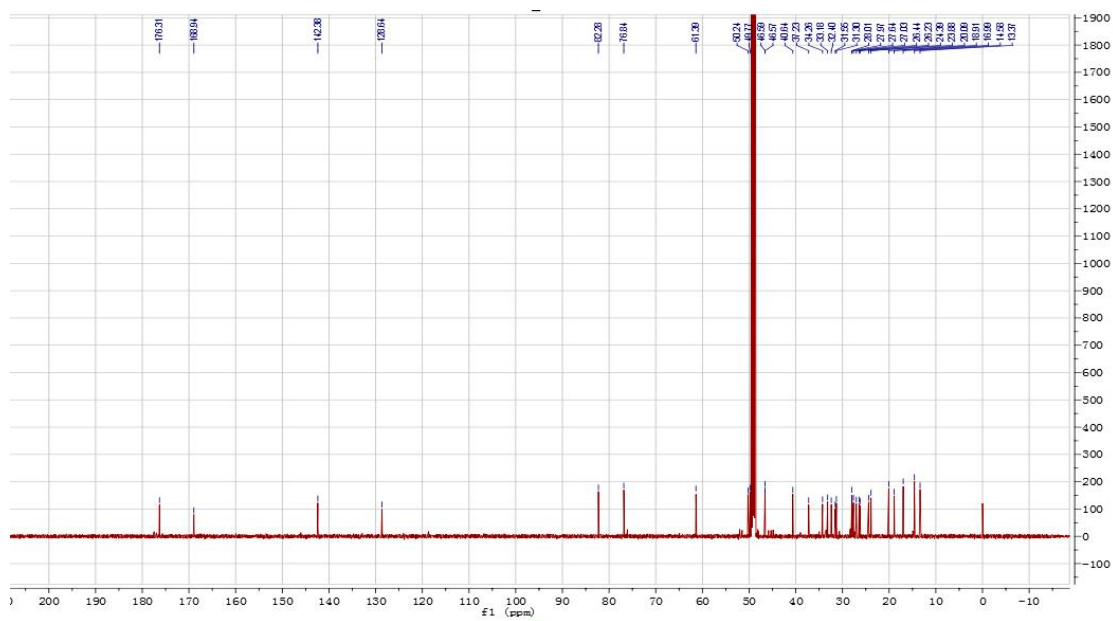
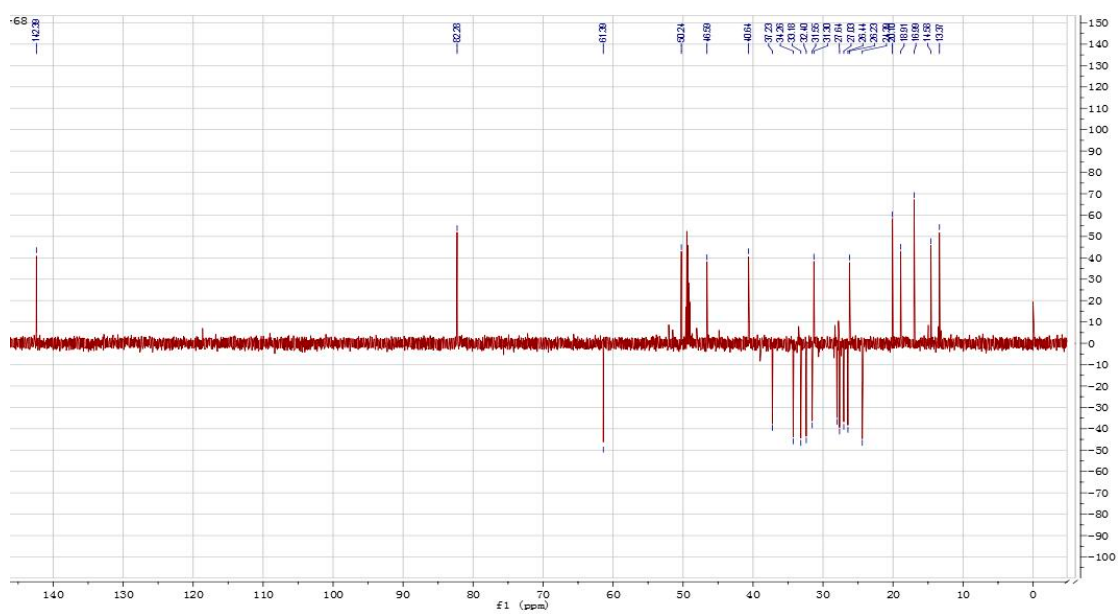
Figure S12. ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound 2

