

Electronic Supplementary Information

Withapubesides A–D, natural inducible nitric oxide synthase (iNOS) inhibitors

from *Physalis pubescens*

Gui-yang Xia,^{ab} Tie Yao,^{ab} Bing-yang Zhang,^a Yang Li,^b Ning Kang,^a Shi-jie Cao,^a Li-qin Ding,^a Li-Xia Chen,^{*b} Feng Qiu^{*a}

^a. Tianjin State Key Laboratory of Modern Chinese Medicine and School of Chinese Materia Medica, Tianjin University of Traditional Chinese Medicine, 312 Anshanxi Road, Nankai District, Tianjin 300193, China. E-mail: fengqiu20070118@163.com.

^b. Department of Natural Products Chemistry, School of Traditional Chinese Materia Medica, Wuya college of innovation, Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China. E-mail: syzyclx@163.com.

Contents of Electronic Supplementary Information

Figure S1. ^{13}C NMR (150 MHz) spectrum of compound 1 in pyridine- d_5	1
Figure S2. ^1H NMR (600 MHz) spectrum of compound 1 in pyridine- d_5	2
Figure S3. HSQC spectrum of compound 1 in pyridine- d_5	3
Figure S4. ^1H - ^1H COSY spectrum of compound 1 in pyridine- d_5	4
Figure S5. HMBC spectrum of compound 1 in pyridine- d_5	5
Figure S6. NOESY spectrum of compound 1 in pyridine- d_5	6
Figure S7. HRESIMS data of compound 1	7
Figure S8. IR spectrum of compound 1	7
Figure S9. ^{13}C NMR (150 MHz) spectrum of compound 1a in pyridine- d_5	8
Figure S10. ^1H NMR (600 MHz) spectrum of compound 1a in pyridine- d_5	9
Figure S11. HRESIMS data of compound 1a	10
Figure S12. IR spectrum of compound 1a	10
Figure S13. ^{13}C NMR (150 MHz) spectrum of compound 2 in pyridine- d_5	11
Figure S14. ^1H NMR (600 MHz) spectrum of compound 2 in pyridine- d_5	12
Figure S15. HSQC spectrum of compound 2 in pyridine- d_5	13
Figure S16. HMBC spectrum of compound 2 in pyridine- d_5	14
Figure S17. NOESY spectrum of compound 2 in pyridine- d_5	15
Figure S18. HRESIMS data of compound 2	16
Figure S19. IR spectrum of compound 2	16
Figure S20. UV spectrum of compound 2	17
Figure S21. ^{13}C NMR (100 MHz) spectrum of compound 3 in pyridine- d_5	18
Figure S22. ^1H NMR (400 MHz) spectrum of compound 3 in pyridine- d_5	19
Figure S23. HSQC spectrum of compound 3 in pyridine- d_5	20
Figure S24. ^1H - ^1H COSY spectrum of compound 3 in pyridine- d_5	21
Figure S25. HMBC spectrum of compound 3 in pyridine- d_5	22
Figure S26. NOESY spectrum of compound 3 in pyridine- d_5	23
Figure S27. HRESIMS data of compound 3	24
Figure S28. IR spectrum of compound 3	24
Figure S29. ^{13}C NMR (150 MHz) spectrum of compound 4 in pyridine- d_5	25
Figure S30. ^1H NMR (600 MHz) spectrum of compound 4 in pyridine- d_5	26
Figure S31. HSQC spectrum of compound 4 in pyridine- d_5	27
Figure S32. ^1H - ^1H COSY spectrum of compound 4 in pyridine- d_5	28
Figure S33. HMBC spectrum of compound 4 in pyridine- d_5	29
Figure S34. NOESY spectrum of compound 4 in pyridine- d_5	30
Figure S35. HRESIMS data of compound 4	31
Figure S36. IR spectrum of compound 4	31
Figure S37. UV spectrum of compound 4	32

