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Data Article

Spectral data for cholestane glycosides from the bulbs of *Ornithogalum saundersiae* Baker



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ABSTRACT

Herein, the spectral data, including nuclear magnetic resonance spectroscopy (NMR) and mass spectral data, and gas chromatography data of eight cholestane glycosides from *Ornithogalum saundersiae* Baker (Asparagaceae) bulbs are described. The data are linked with the article entitled "Structure and bioactivity of cholestane glycosides from the bulbs of *Ornithogalum saundersiae* Baker" (Chen et al., 2019).

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Specifications Table

Subject	Chemistry
Specific subject area	Natural products research
Type of data	Figures
How data were acquired	High-resolution electrospray ionization mass spectrometry (HRESIMS), NMR, Gas chromatography (GC)
Data format	Raw, filtered and analyzed
Parameters for data collection	The purified isolates were subjected to HRESIMS analysis. Cholestane glycosides were dissolved in C5D5N prior to NMR analysis. The acidified compounds must be derivatized before GC analysis.
Description of data collection	HRESIMS was performed on an Agilent 6520 HPLC-Q-TOF. NMR data were recorded with Bruker AV-III-500 spectrometer or a Bruker-600 NMR spectrometer. GC analysis were conducted in Agilent 7890 system.
Data source location	Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College Beijing P. R. China
Data accessibility	Data is with this article
Related research article	Qing-Wei Chen, Xu Zhang, Ting Gong, Wan Gao, Shuai Yuan, Pei-Cheng Zhang, Jian-Qiang Kong Structure and bioactivity of cholestane glycosides from the bulbs of <i>Ornithogalum saundersiae</i> Baker <i>Phytochemistry</i> , 2019, 164:206-214

Value of the data

- Spectral data of cholestane glycosides are useful for elucidating their chemical structures.
- The presented data benefit the chemical researchers, especially those working on the structural identification of steroidal glycosides.
- The presented data can provide references for the structural characterization of related cholestane glycosides in other species.
- The method described in this article can provide references for the isolation of related compounds.

1. Data

Eight new cholestane glycosides were isolated from the bulbs of *Ornithogalum saundersiae* Baker [1]. Their spectral data, including NMR and mass spectral data, and gas chromatography data were presented in this article. See Figs. 1–66 with this article.

1.1. MS data for compounds 1-8

HRESIMS was performed for purified compounds 1–8. MS data was provided in Figs. 1–8.

1.2. NMR data for compounds 1-8

1D and 2D NMR spectroscopy data of isolates 1–8 were recorded in Figs. 9–56. These data include ¹H-NMR, ¹³C-NMR, ¹H-¹H correlated spectroscopy (COSY), ¹H-¹³C heteronuclear multiple bond correlation (HMBC), heteronuclear singular quantum correlation (HSQC) and rotating-frame overhauser effect spectroscopy (ROESY) (Figs. 9–56).

1.3. GC data

Gas chromatography analysis were performed to determine the absolute configuration of sugar moieties in compounds 1–8 (Figs. 57–66).

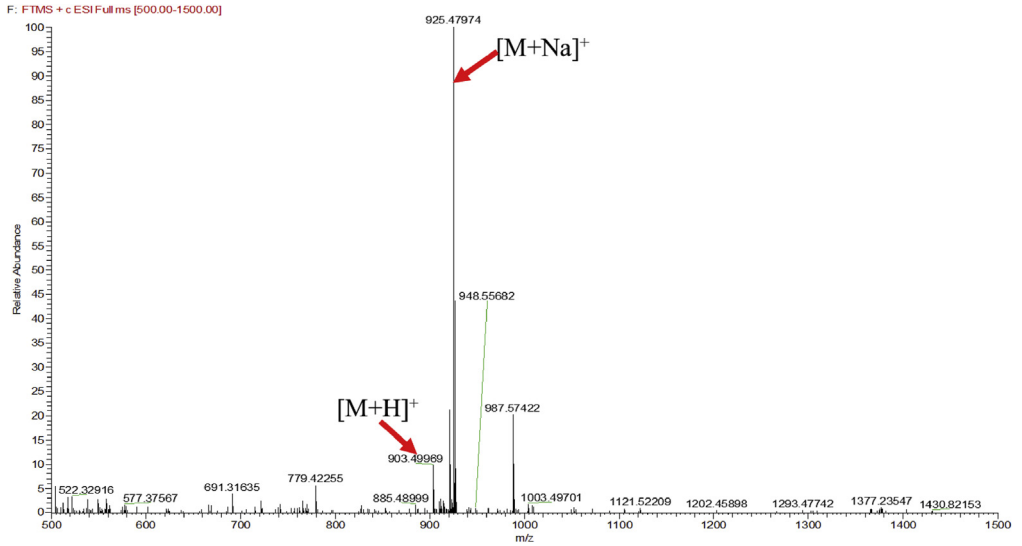


Fig. 1. HRESIMS spectra of 1.