Figure S13. DEPT 135° spectrum of compound 2

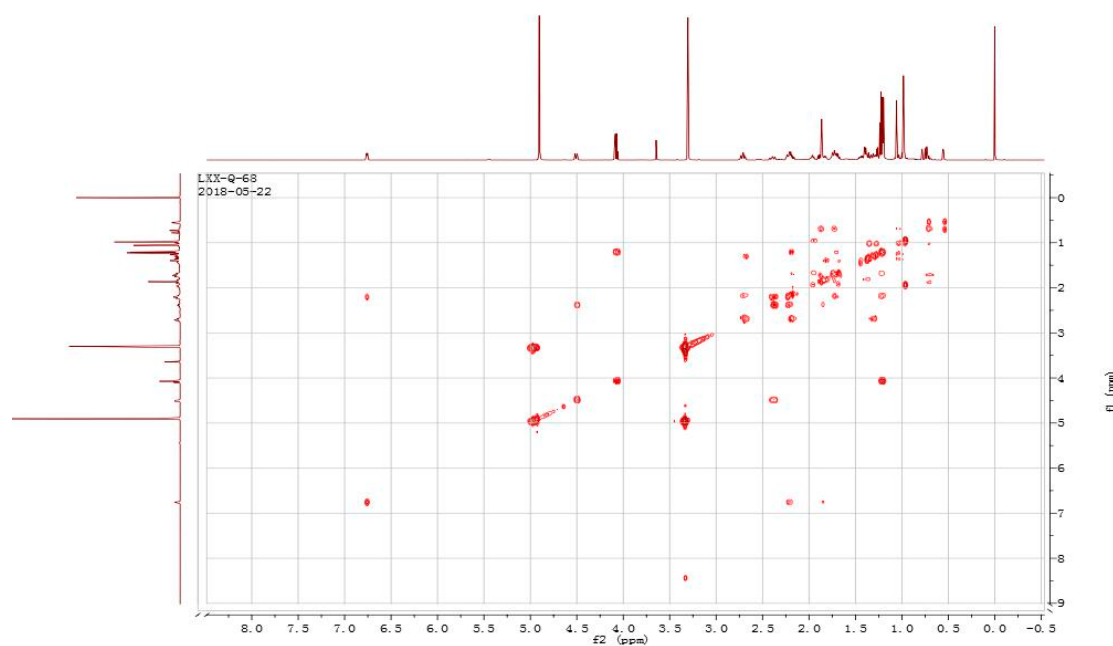
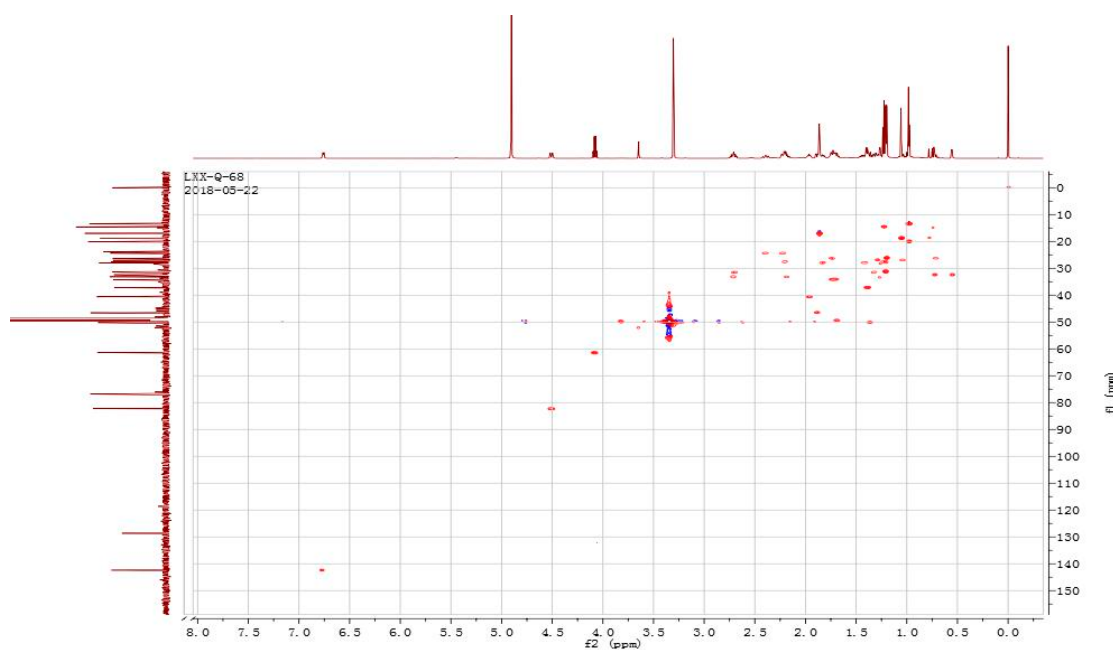
Figure S14. ^1H - ^1H COSY spectrum of compound 2