Figure S1. ^{13}C NMR (150 MHz) spectrum of compound **1** in pyridine- d_5

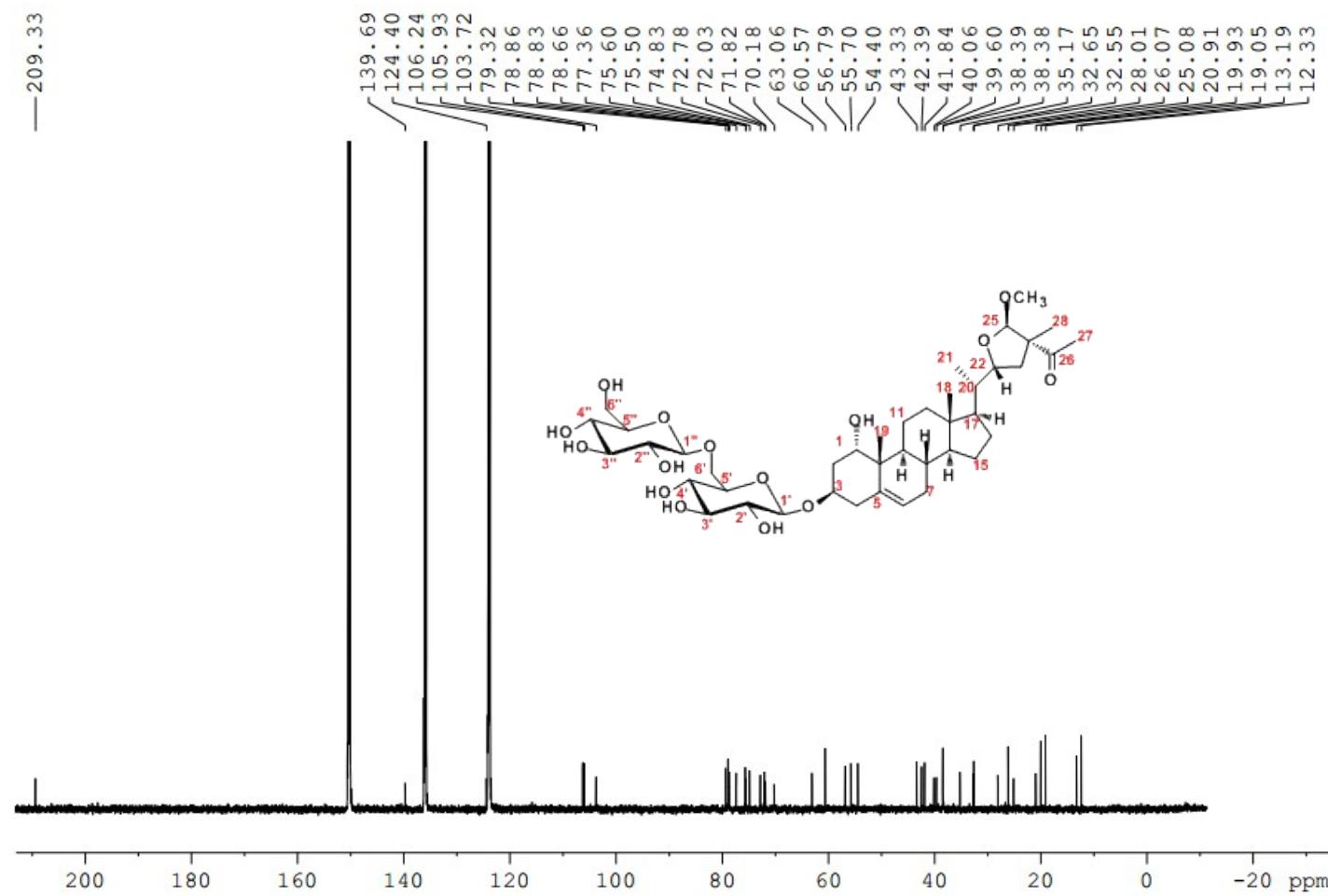


Figure S2. ^1H NMR (600 MHz) spectrum of compound **1** in pyridine- d_5

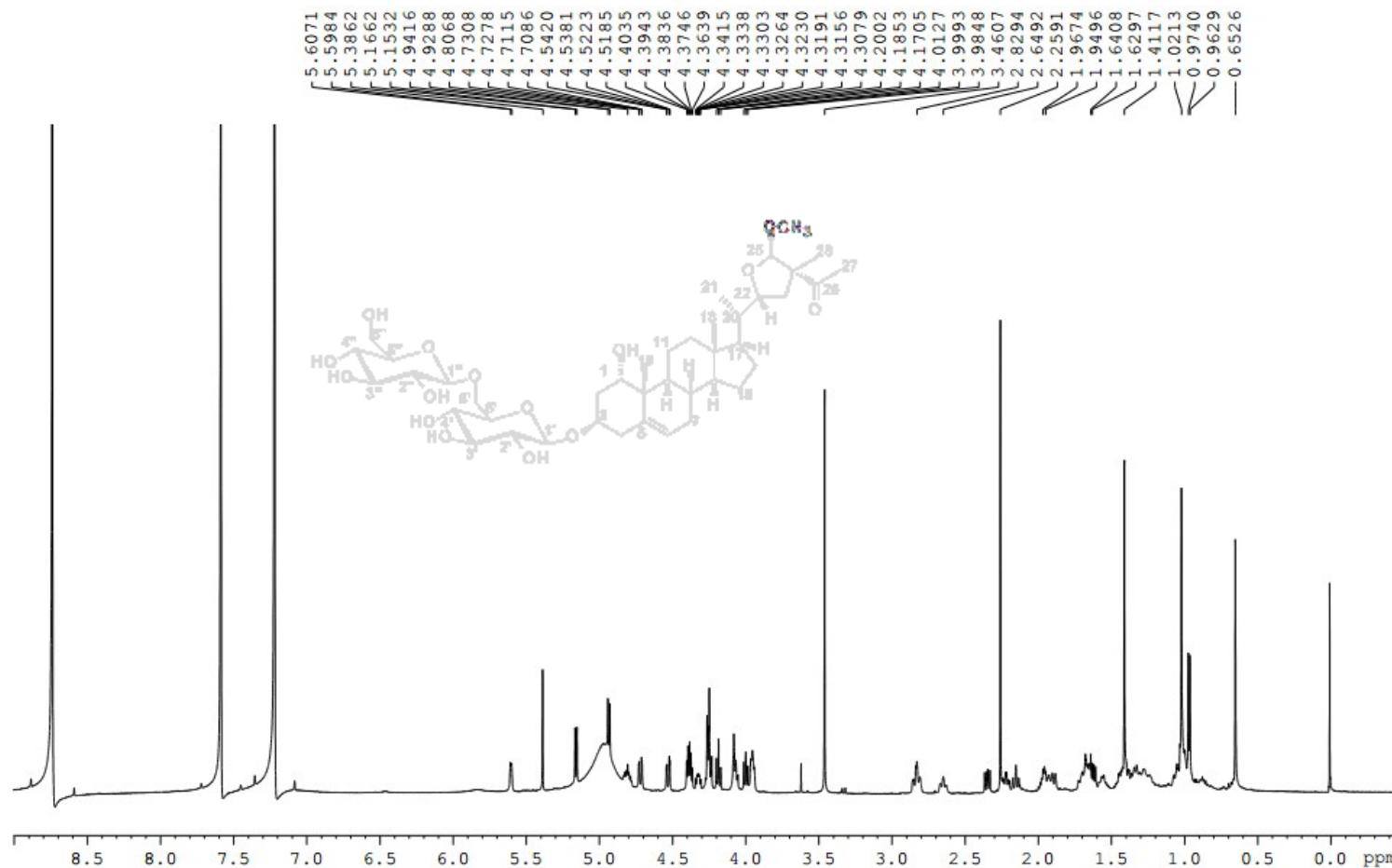


Figure S3. HSQC spectrum of compound **1** in pyridine-*d*₅

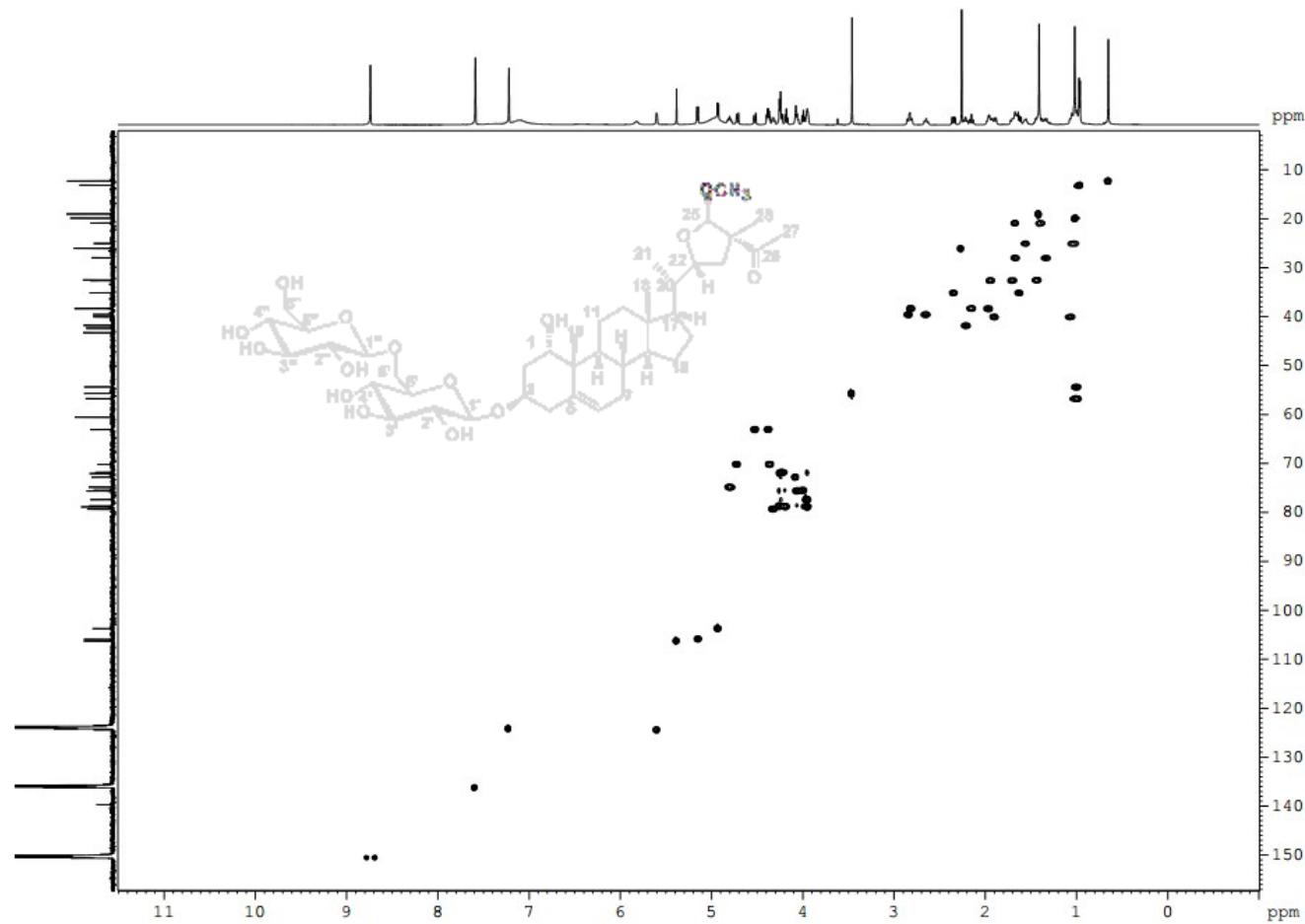


Figure S4. ^1H - ^1H COSY spectrum of compound **1** in pyridine- d_5

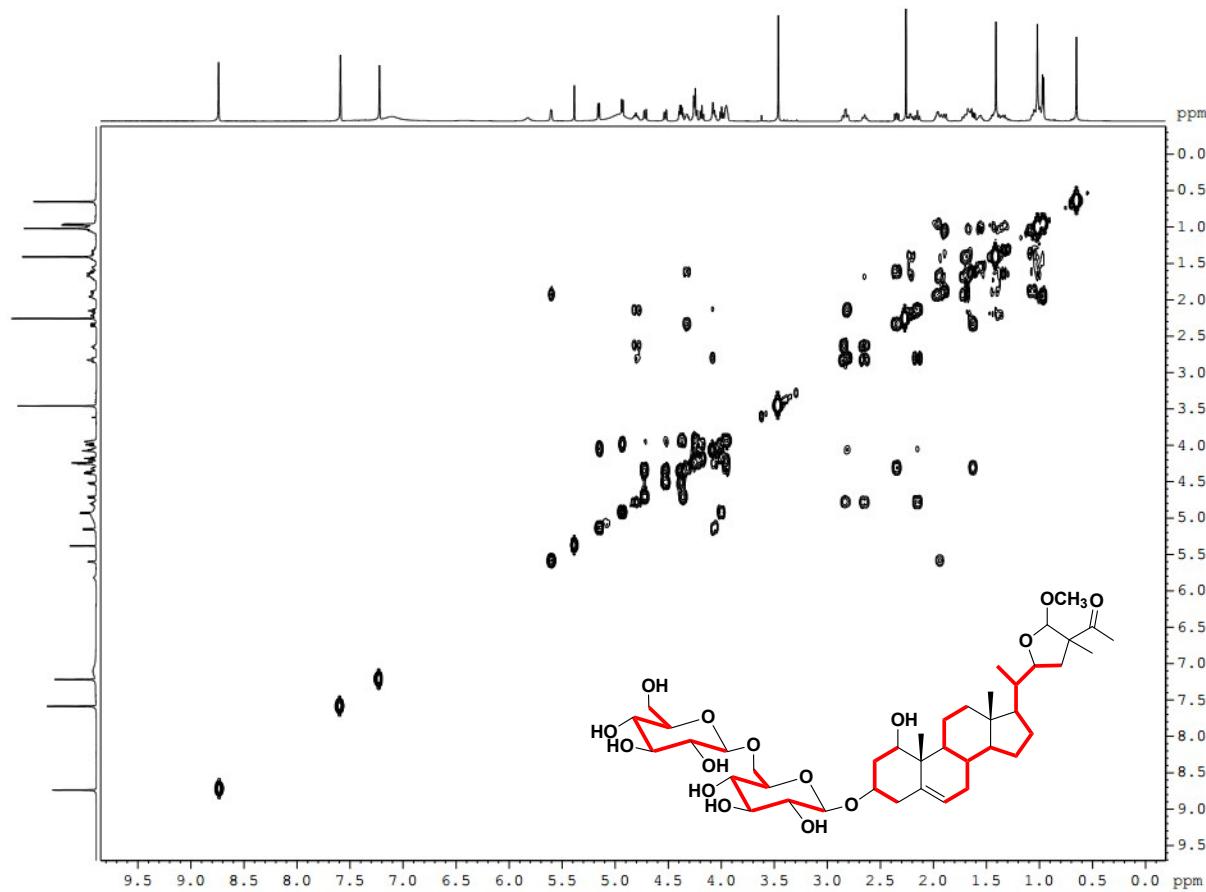


Figure S5. HMBC spectrum of compound **1** in pyridine-*d*₅

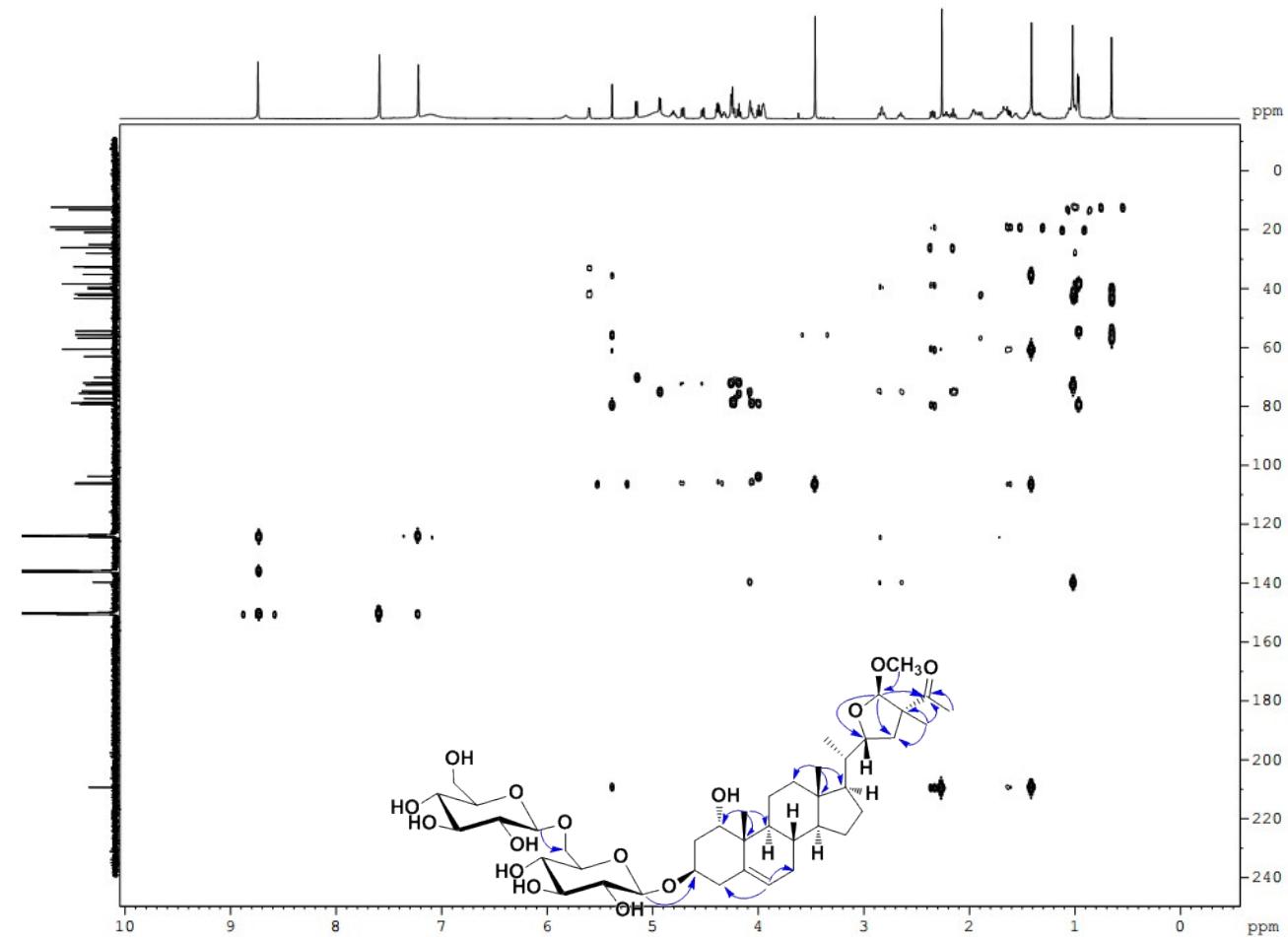


Figure S6. NOESY spectrum of compound **1** in pyridine-*d*₅

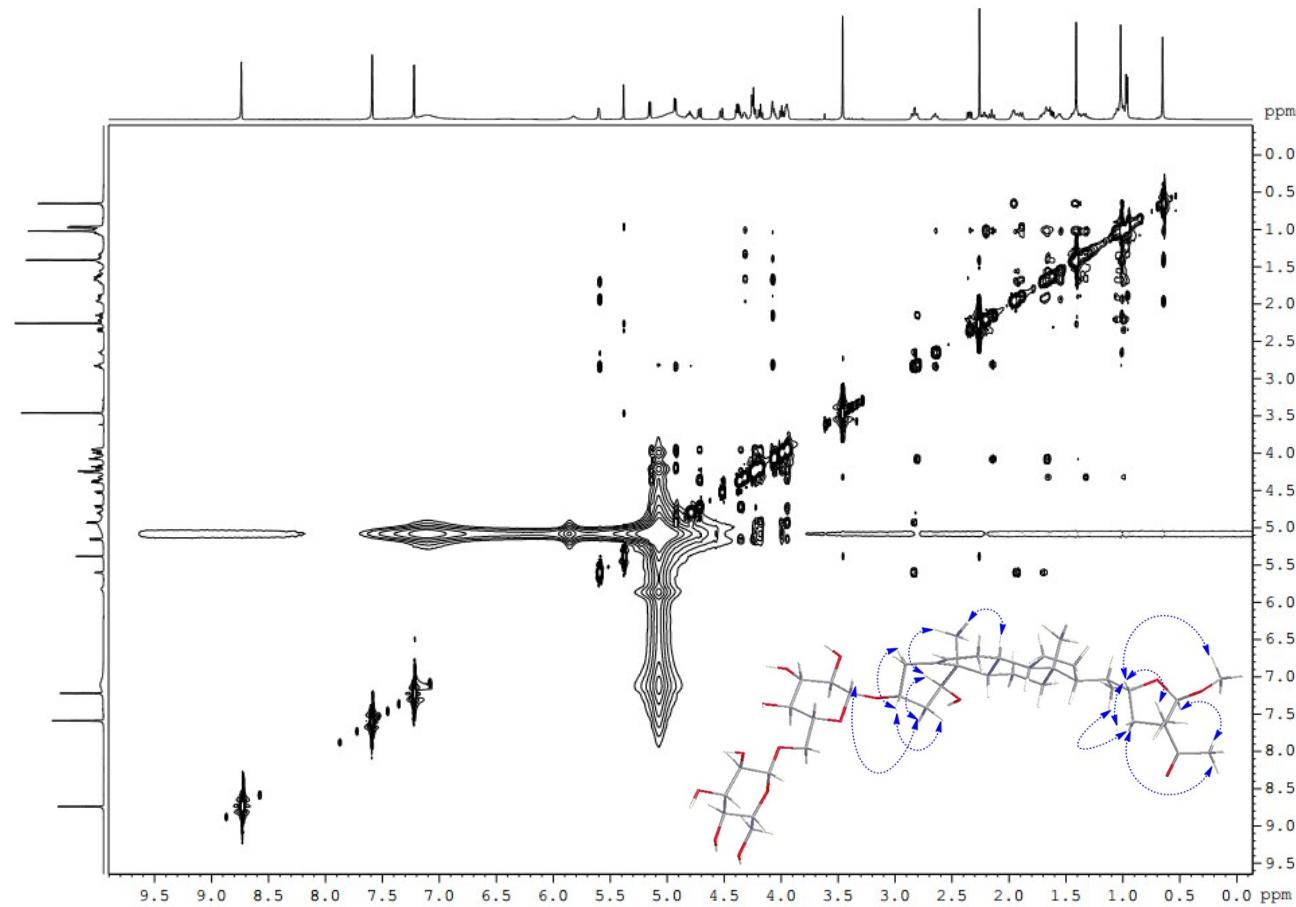


Figure S7. HRESIMS data of compound 1