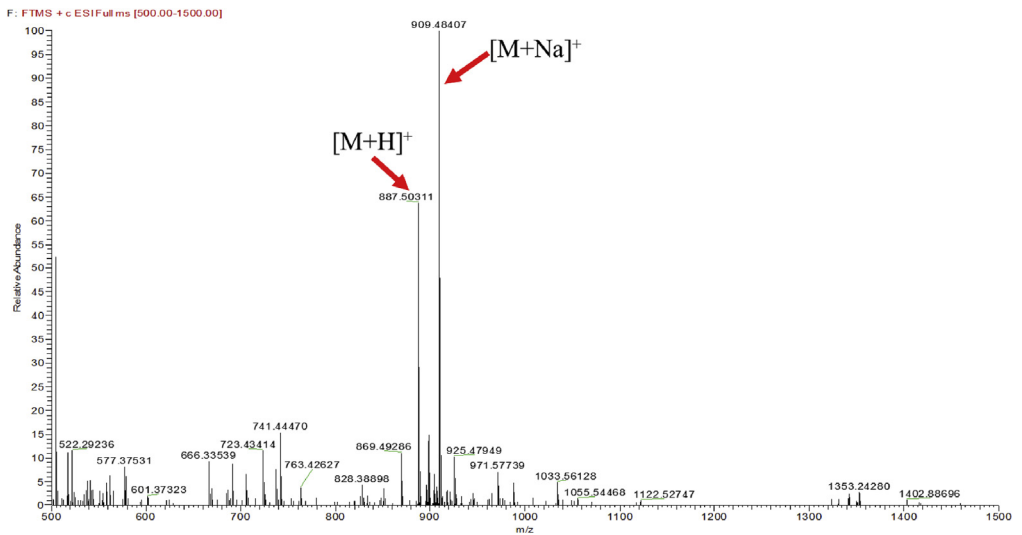


Fig. 2. HRESIMS spectra of 2.

2. Experimental design, materials and methods

2.1. HRESIMS analysis

After isolation and purification from the bulbs of *O. saundersiae* Baker, eight cholestane glycosides were subjected to HRESIMS analysis, which was performed using an Agilent 6520 HPLC-Q-TOF (Agilent Technologies, Waldbronn, Germany).

F: FTMS + c ESI Full ms [500.00-1500.00]

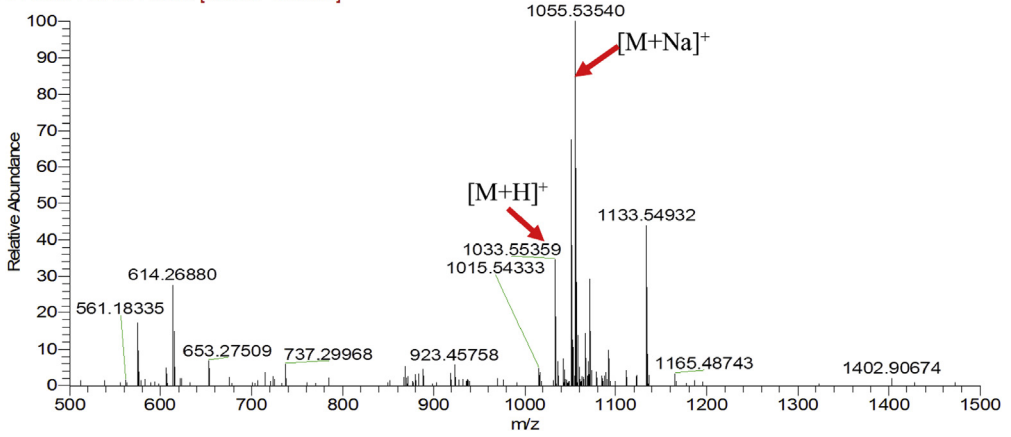


Fig. 3. HRESIMS spectra of 3.

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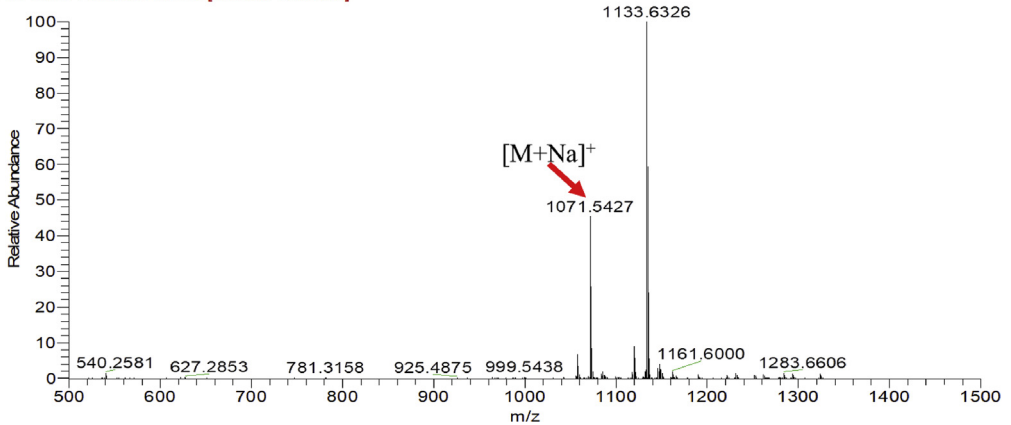


Fig. 4. HRESIMS spectra of 4.

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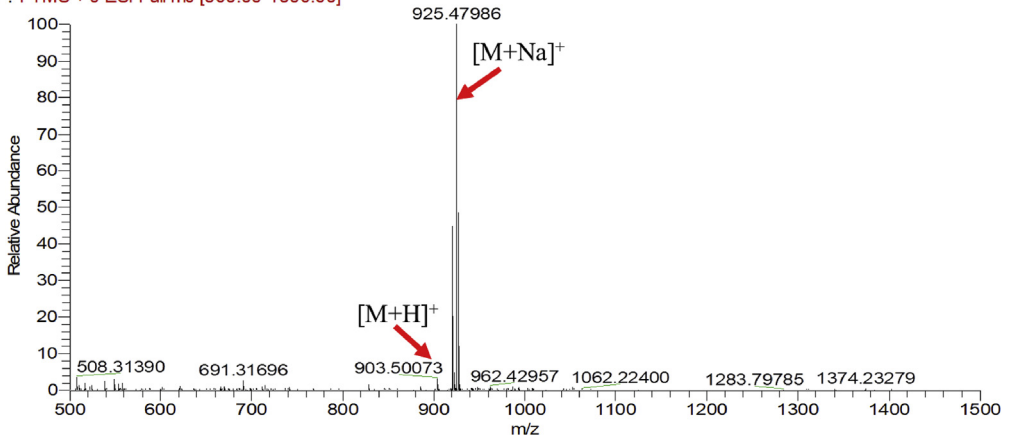


Fig. 5. HRESIMS spectra of 5.