Figure S15. HSQC spectrum of compound 2

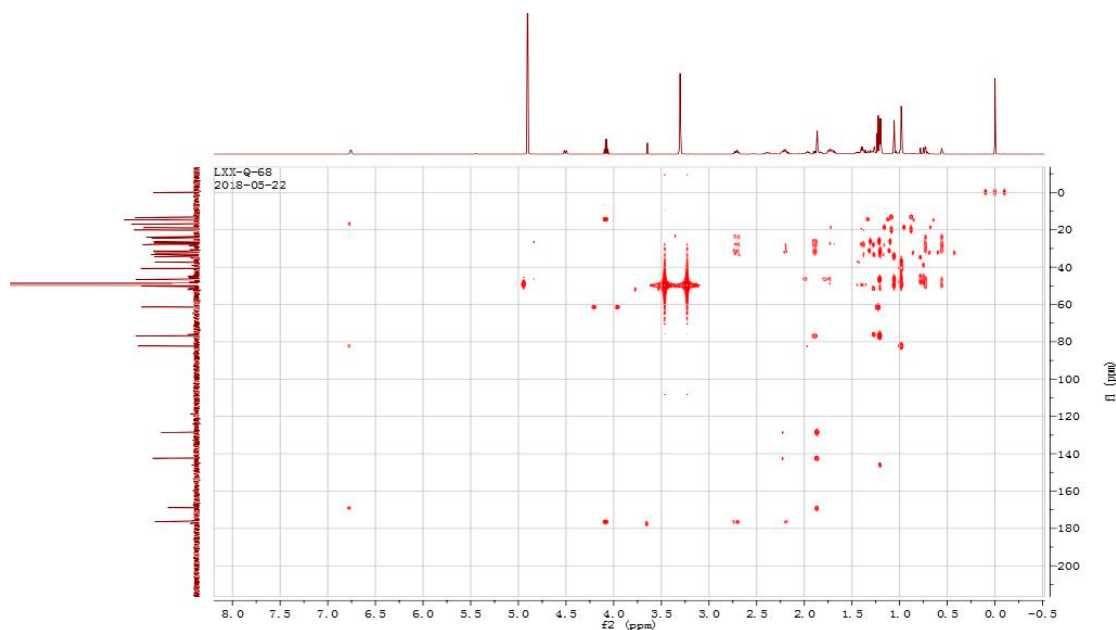
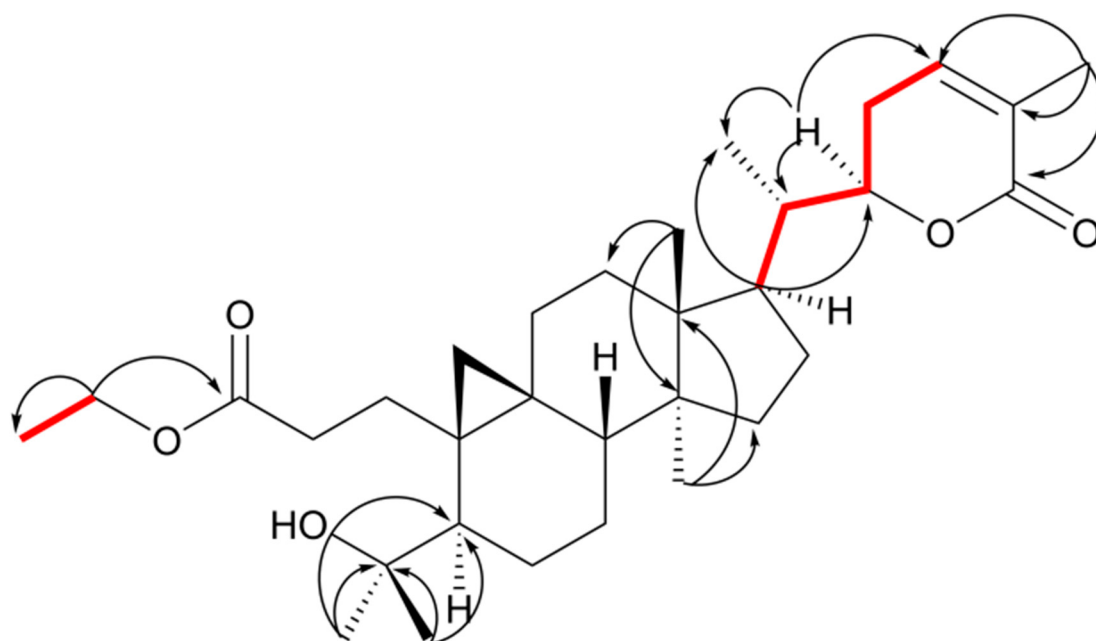


Figure S16. HMBC spectrum of compound 2

Figure S17. Key HMBC correlations and ^1H - ^1H COSY correlations of compound 2

lxx-Q-68 #11 RT: 0.14 AV: 1 NL: 2.25E8
T: FTMS + p ESI Full ms [100.0000-1100.0000]