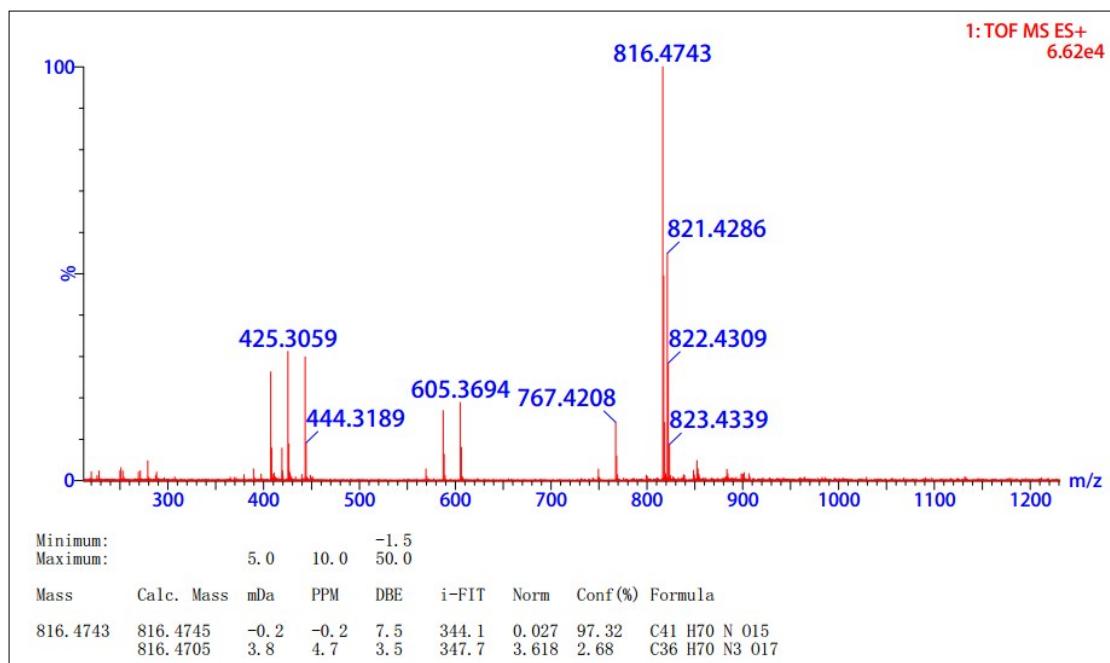


Figure S8. IR spectrum of compound 1

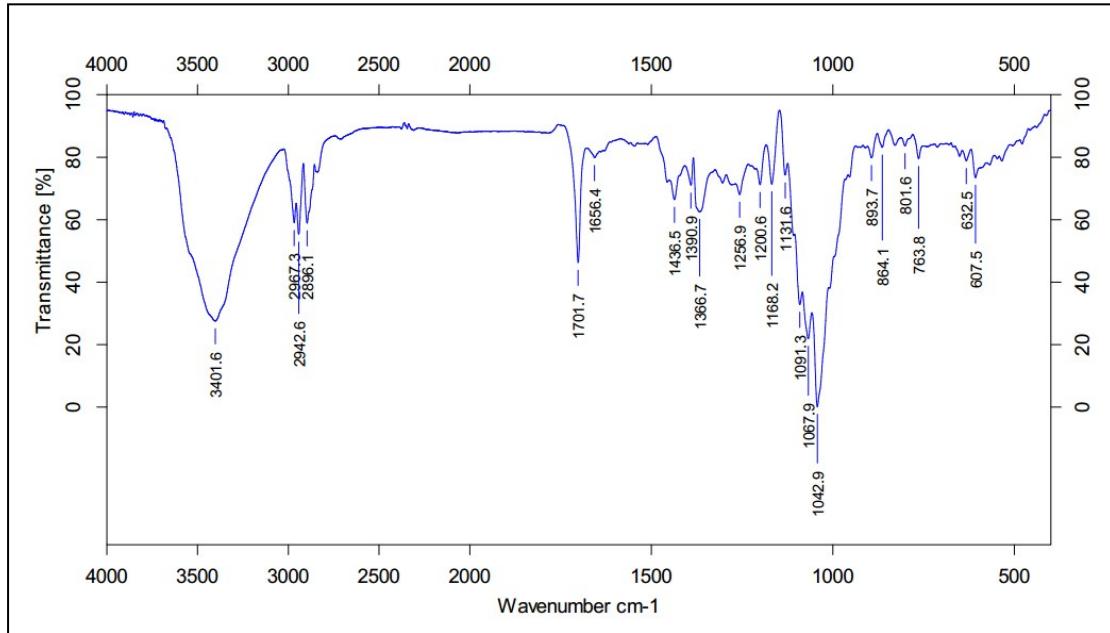


Figure S9. ^{13}C NMR (150 MHz) spectrum of compound **1a** in pyridine- d_5

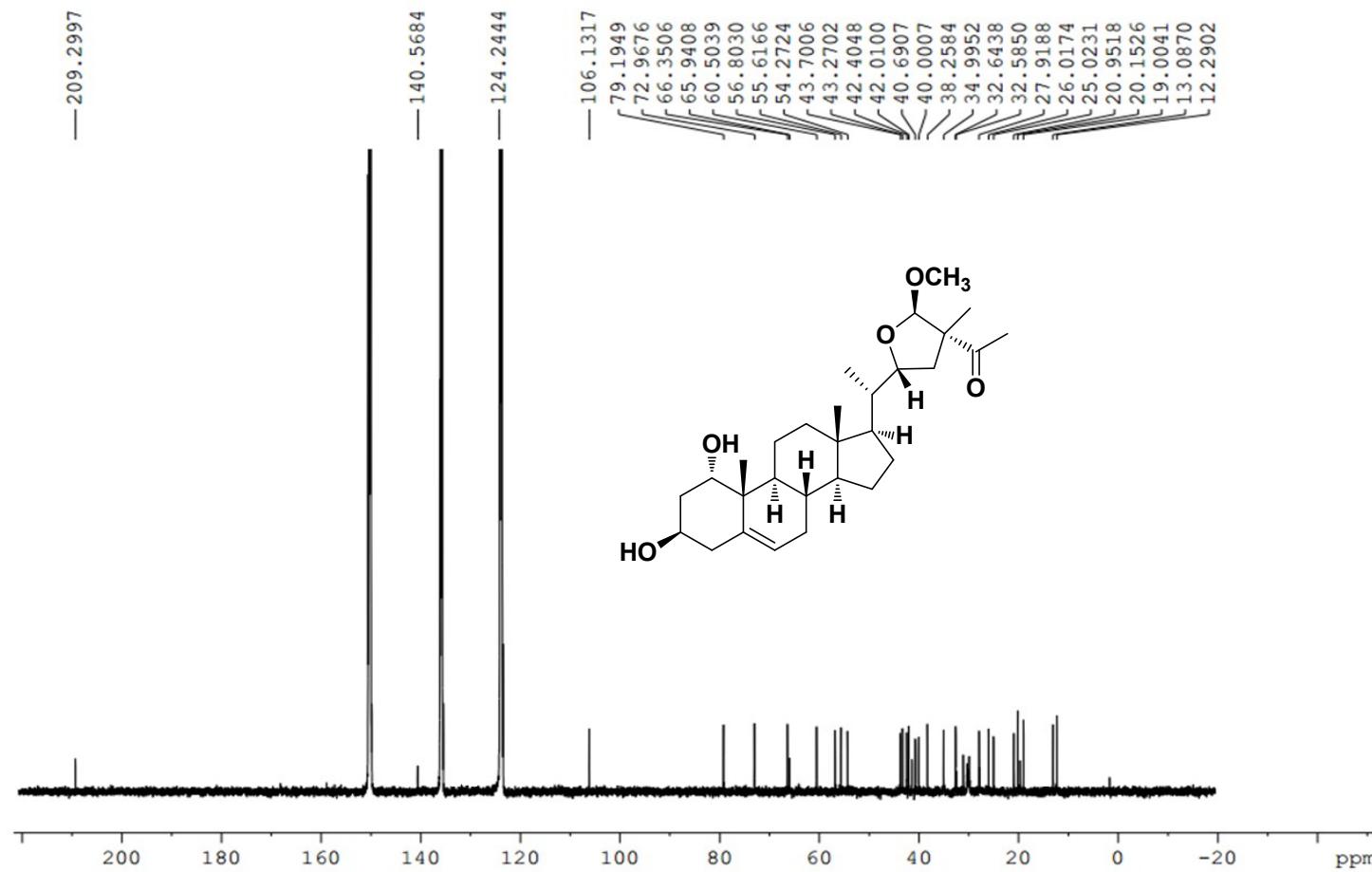


Figure S10. ^1H NMR (600 MHz) spectrum of compound **1a** in pyridine- d_5

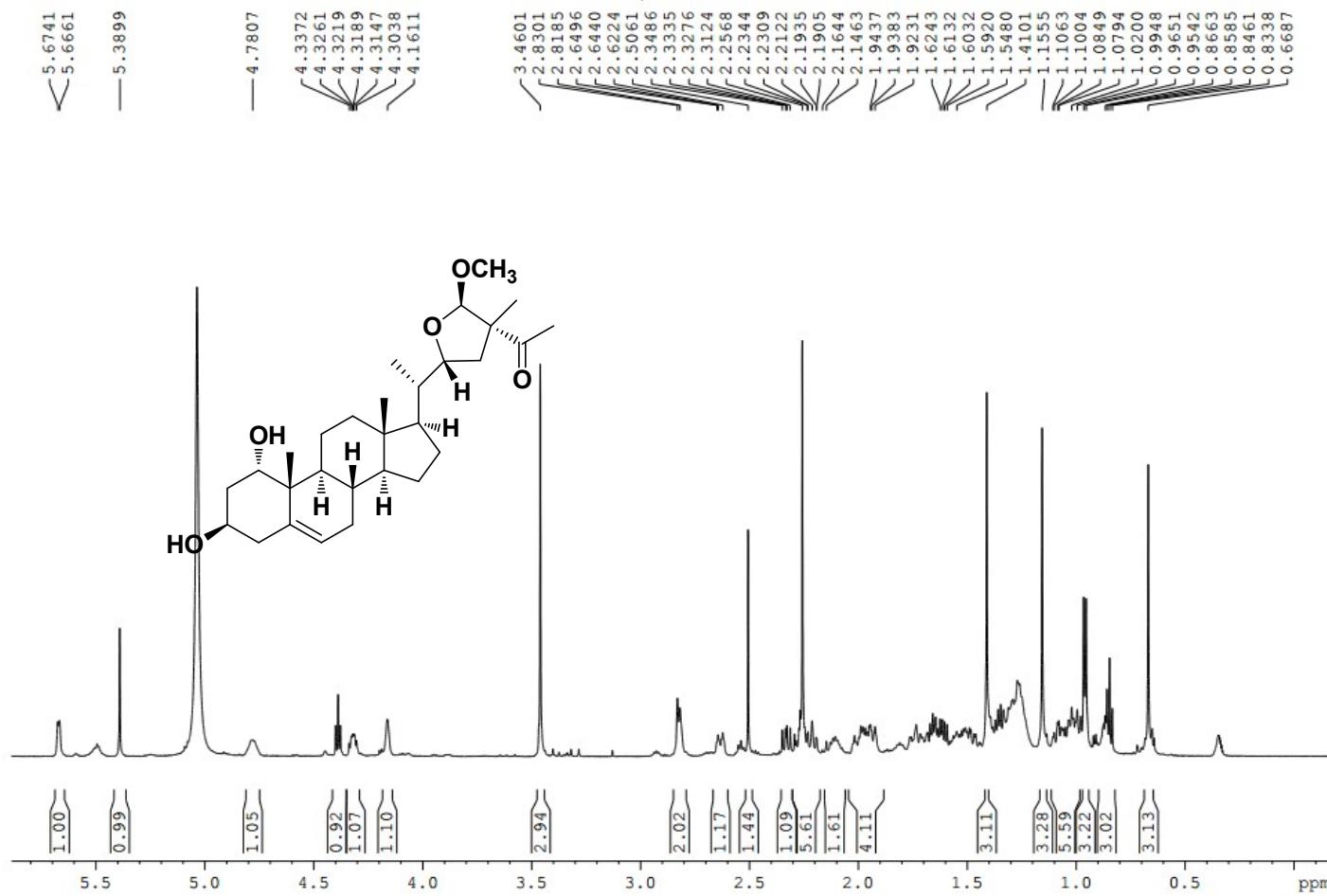


Figure S11. HRESIMS data of compound **1a**

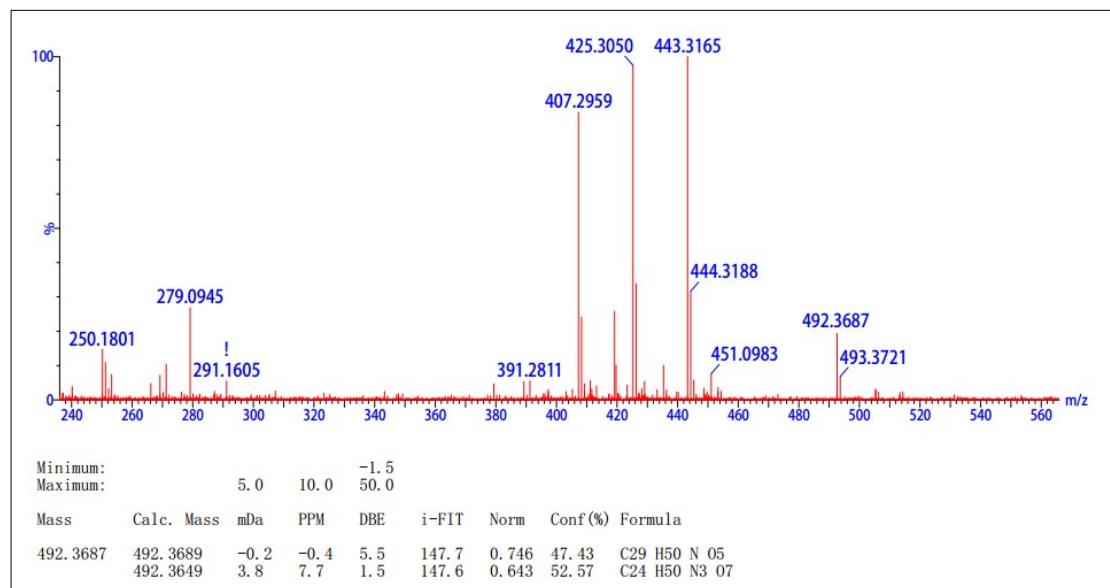


Figure S12. IR spectrum of compound **1a**

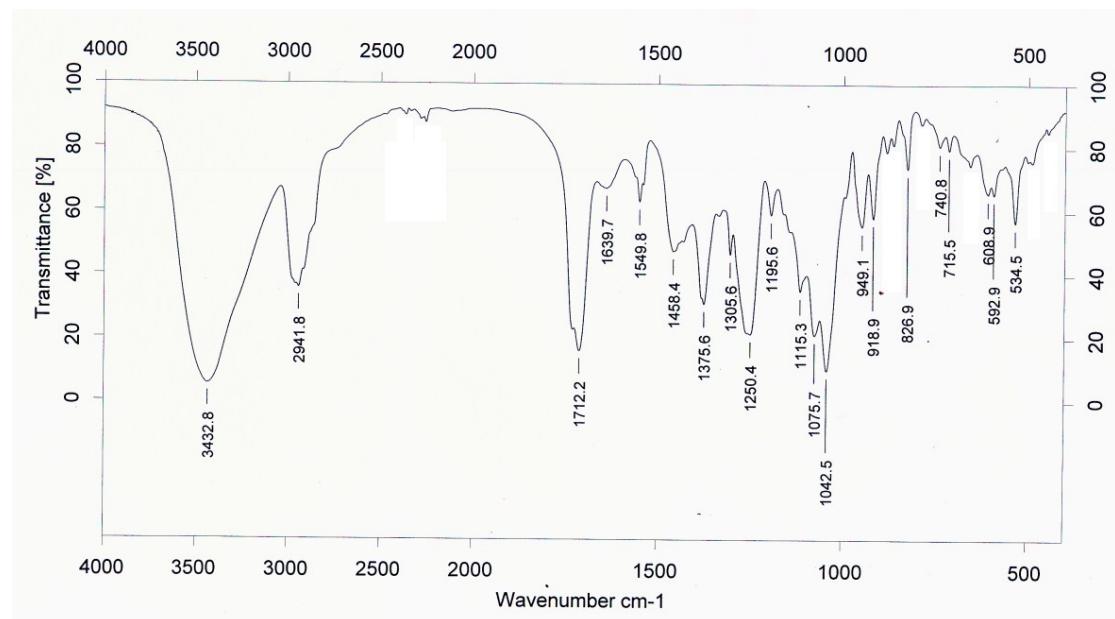


Figure S13. ^{13}C NMR (150 MHz) spectrum of compound **2** in pyridine- d_5 .

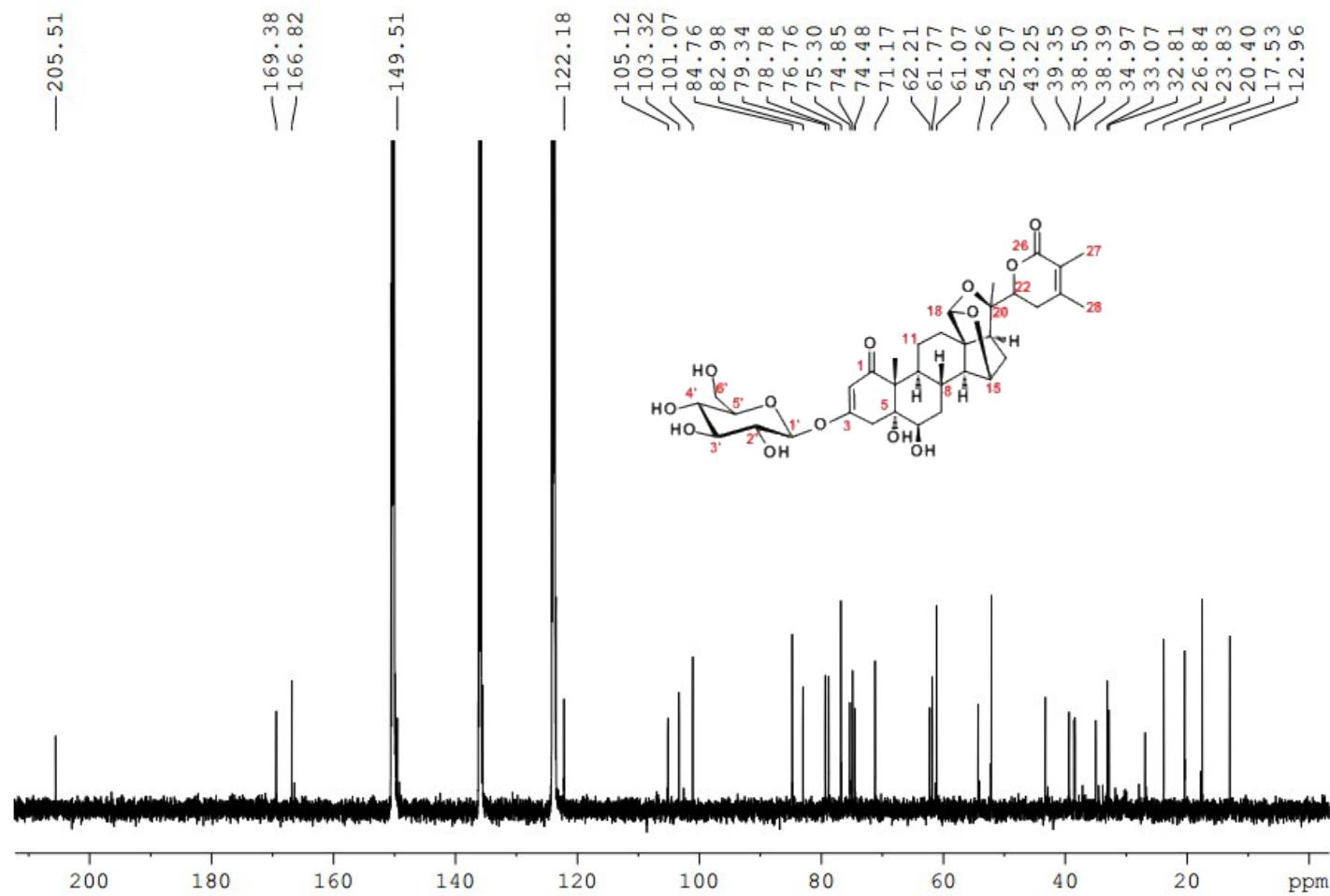


Figure S14. ^1H NMR (600 MHz) spectrum of compound **2** in pyridine- d_5 .