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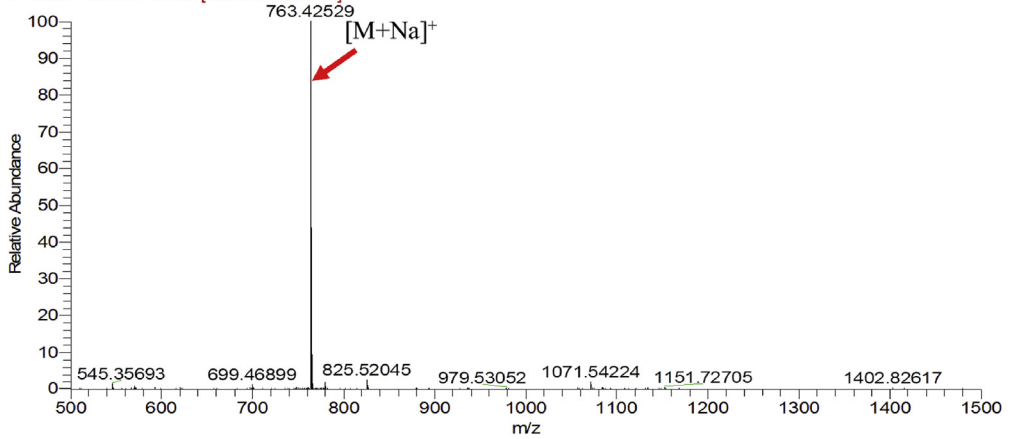


Fig. 6. HRESIMS spectra of 6.

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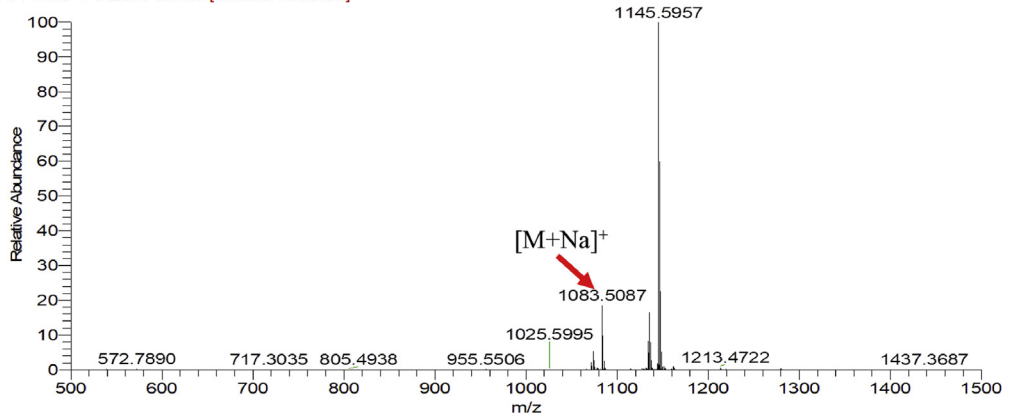


Fig. 7. HRESIMS spectra of 7.

F: FTMS + c ESI Full ms [500.00-1500.00]

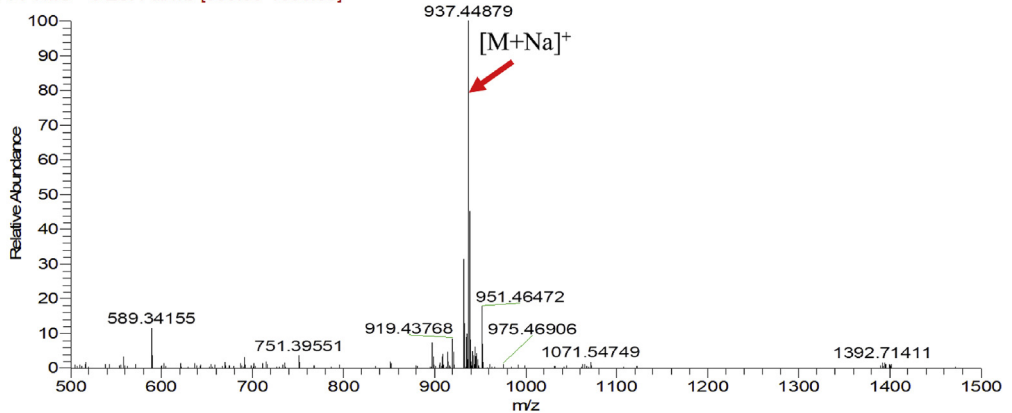


Fig. 8. HRESIMS spectra of 8.