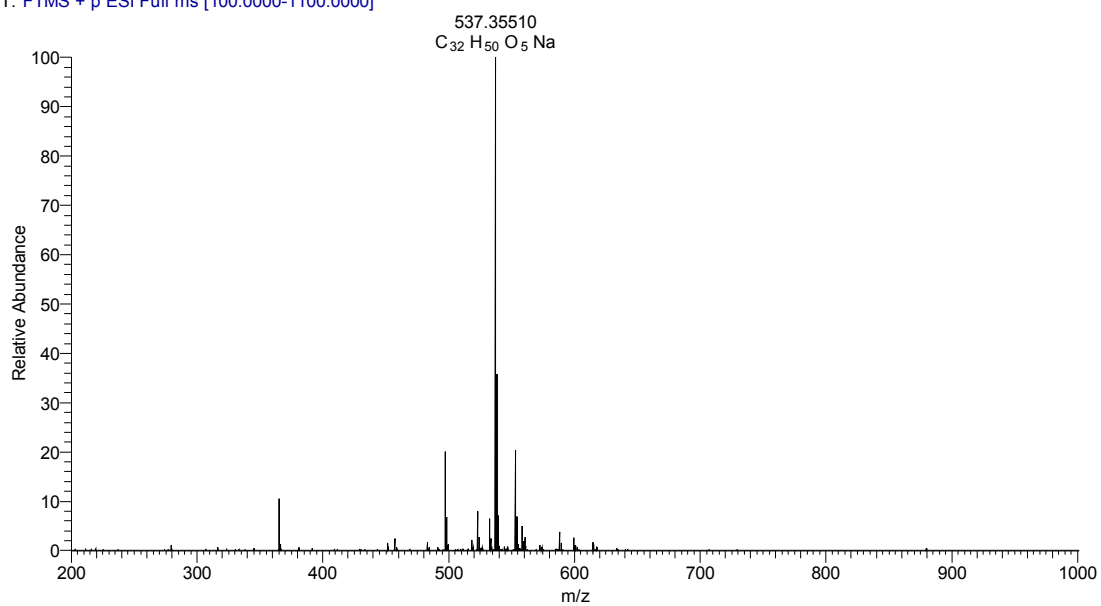


Figure S18. HR-ESI-MS spectrum of compound 2

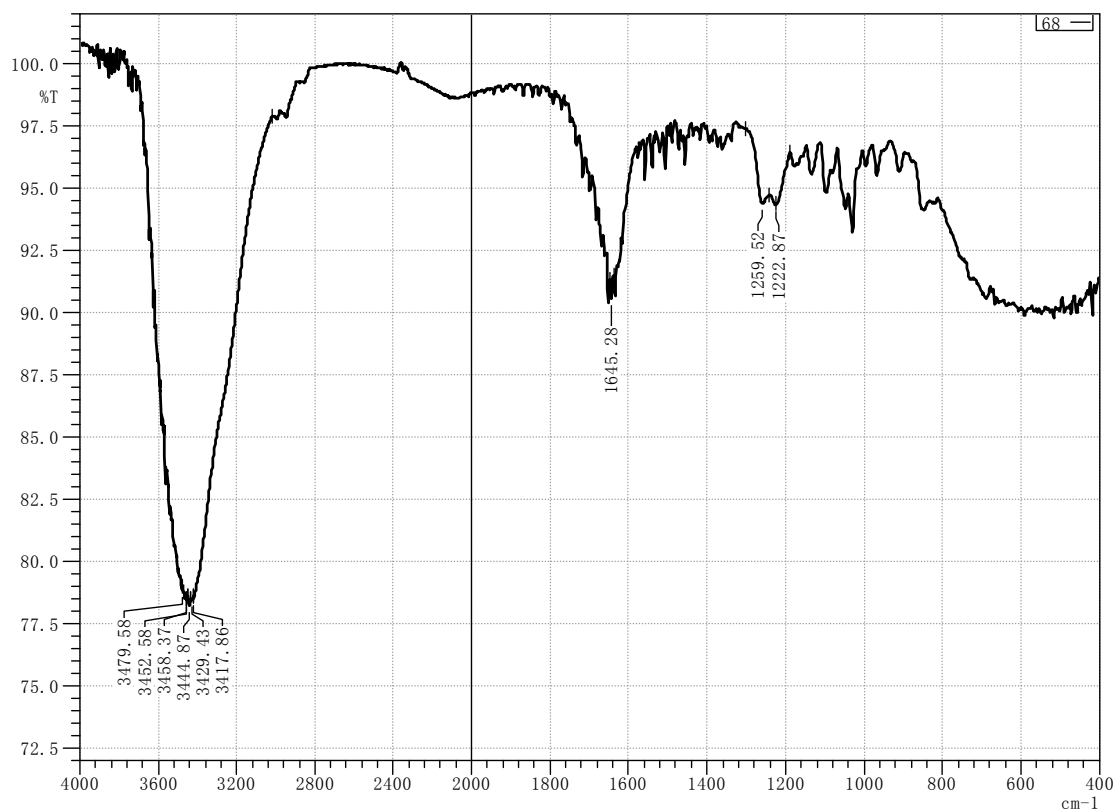


Figure S19. IR spectrum of compound 2