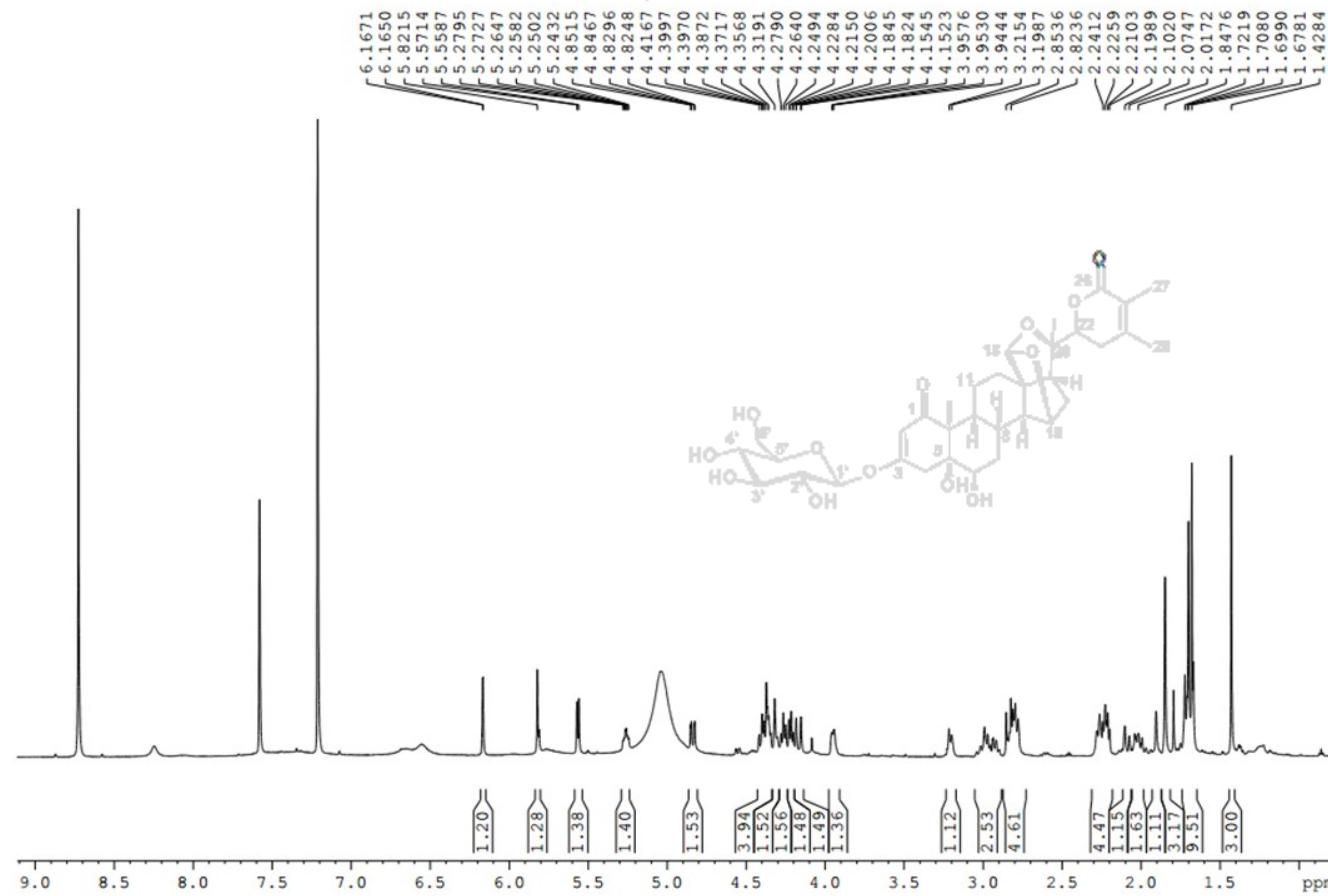


Figure S15. HSQC spectrum of compound **2** in pyridine-*d*₅

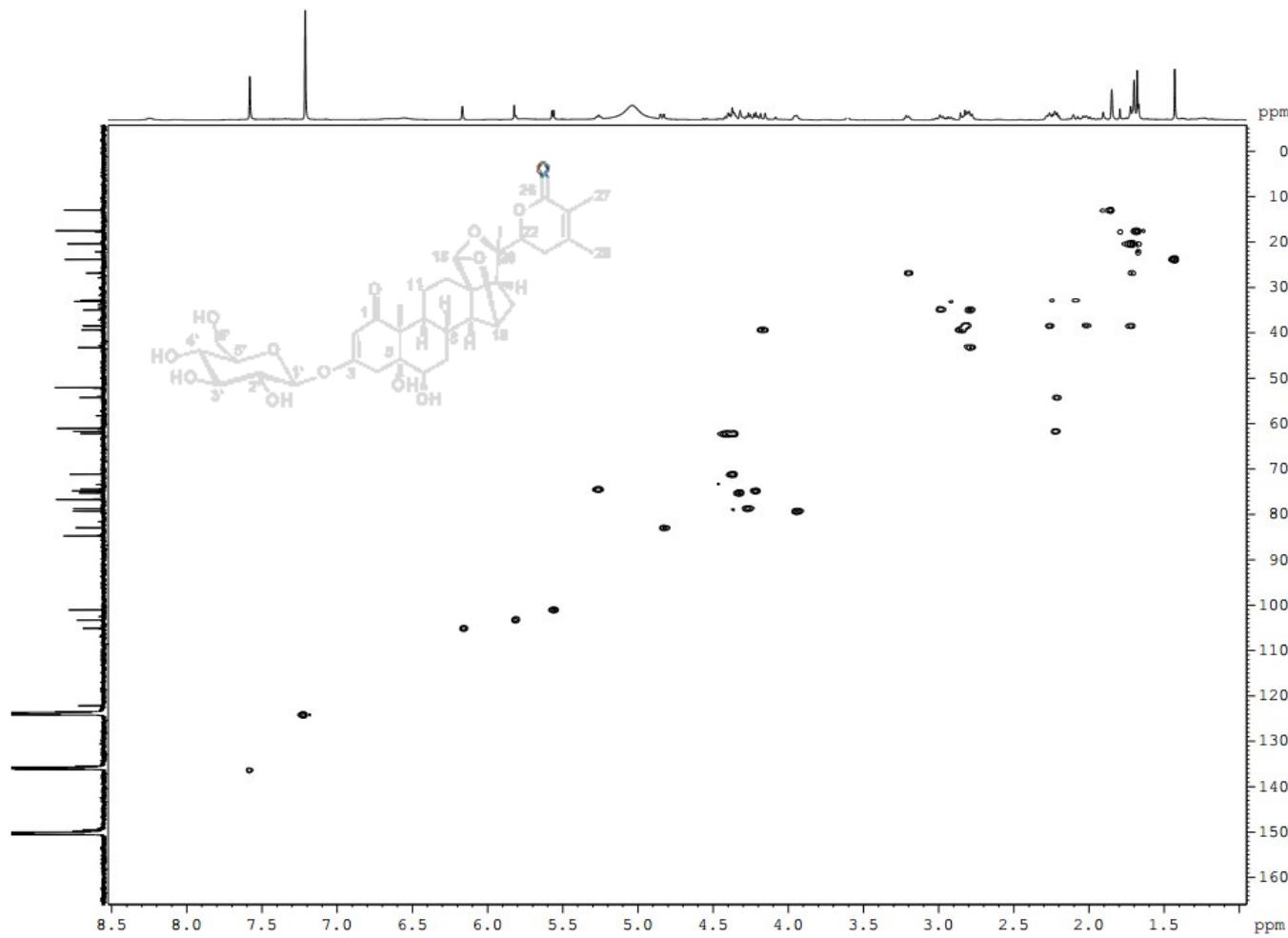


Figure S16. HMBC spectrum of compound **2** in pyridine-*d*₅.

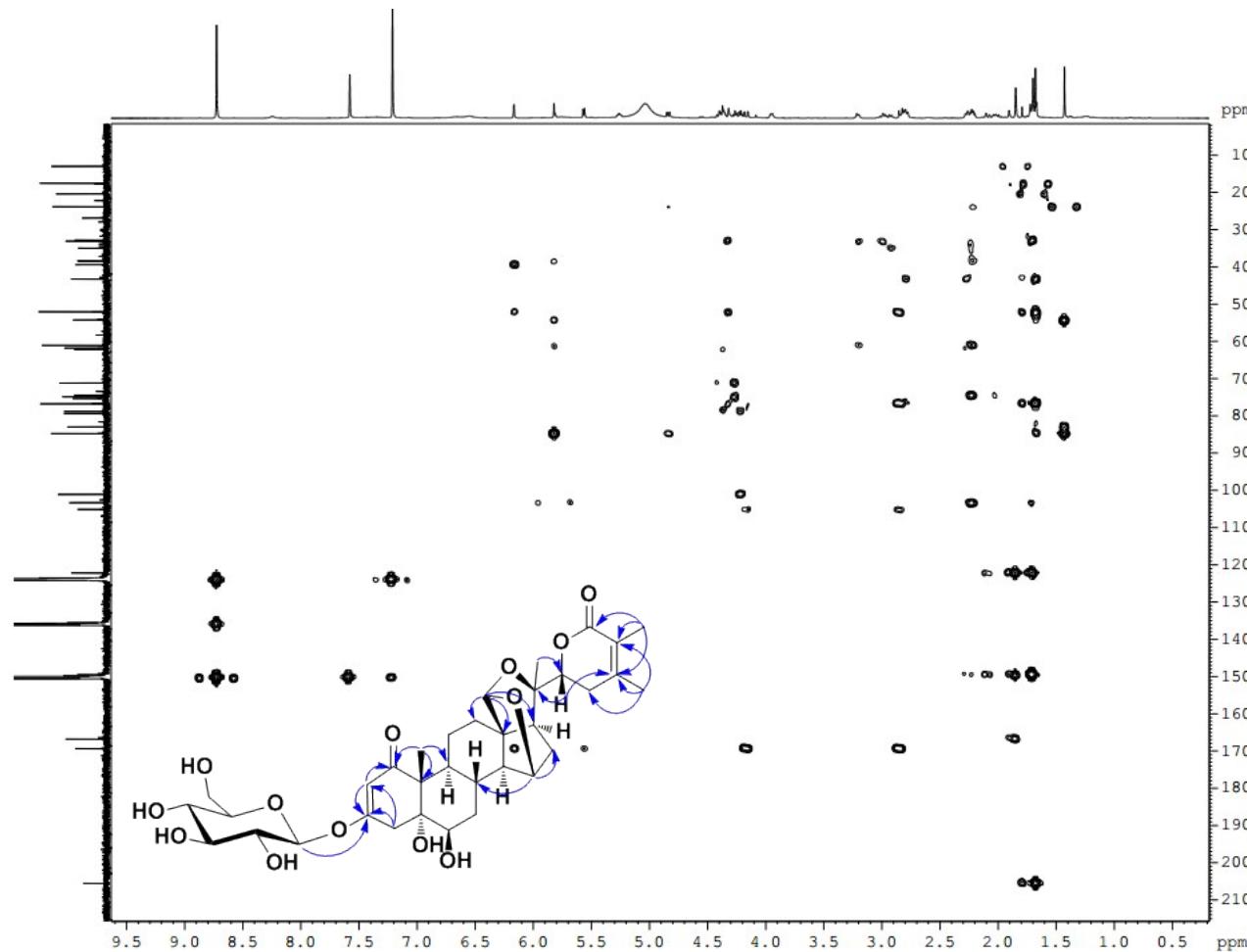


Figure S17. NOESY spectrum of compound **2** in pyridine-*d*₅.

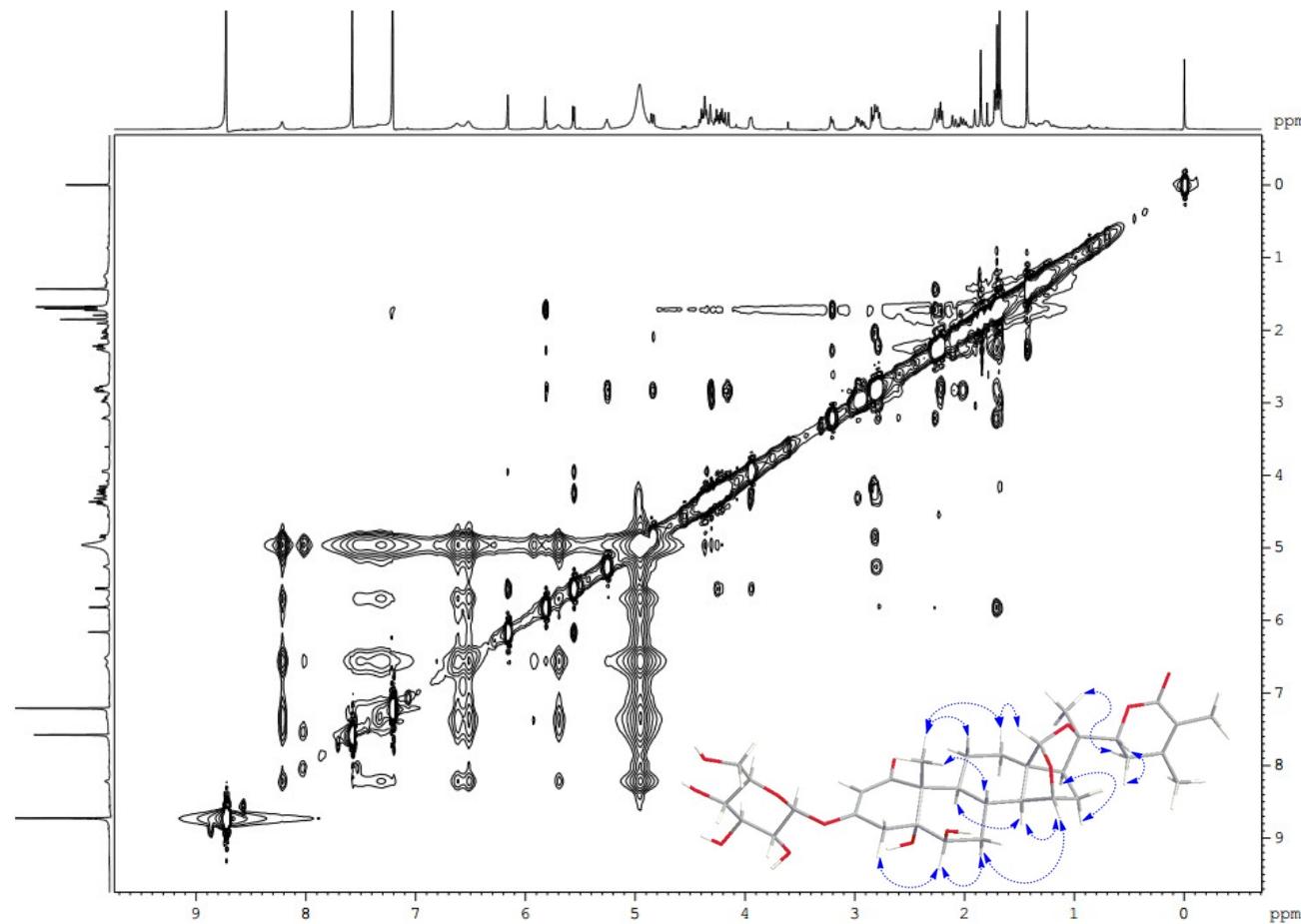


Figure S18. HRESIMS data of compound 2.