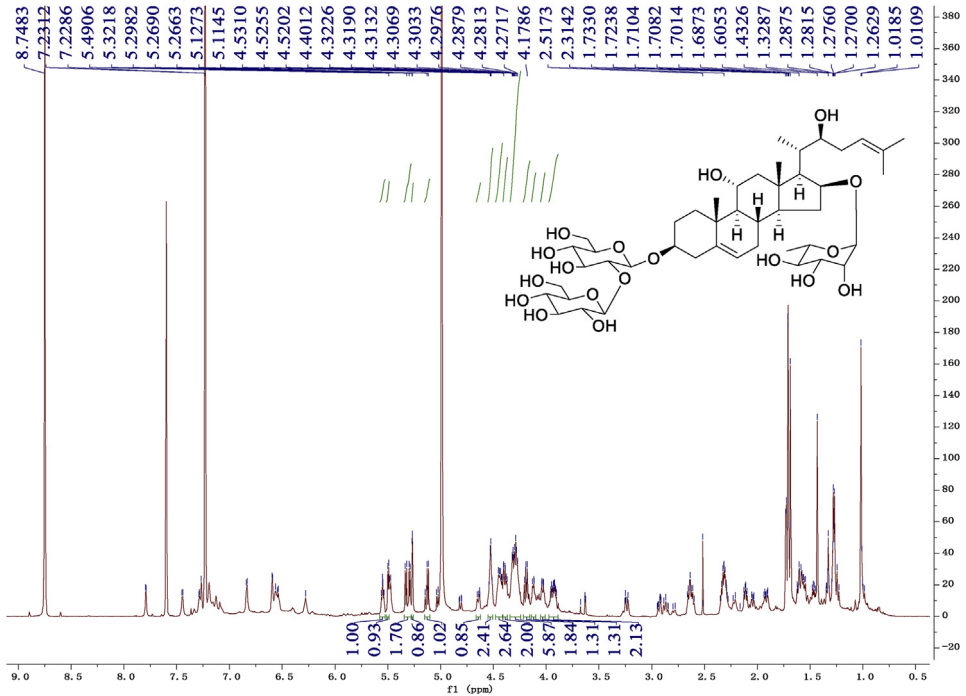


Fig. 9. $^1\text{H-NMR}$ (600 MHz) spectrum in pyridine- d_5 of 1.

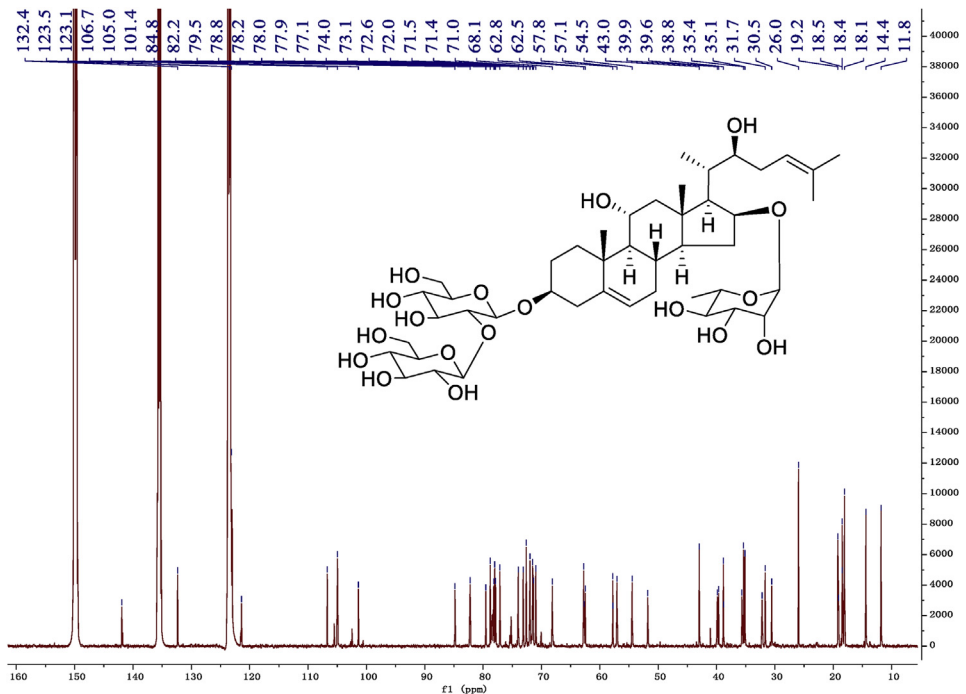


Fig. 10. $^{13}\text{C-NMR}$ (150 MHz) spectrum in pyridine- d_5 of 1.

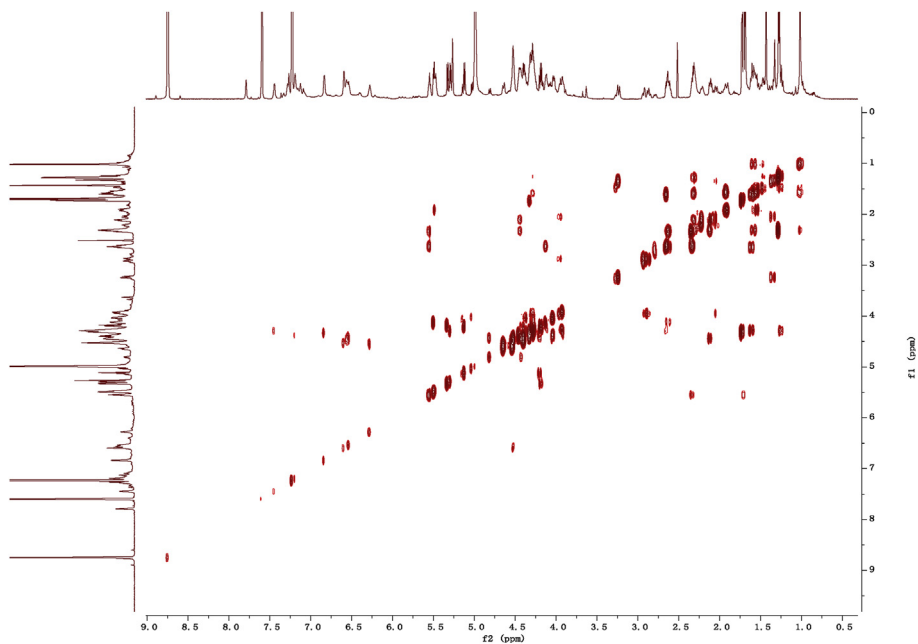


Fig. 11. 2D COSY NMR spectrum in pyridine-*d*₅ of 1.