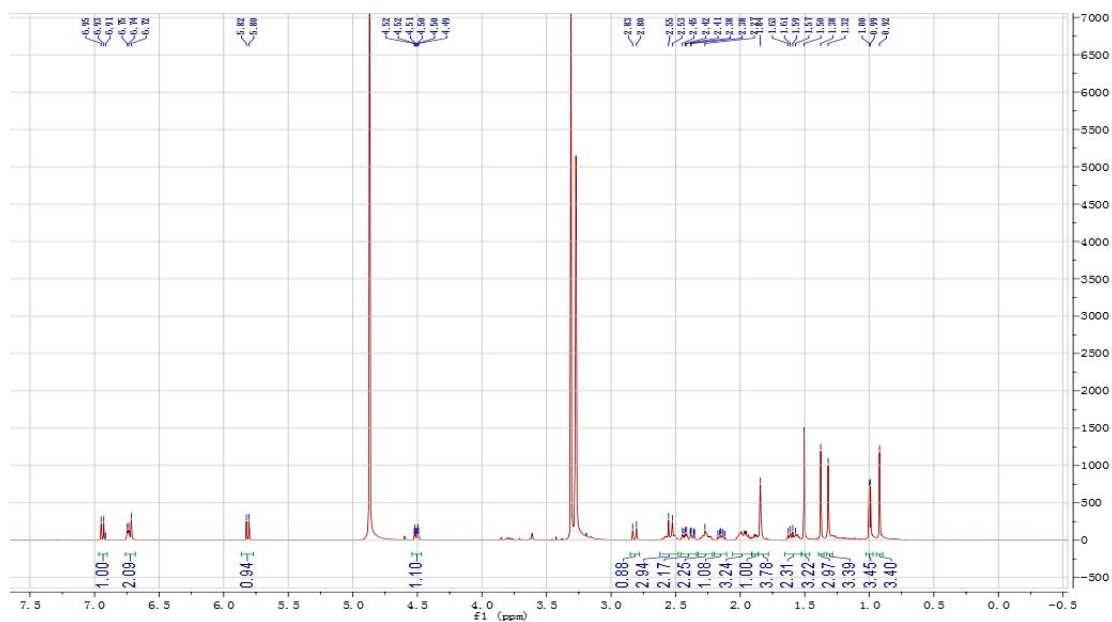


Figure S20. ¹H-NMR (600 MHz, CD₃OD) spectrum of compound **3**

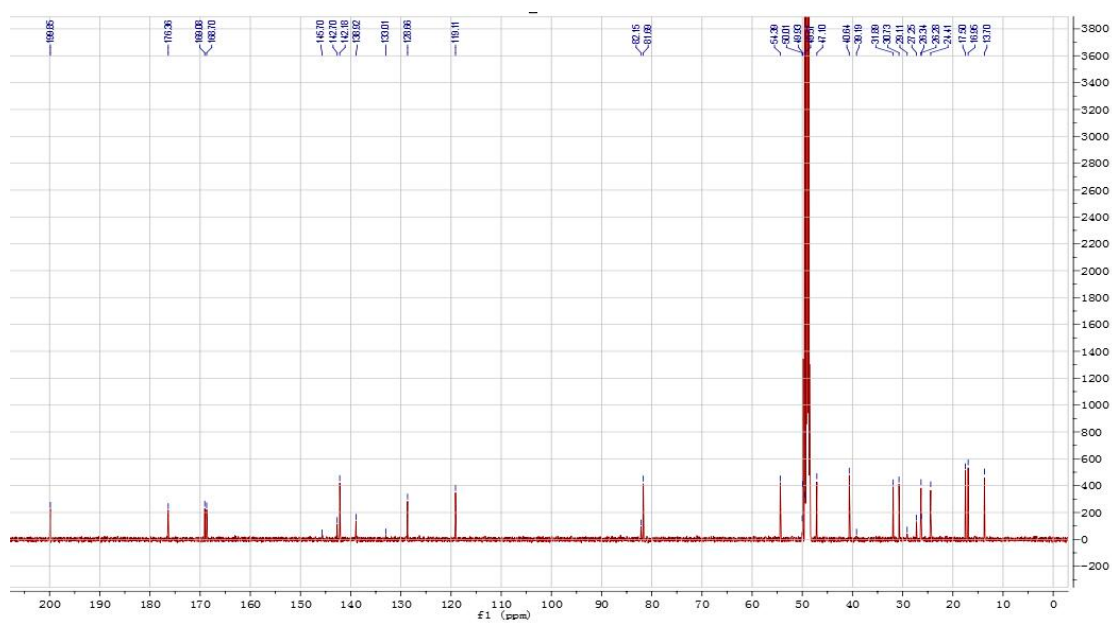