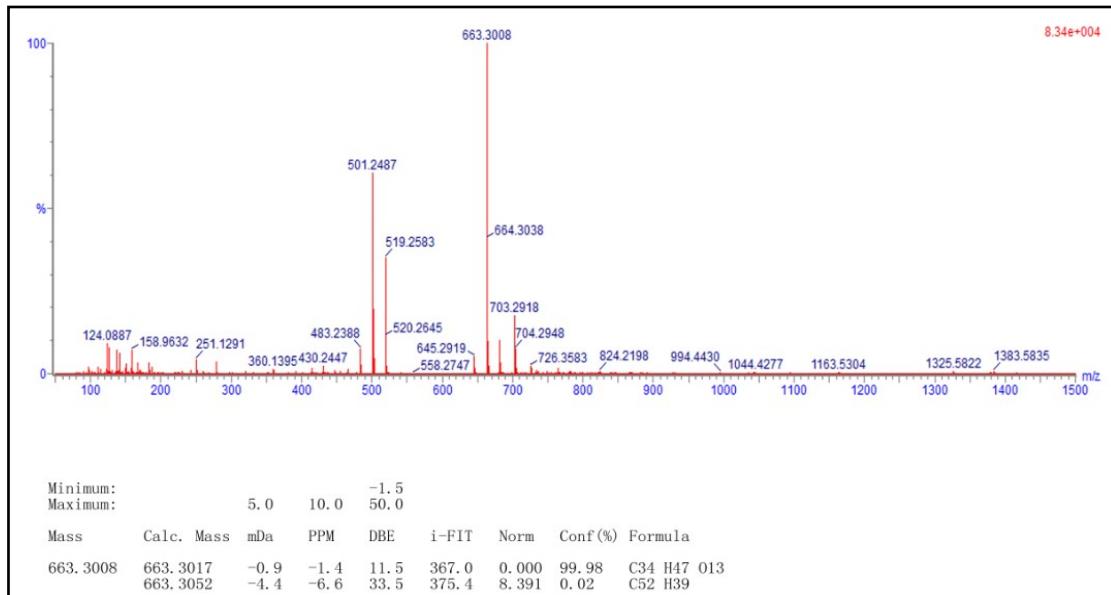


Figure S19. IR spectrum of compound 2.

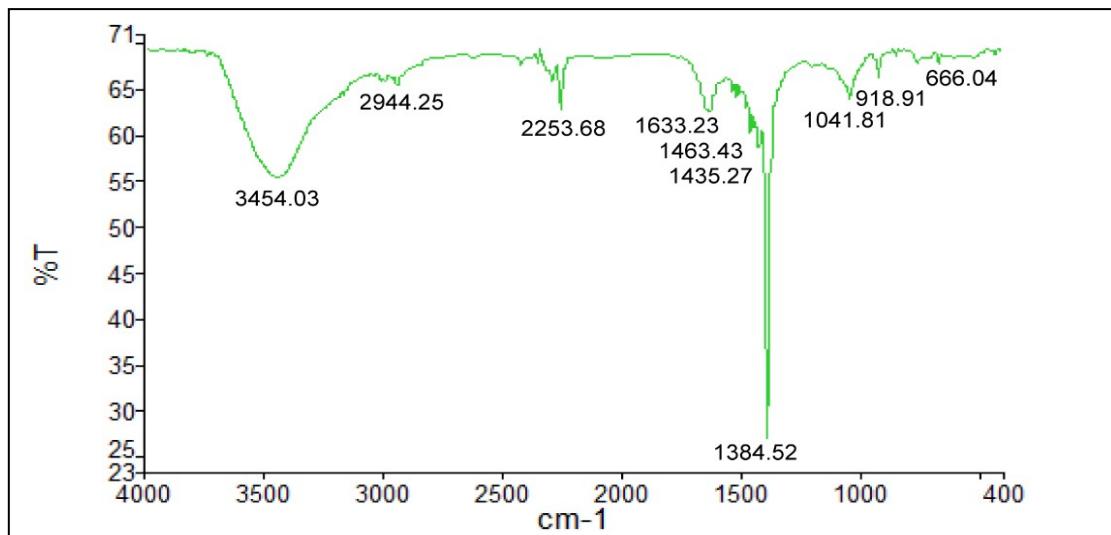


Figure S20. UV spectrum of compound 2.