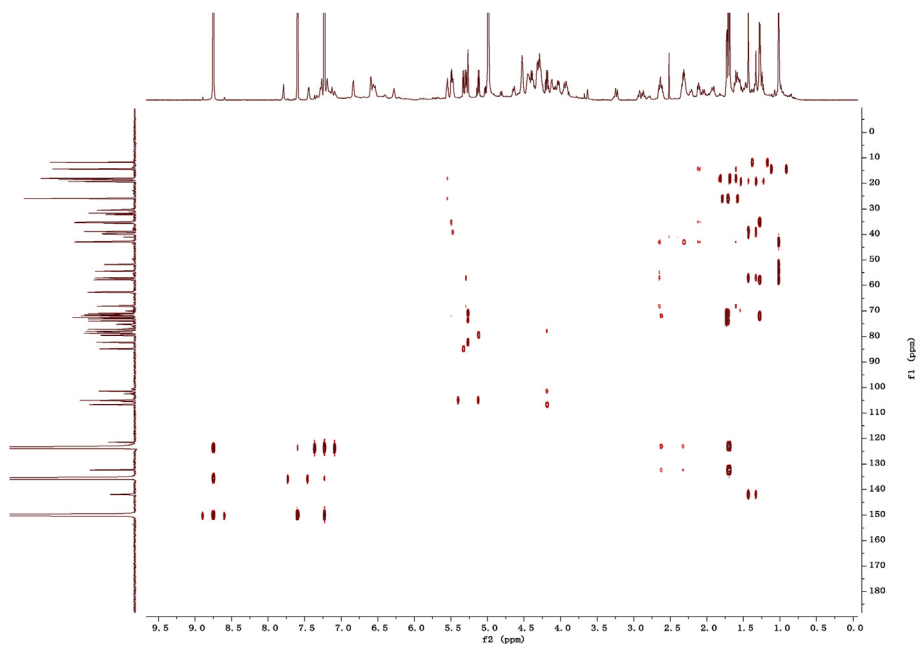


Fig. 12. 2D HMBC NMR spectrum in pyridine-*d*₅ of 1.

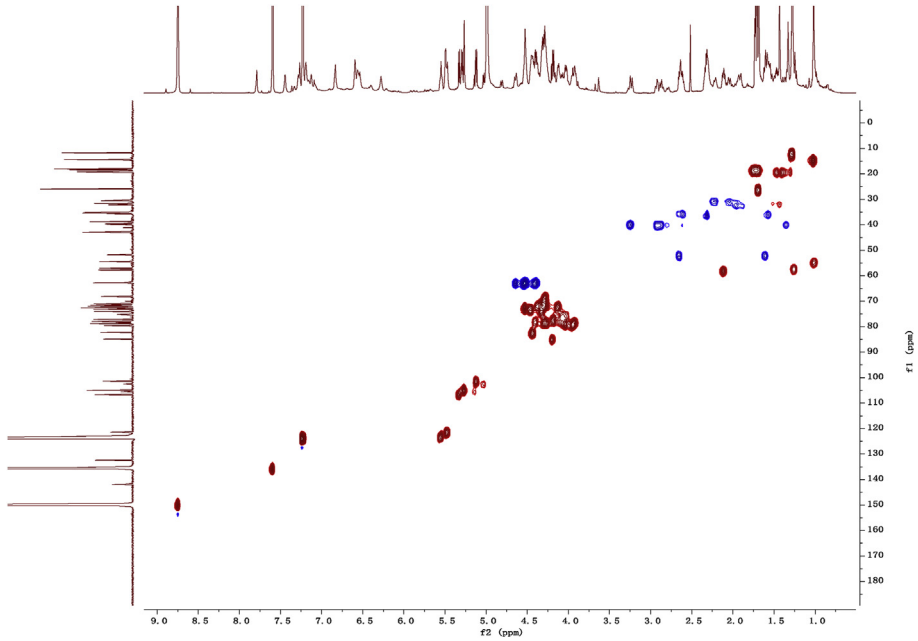


Fig. 13. 2D HSQC NMR spectrum in pyridine- d_5 of 1.

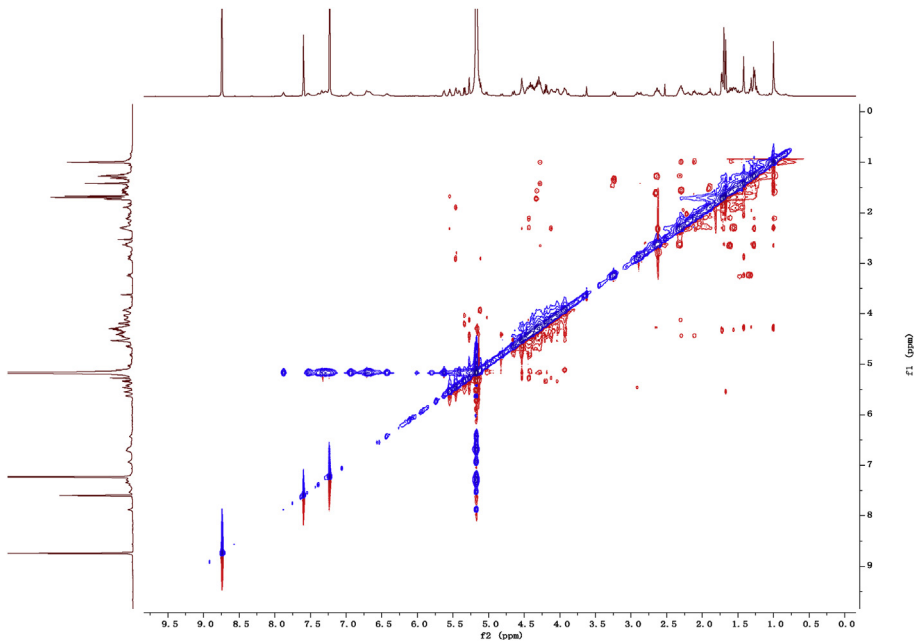


Fig. 14. 2D ROESY NMR spectrum in pyridine- d_5 of 1.