Figure S21. ^{13}C -NMR (150 MHz, CD_3OD) spectrum of compound **3**

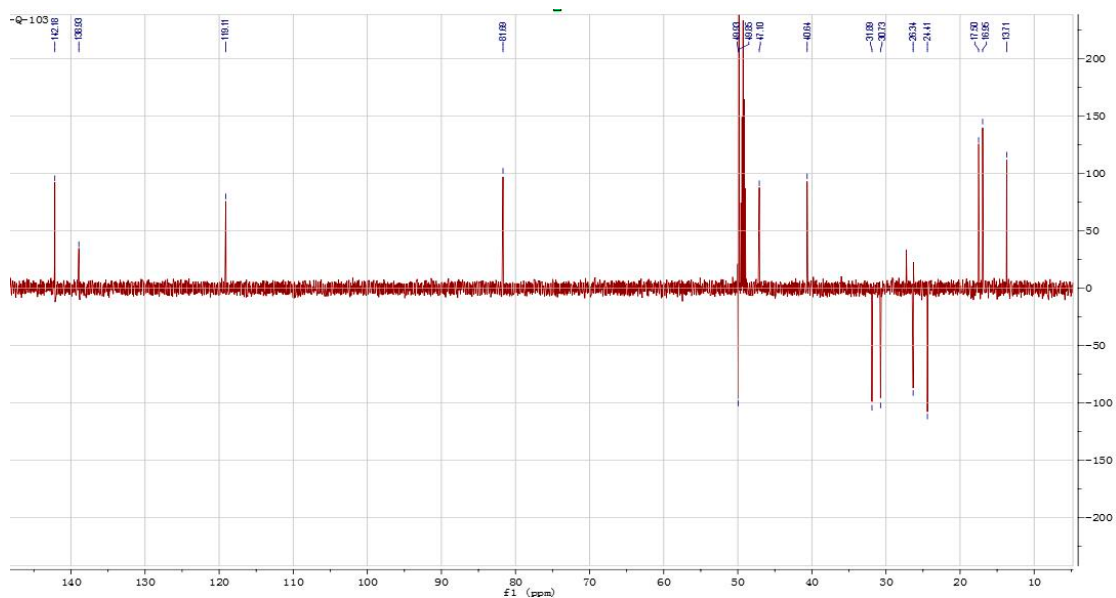
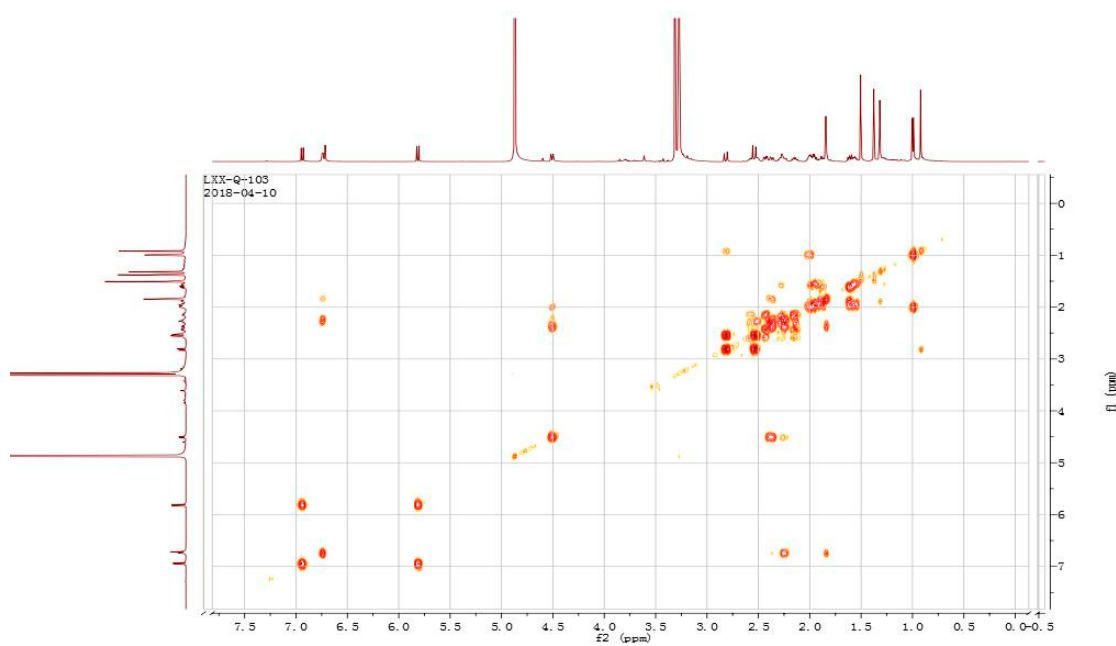