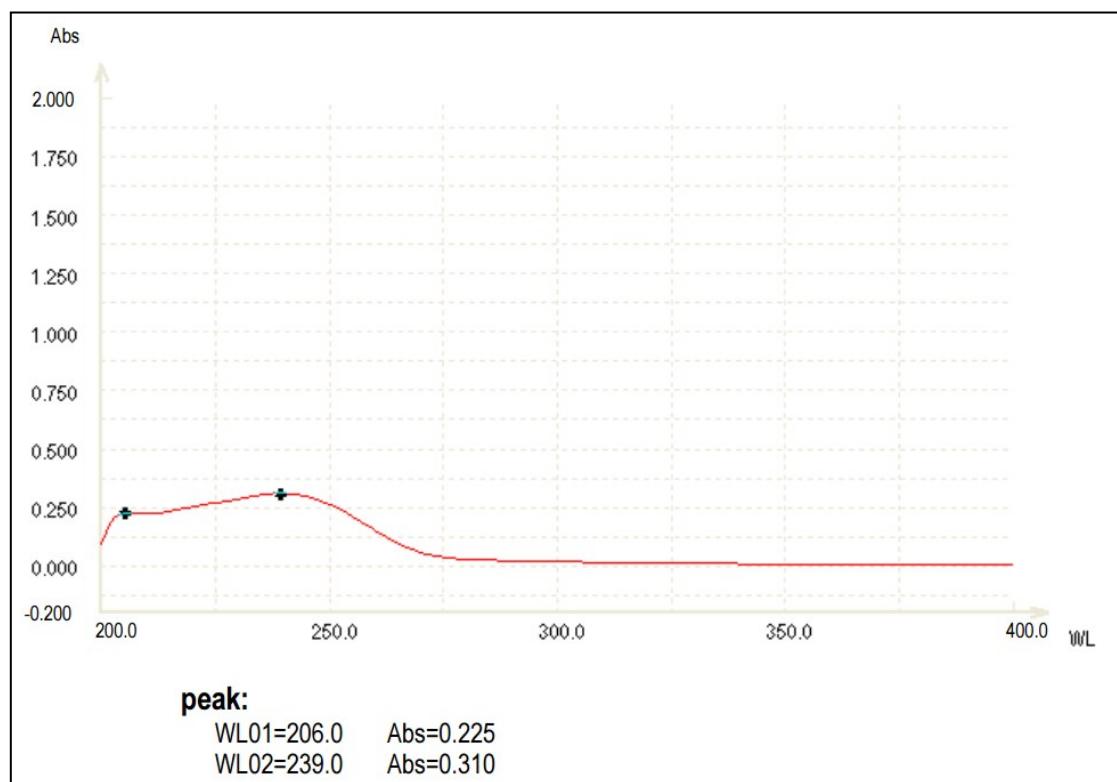


Figure S21. ^{13}C NMR (100 MHz) spectrum of compound **3** in pyridine- d_5

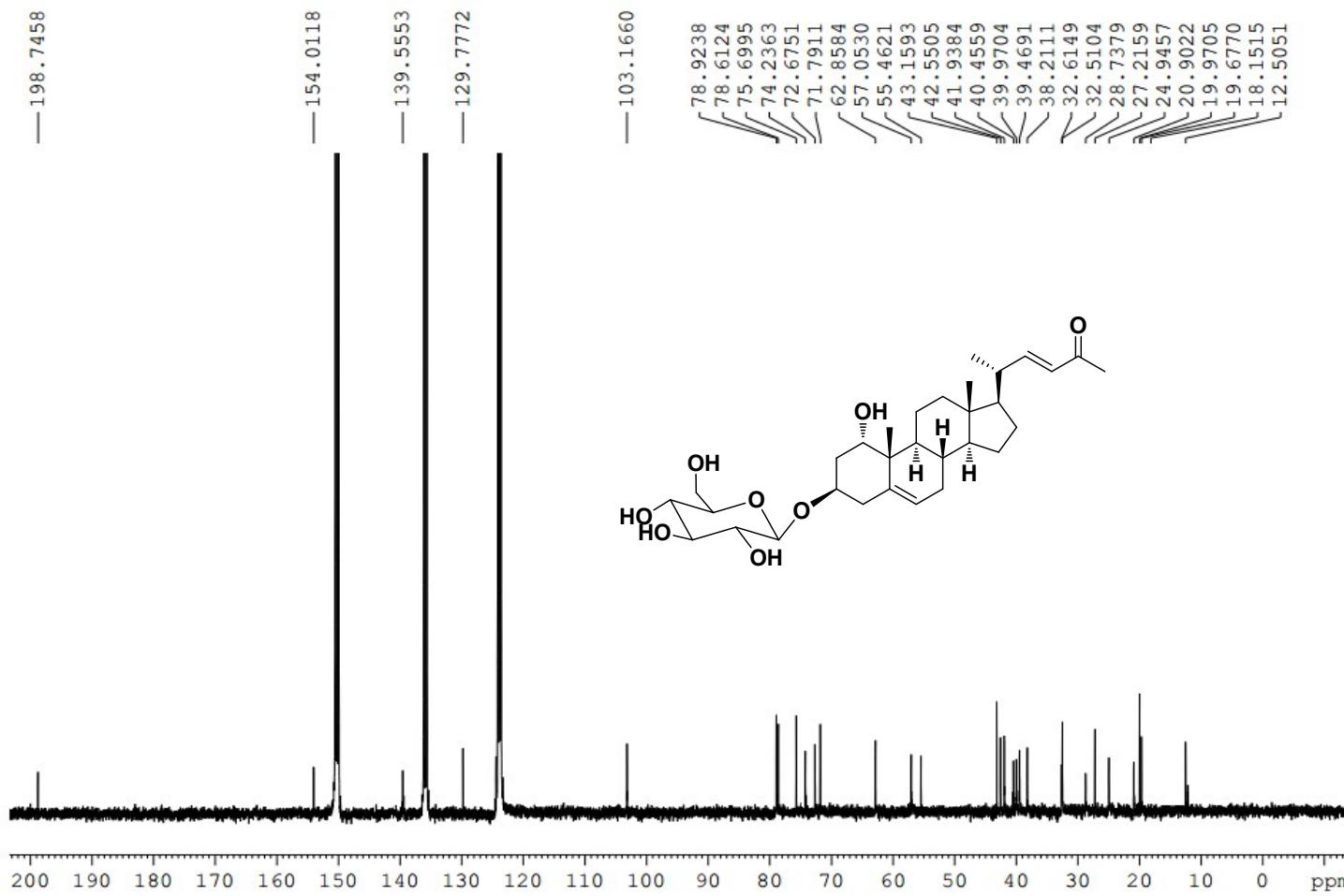


Figure S22. ^1H NMR (400 MHz) spectrum of compound **3** in pyridine- d_5

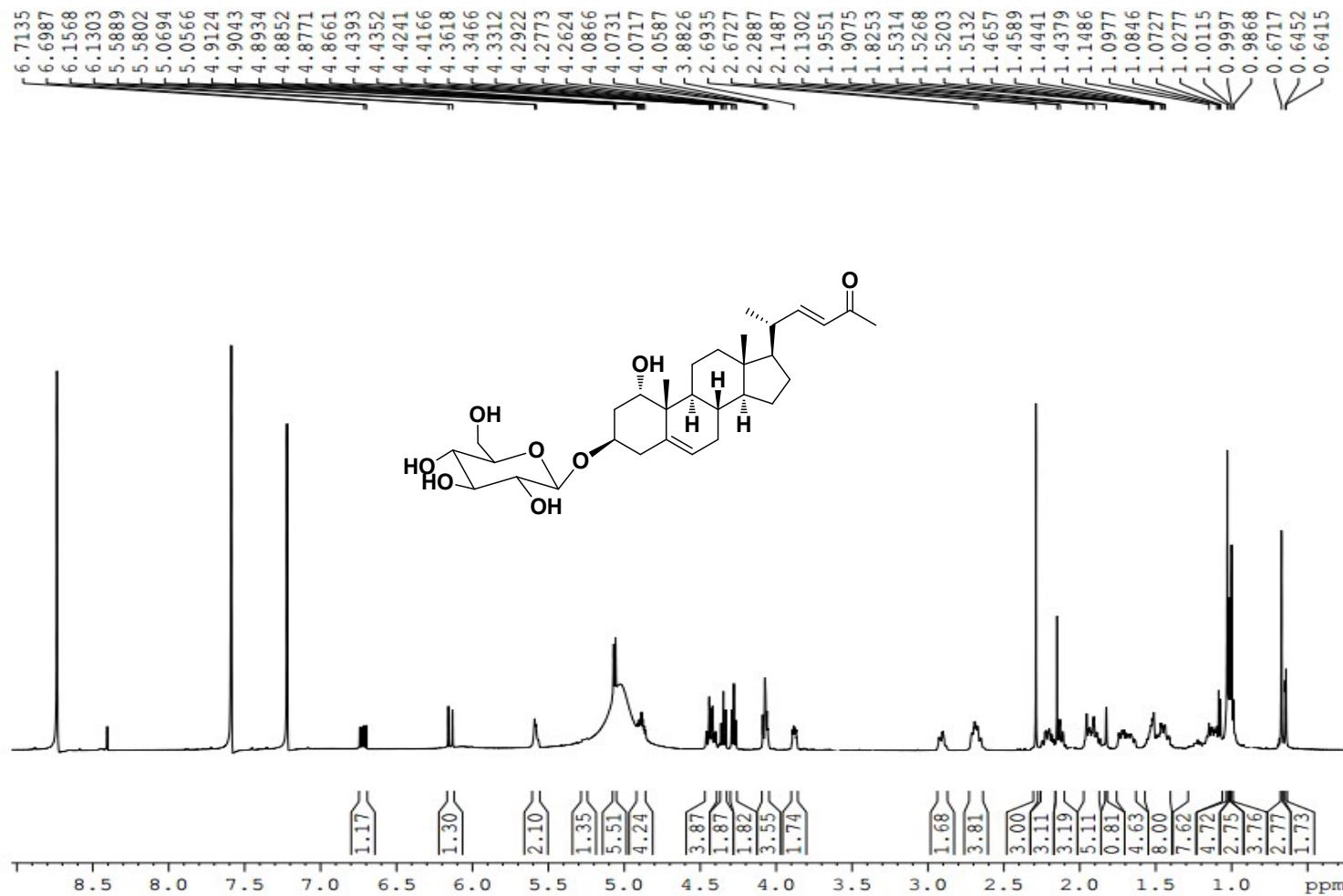


Figure S23. HSQC spectrum of compound **3** in pyridine-*d*₅

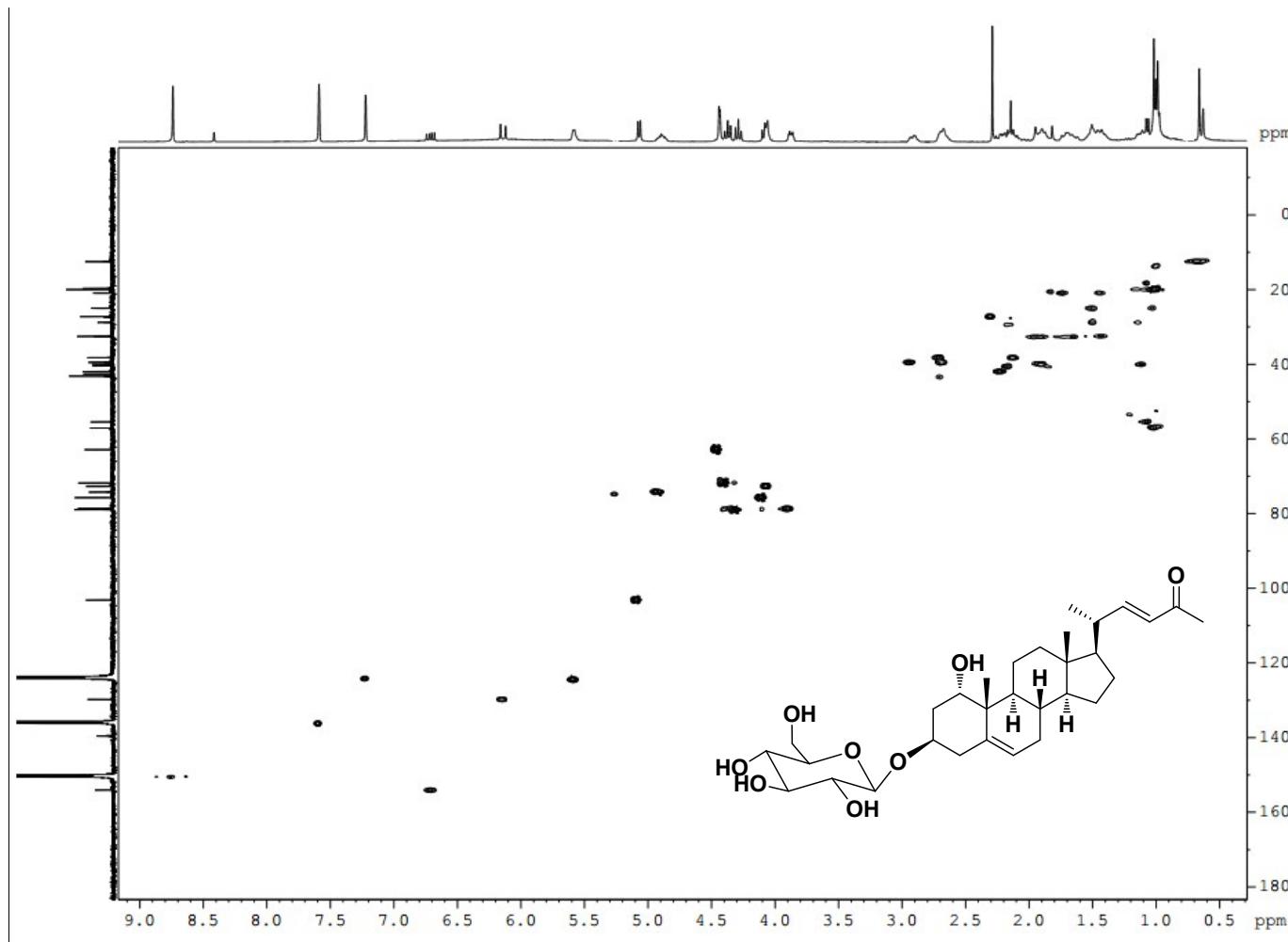


Figure S24. ^1H - ^1H COSY spectrum of compound **3** in pyridine-*d*₅.

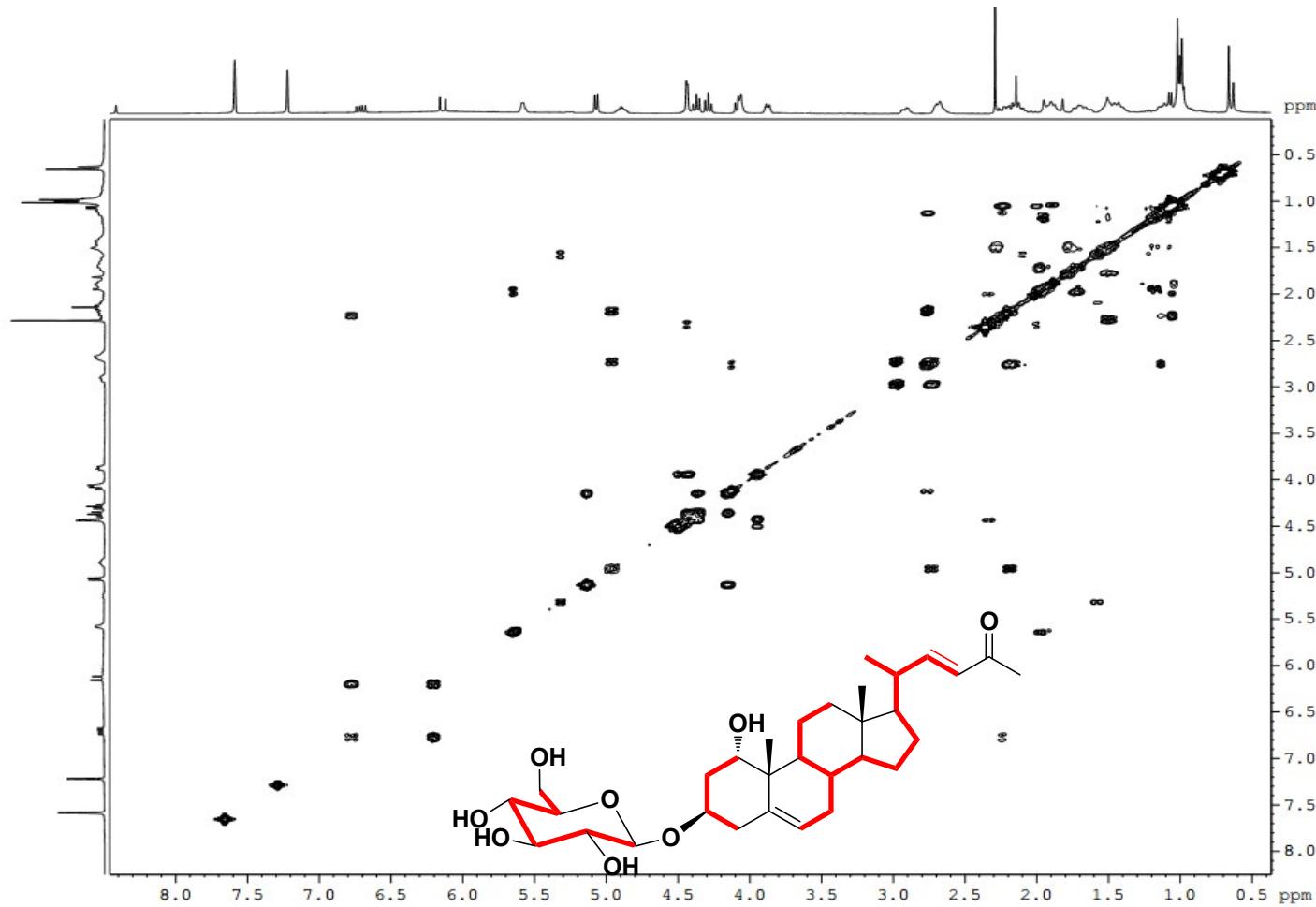


Figure S25. HMBC spectrum of compound **3** in pyridine-*d*₅.

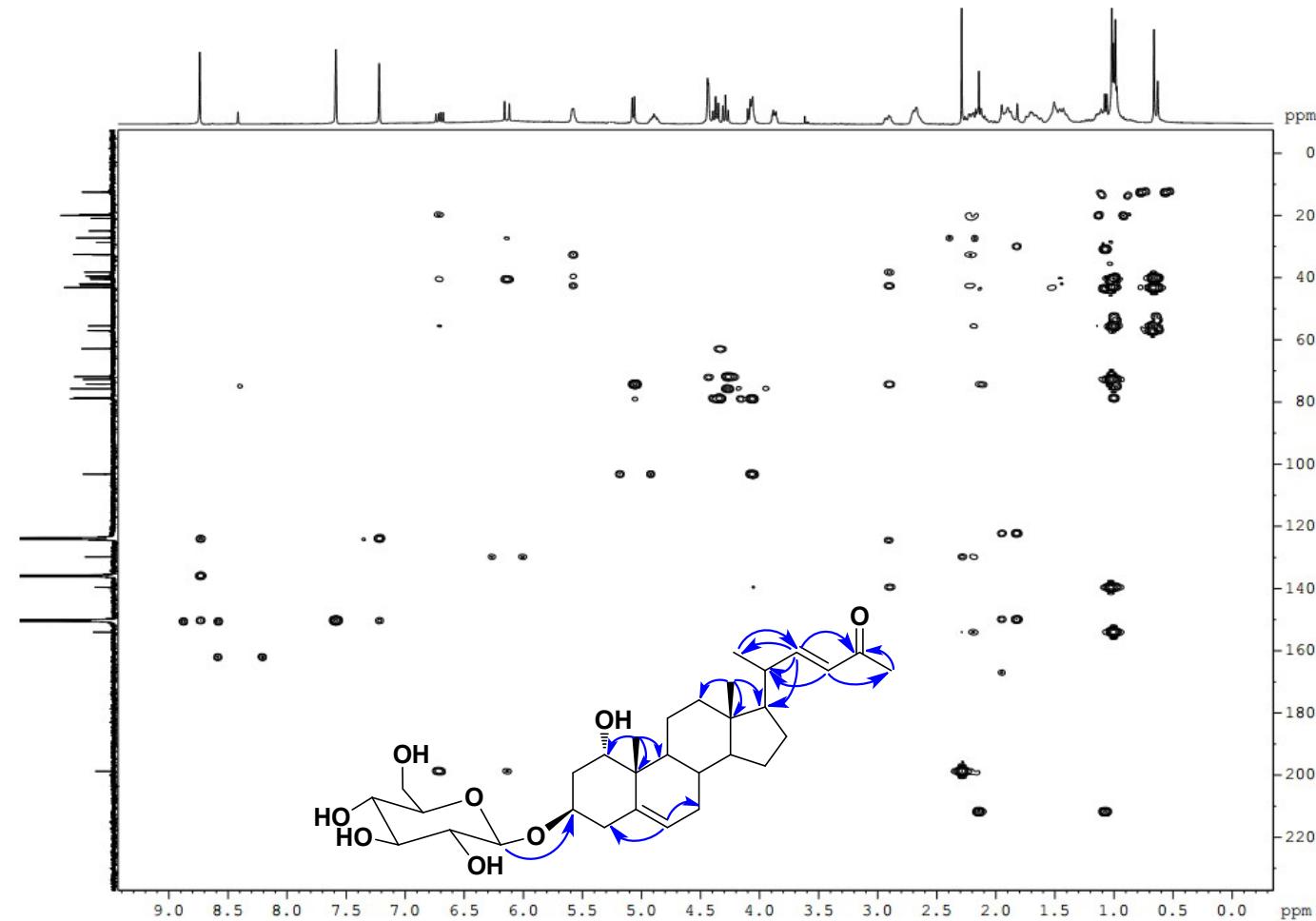


Figure S26. NOESY spectrum of compound **3** in pyridine-*d*₅.

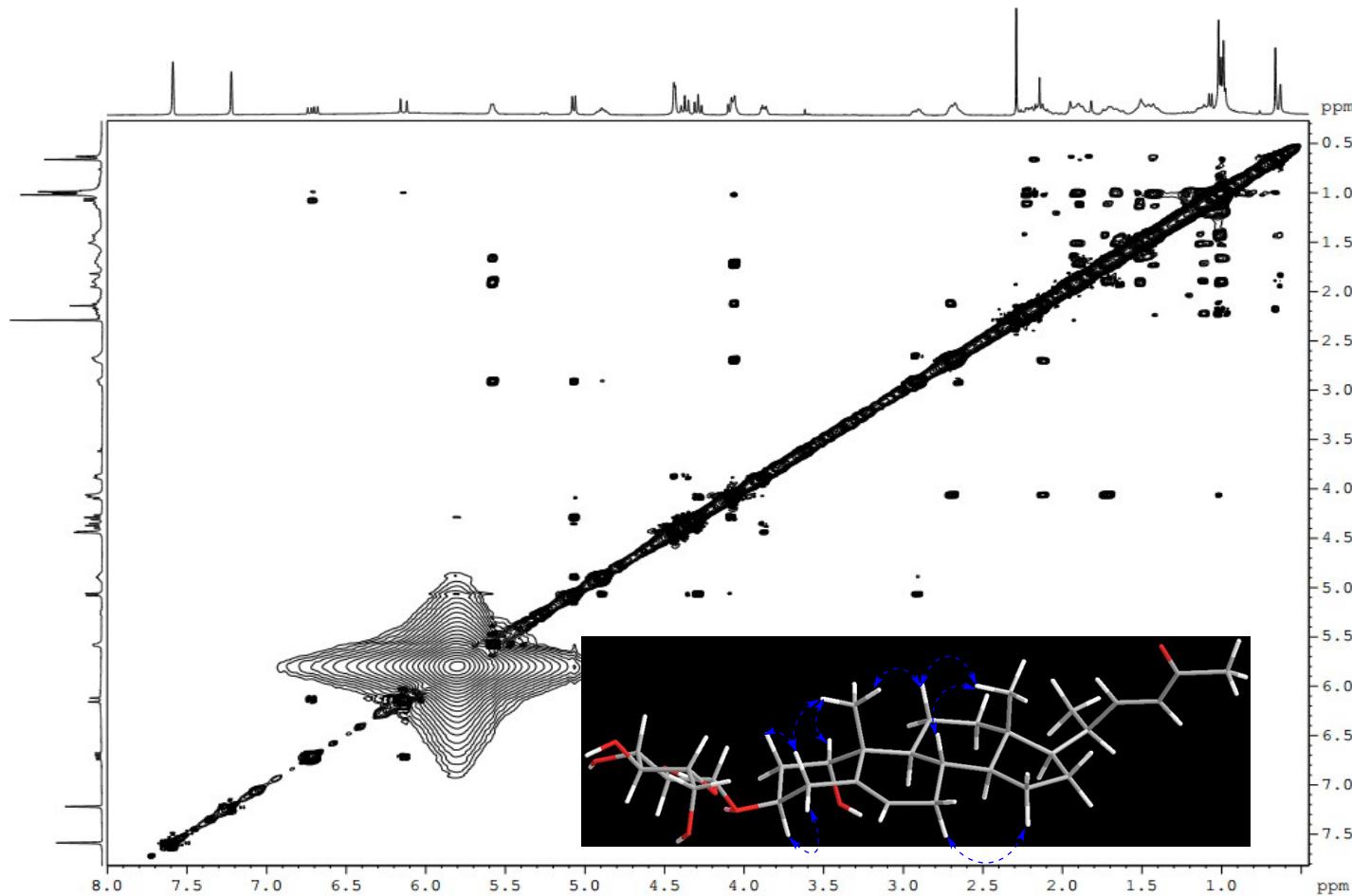


Figure S27. HRESIMS data of compound 3.