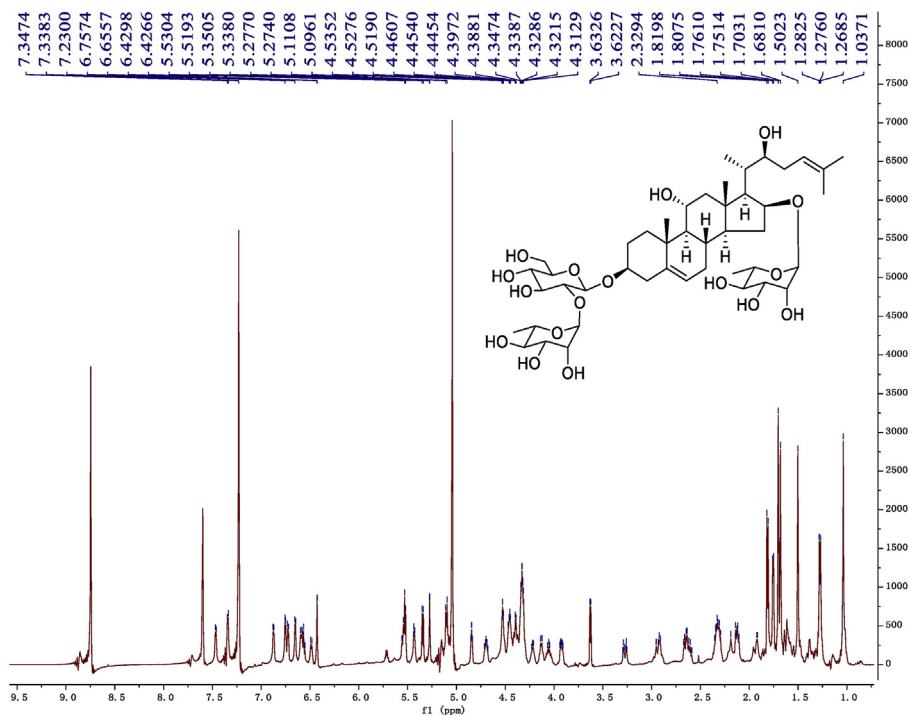


Fig. 15. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 2.

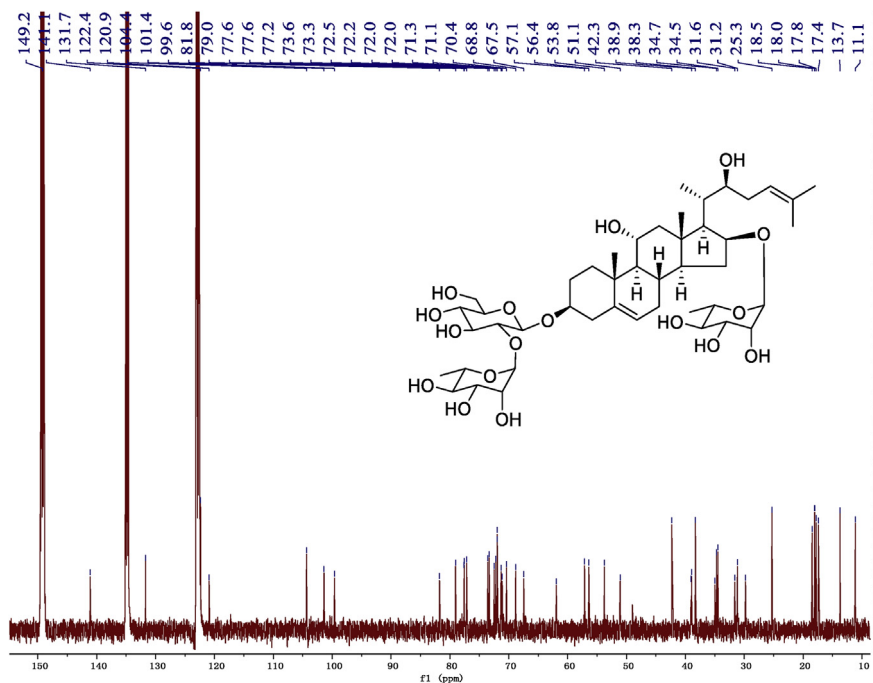


Fig. 16. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 2.