Figure S22. DEPT 135° spectrum of compound 3

Figure S23. ¹H-¹H COSY spectrum of compound 3

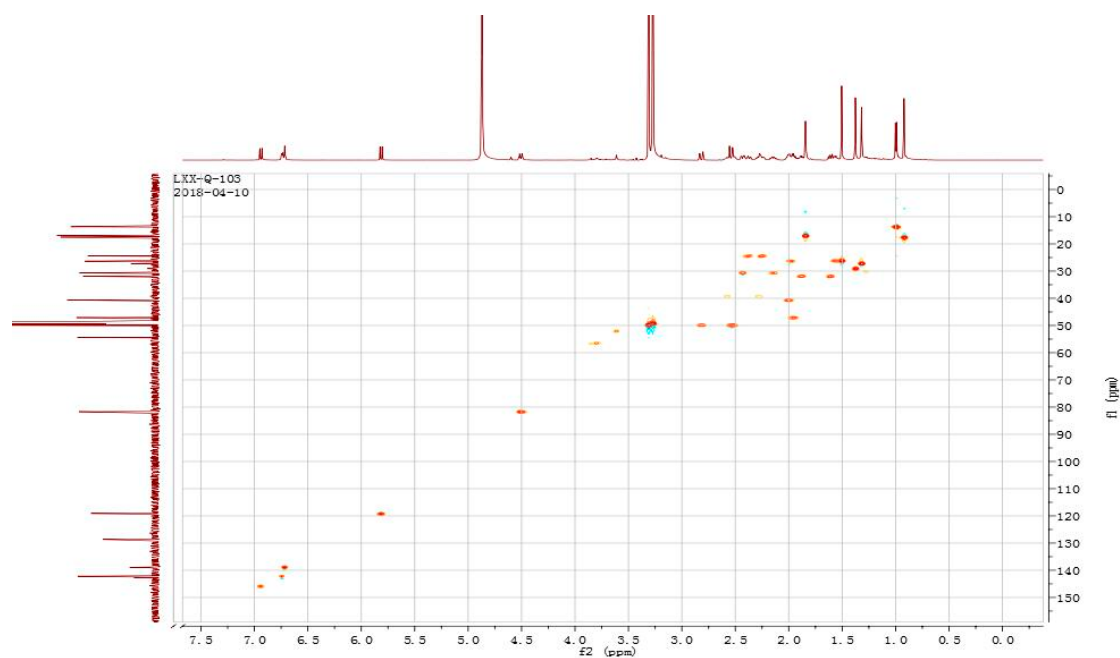


Figure S24. HSQC spectrum of compound 3

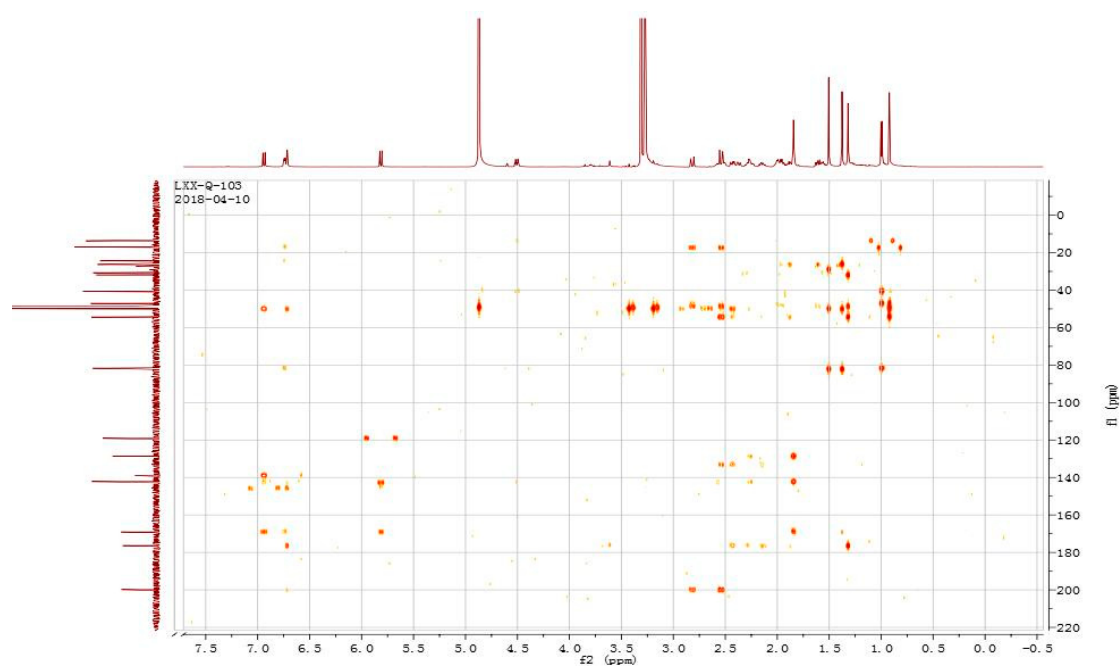


Figure S25. HMBC spectrum of compound 3

103 #11 RT: 0.14 AV: 1 NL: 3.31E8

T: FTMS + p ESI Full lock ms [100.0000-1100.0000]