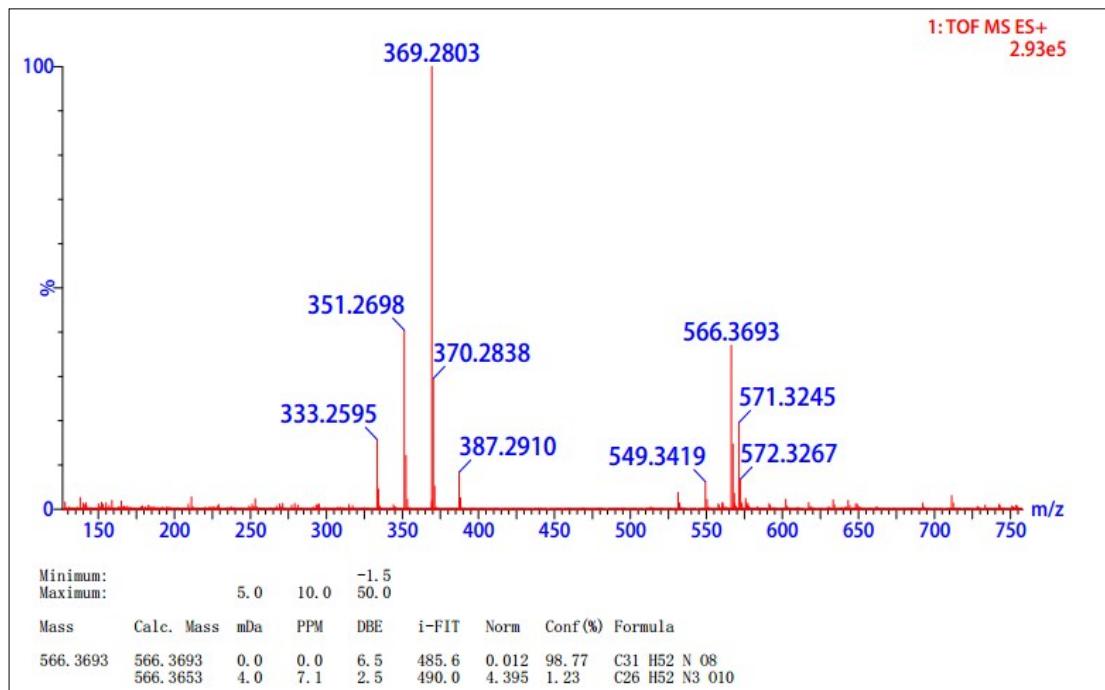


Figure S28. IR spectrum of compound 3.

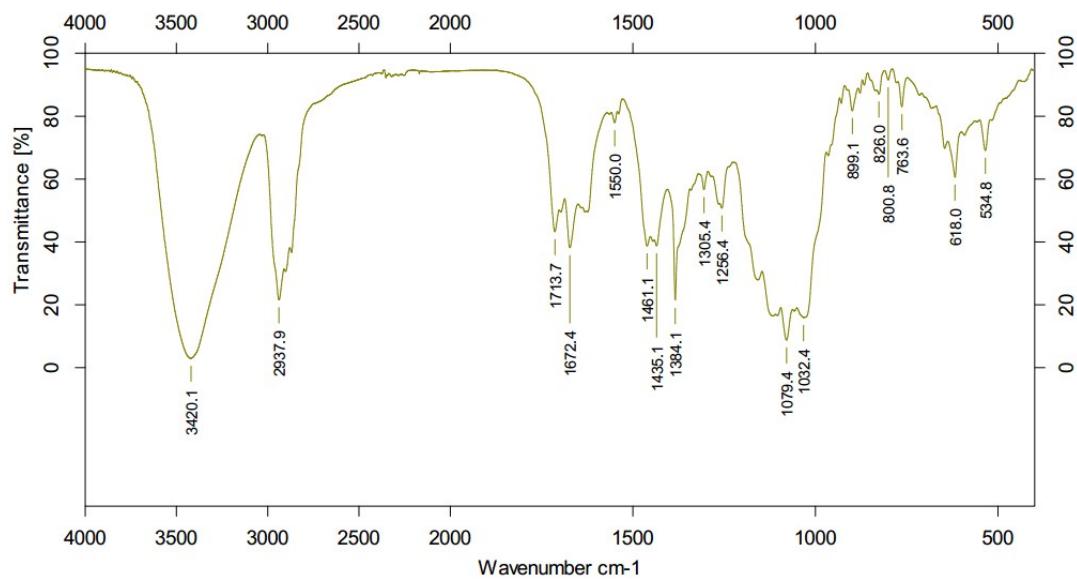


Figure S29. ^{13}C NMR (150 MHz) spectrum of compound **4** in pyridine- d_5 .

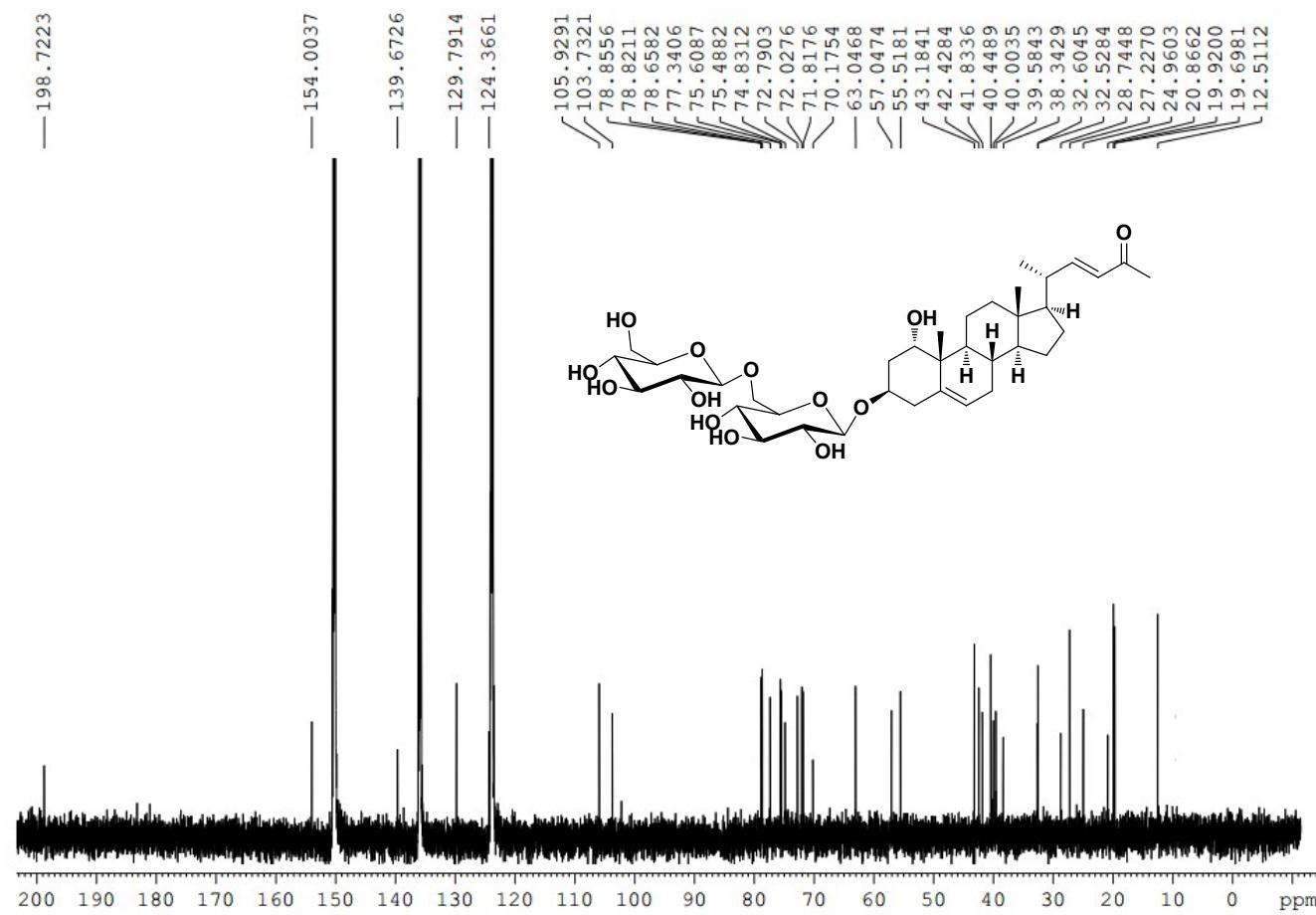


Figure S30. ^1H NMR (600 MHz) spectrum of compound **4** in pyridine- d_5 .

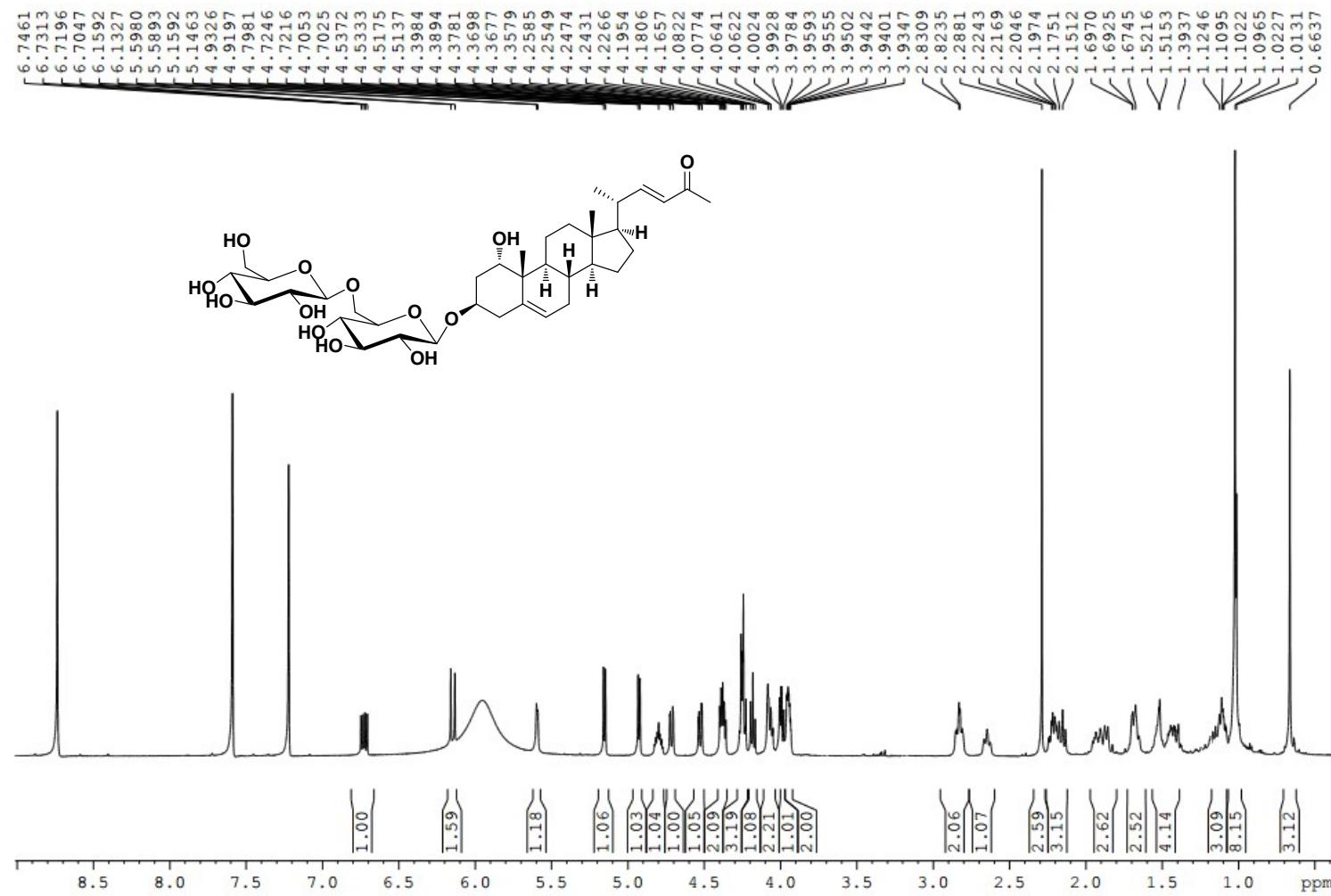


Figure S31. HSQC spectrum of compound **4** in pyridine-*d*₅.

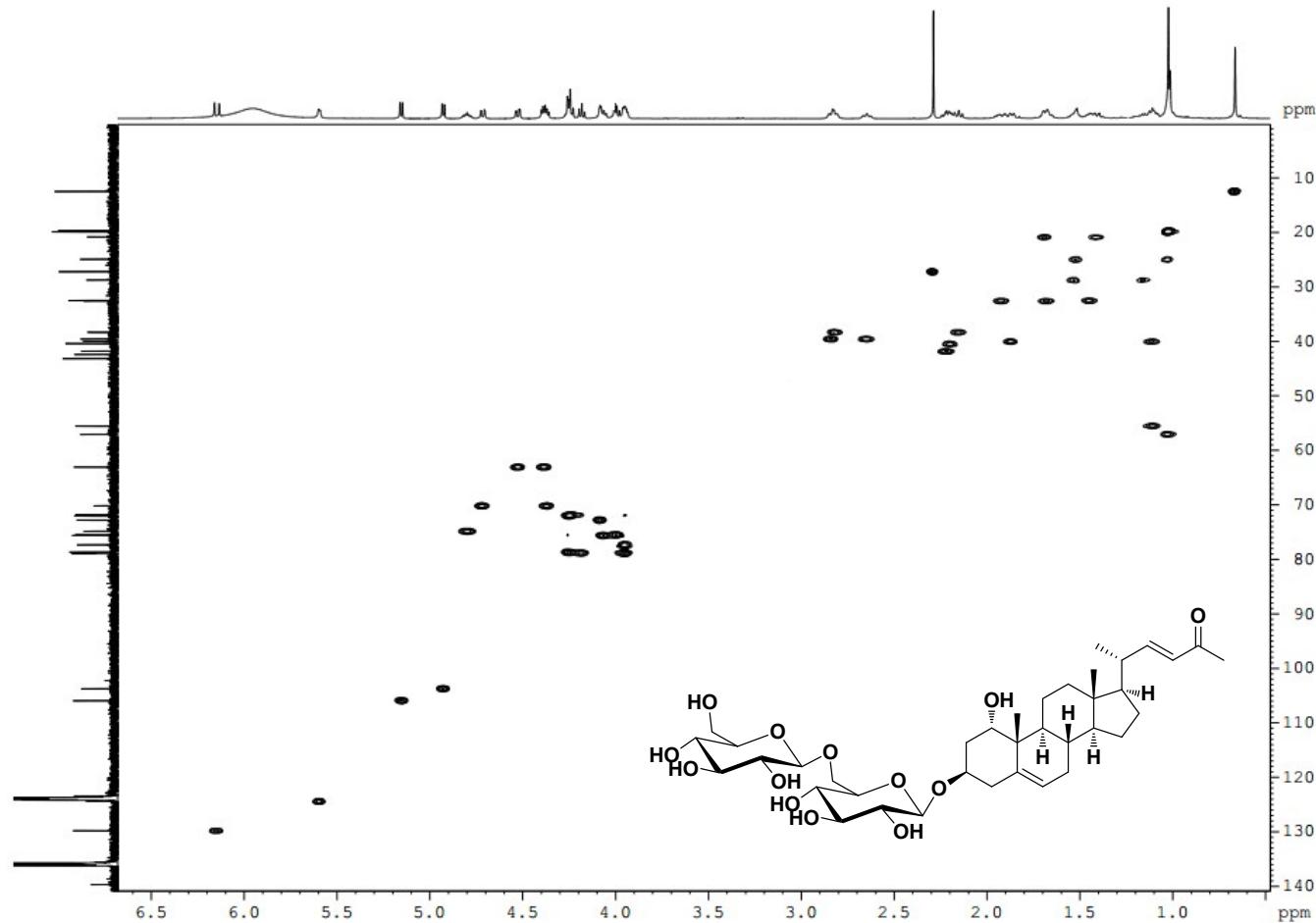


Figure S32. ^1H - ^1H COSY spectrum of compound **4** in pyridine- d_5 .