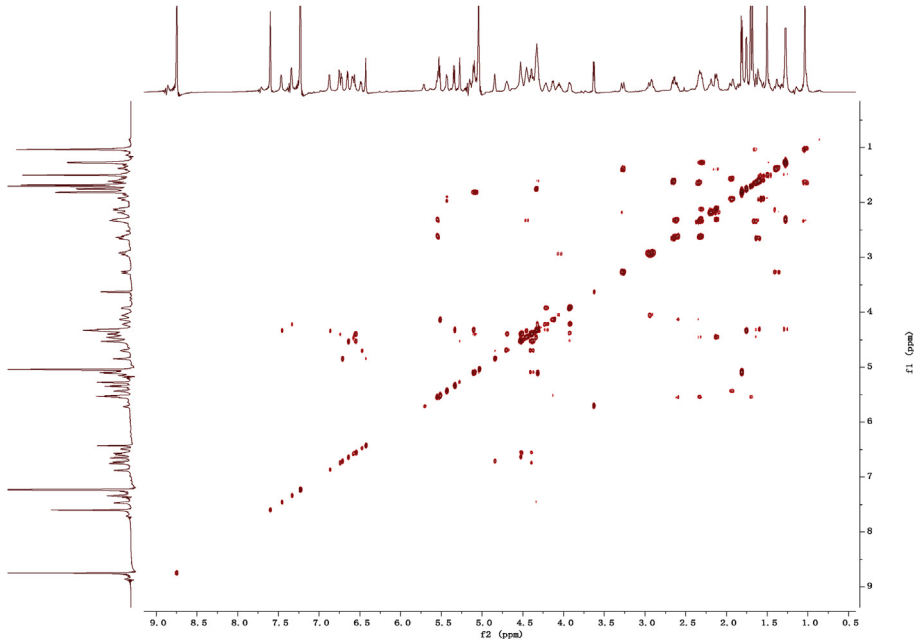


Fig. 17. 2D COSY NMR spectrum in pyridine-*d*₅ of 2.

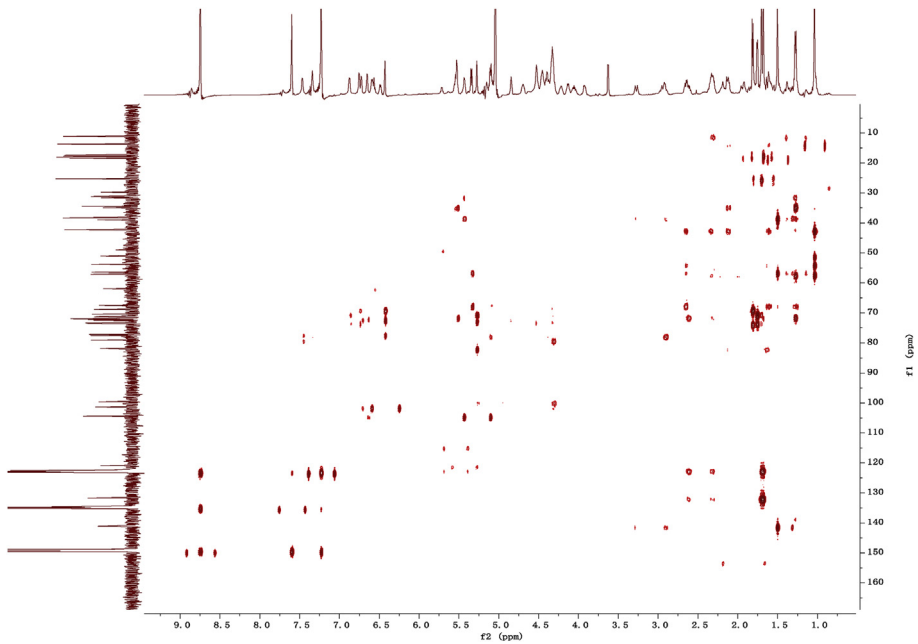


Fig. 18. 2D HMBC NMR spectrum in pyridine-*d*₅ of 2.

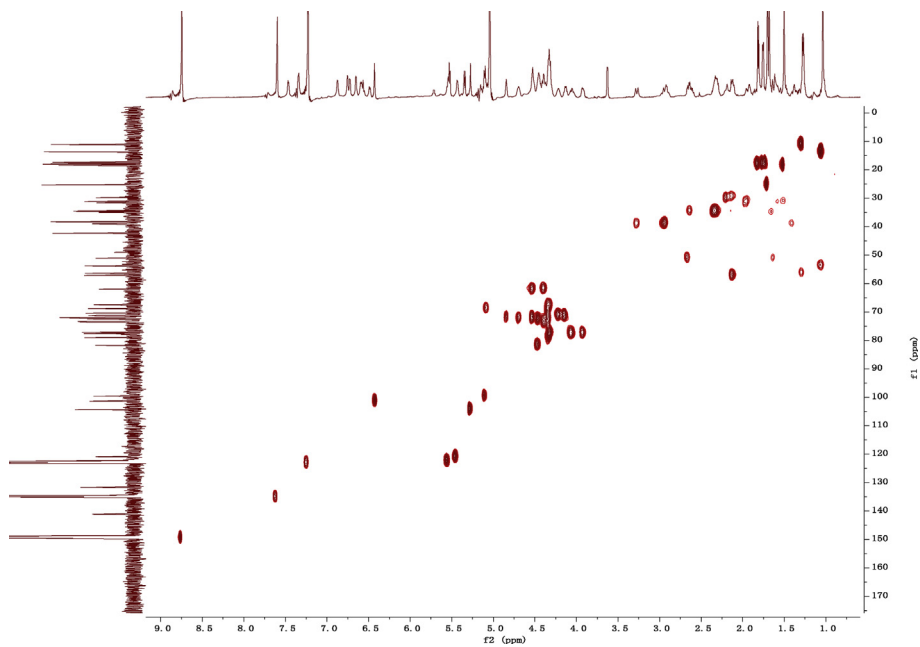


Fig. 19. 2D HSQC NMR spectrum in pyridine- d_5 of 2.