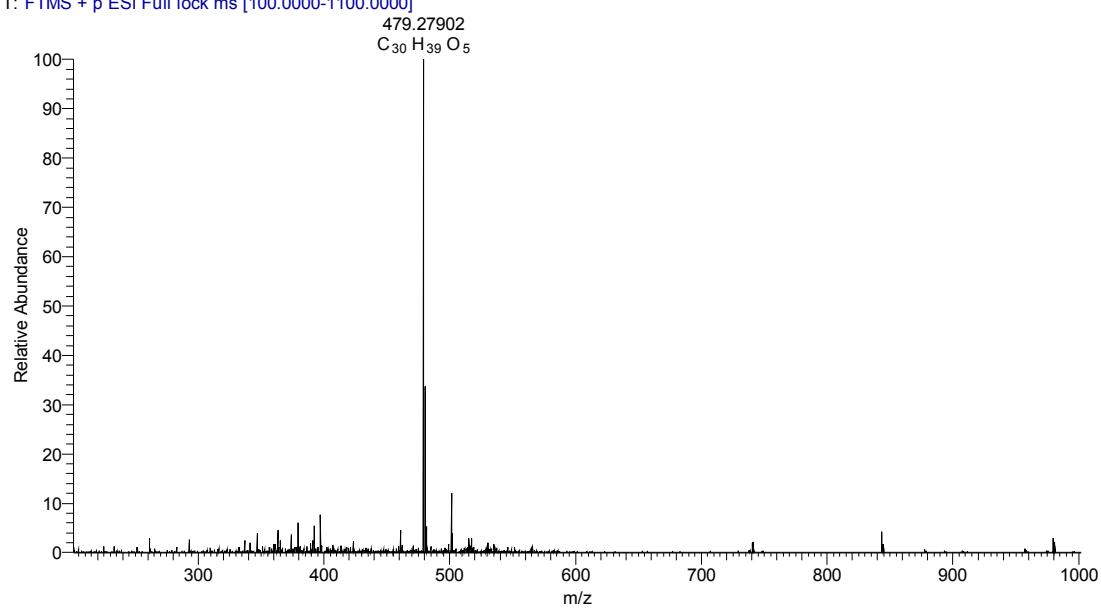


Figure S26. HR-ESI-MS spectrum of compound 3

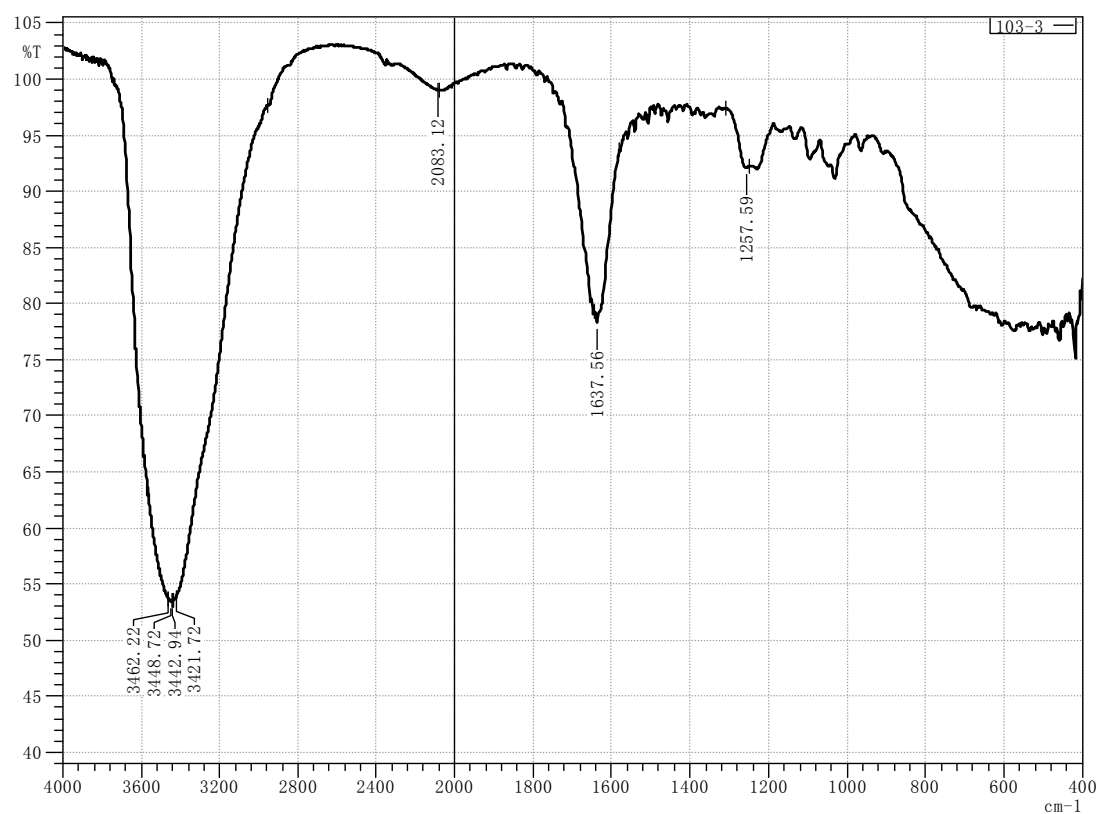


Figure S27. IR spectrum of compound 3