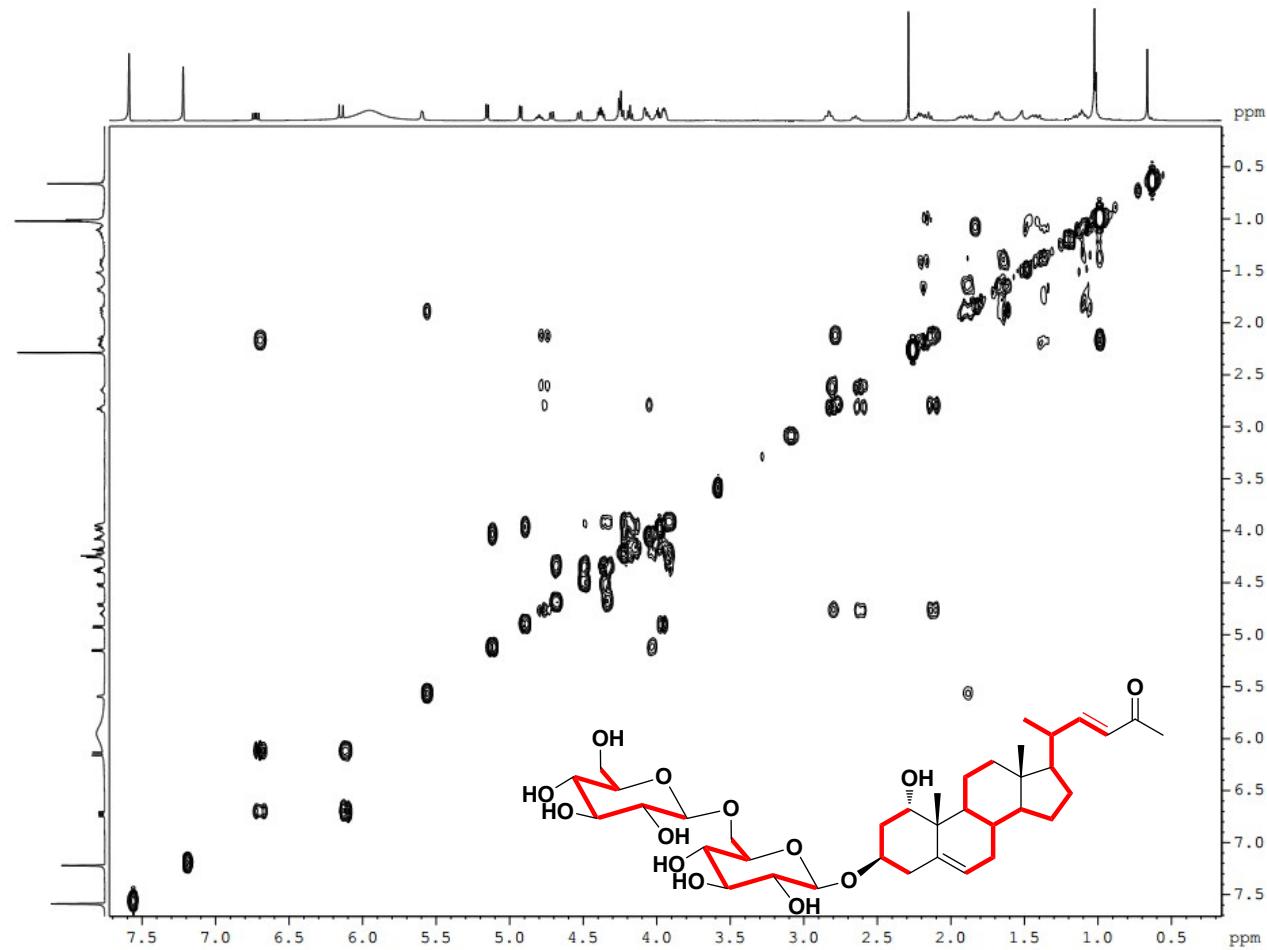


Figure S33. HMBC spectrum of compound **4** in pyridine-*d*₅.

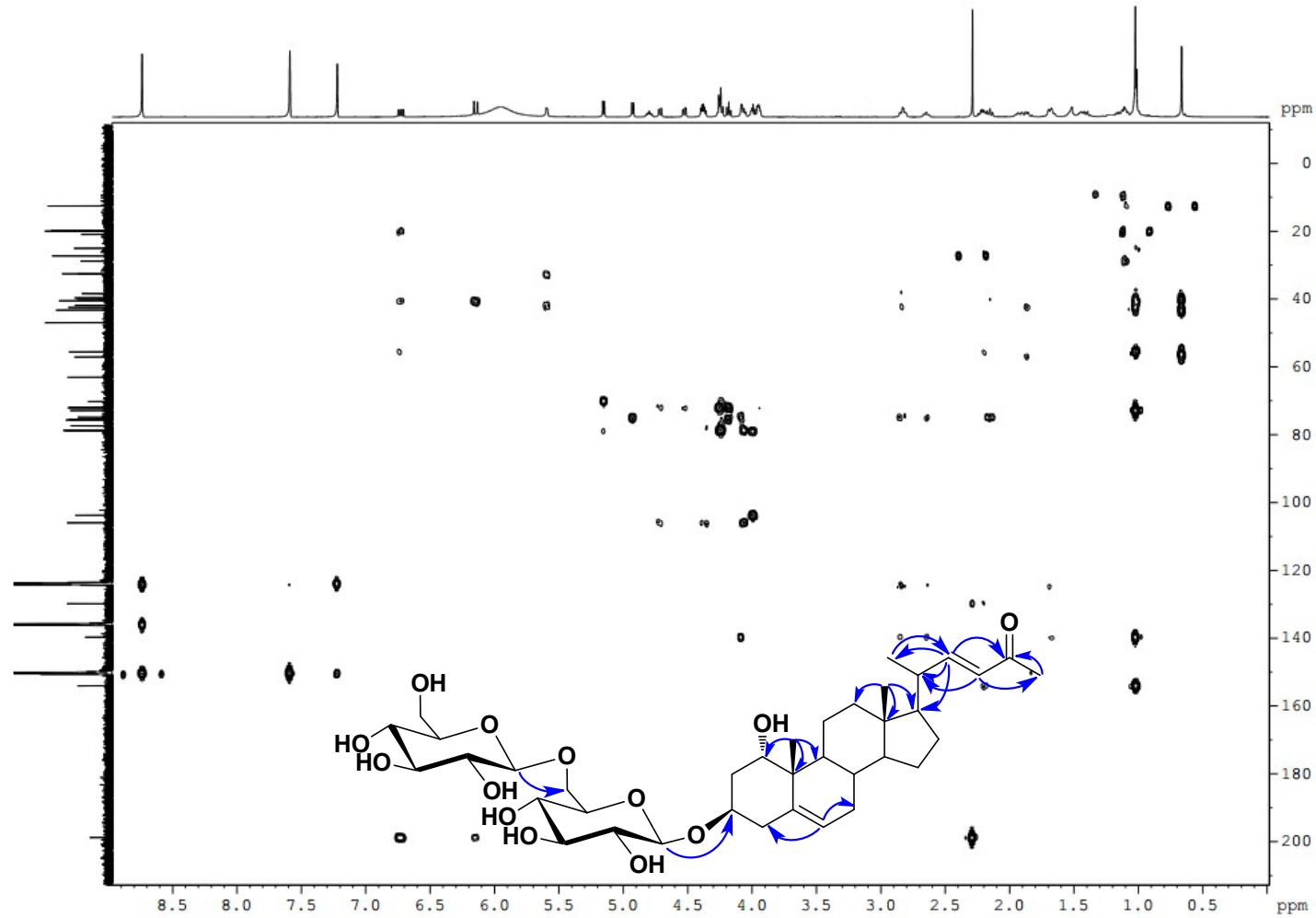


Figure S34. NOESY spectrum of compound 4 in pyridine-*d*₅.

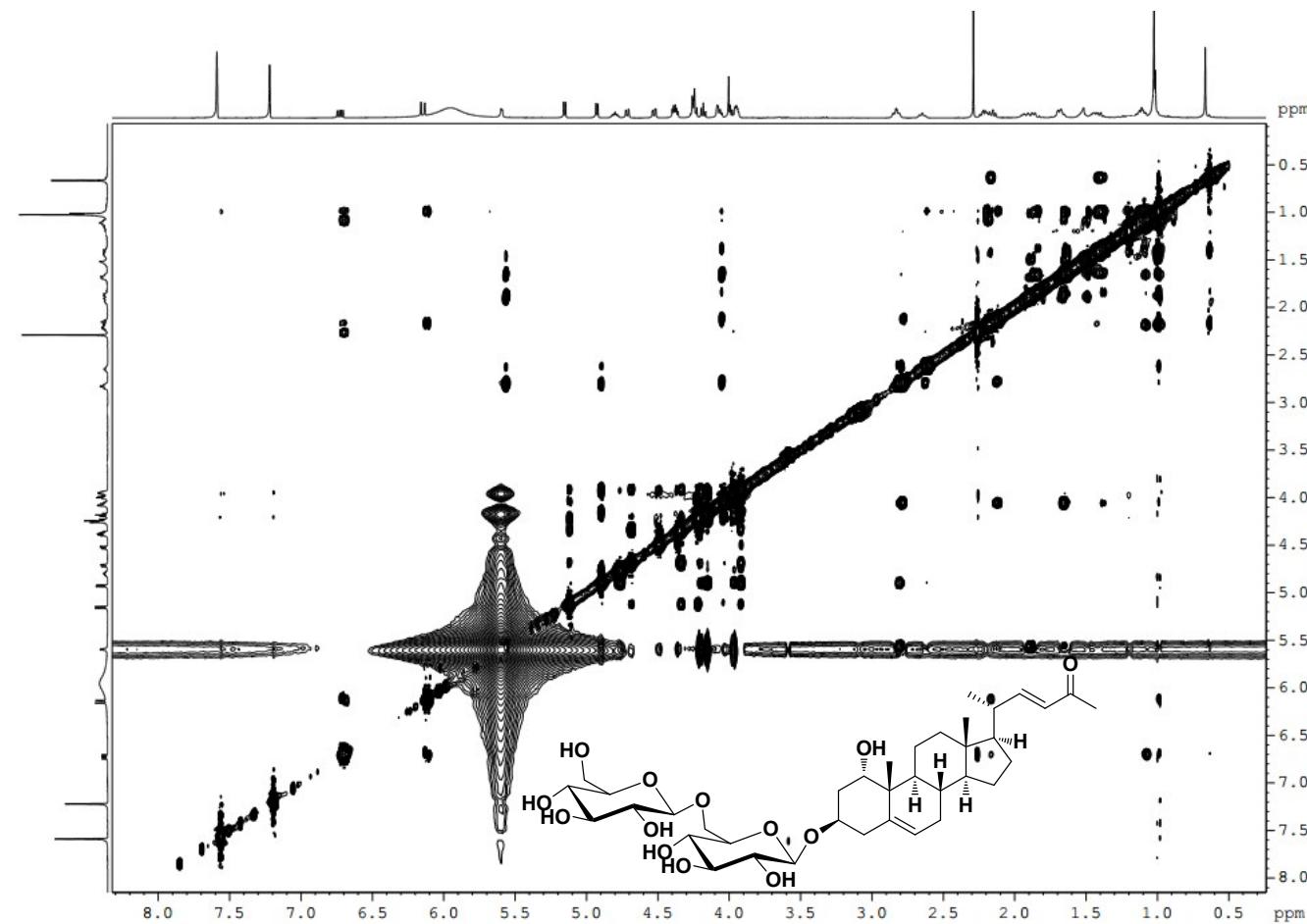


Figure S35. HRESIMS data of compound 4.

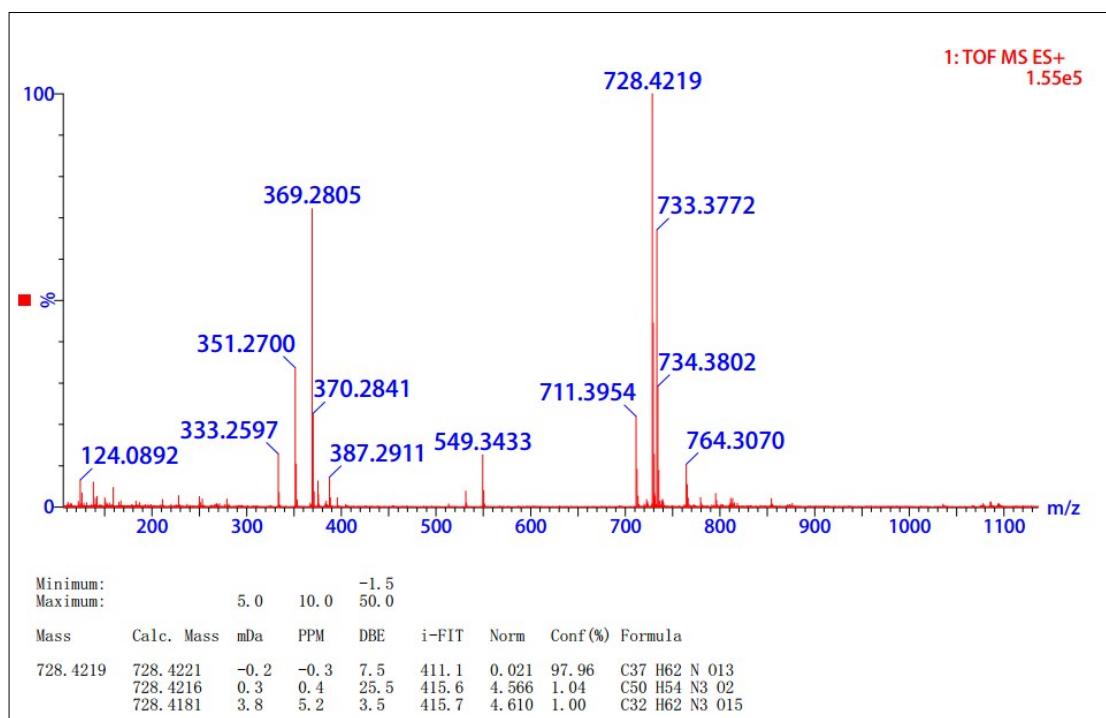


Figure S36. IR spectrum of compound 4.

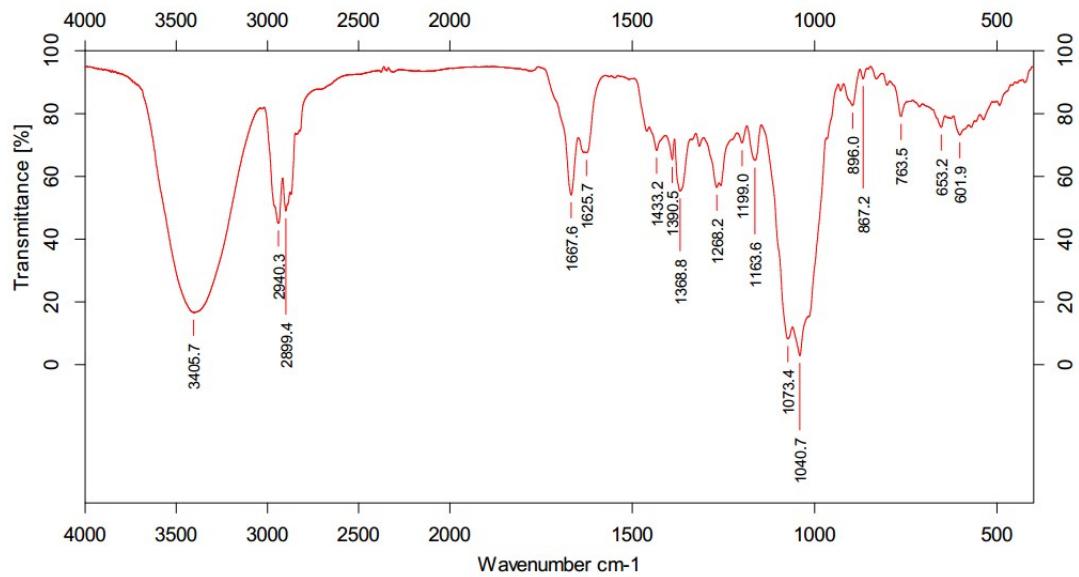


Figure S37. UV spectrum of compound 4.