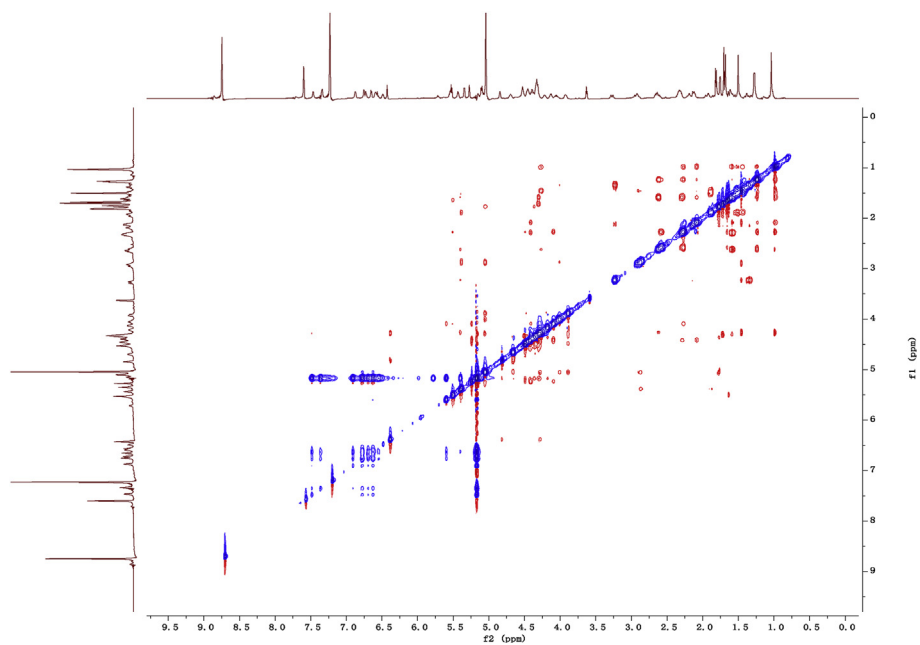


Fig. 20. 2D ROESY NMR spectrum in pyridine- d_5 of 2.

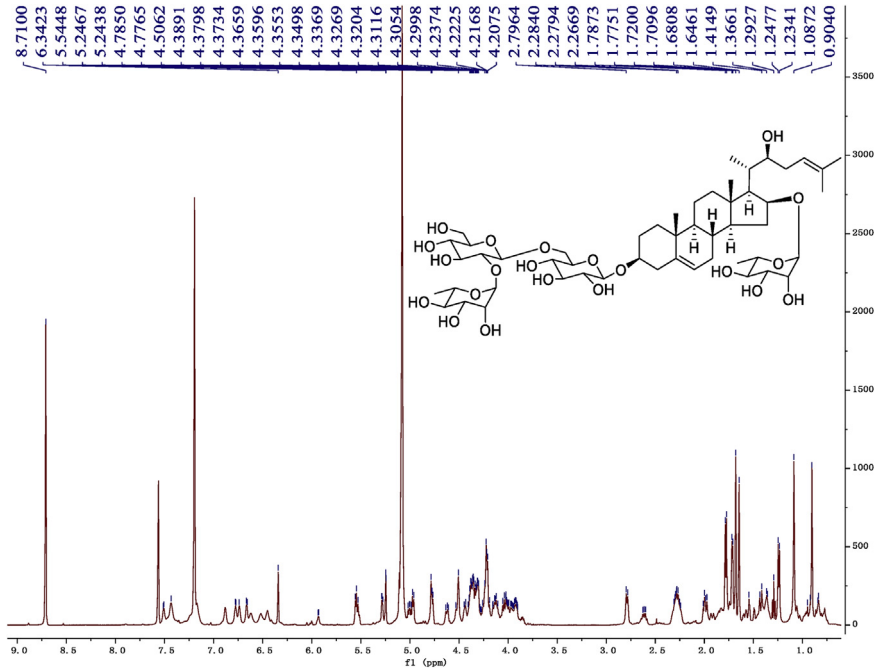


Fig. 21. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 3.

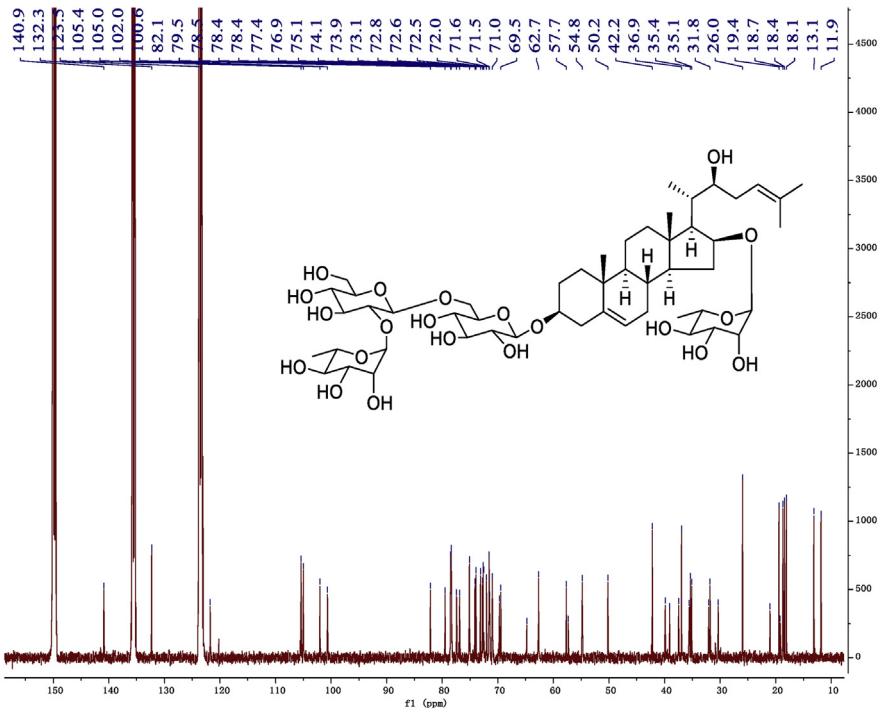


Fig. 22. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 3.

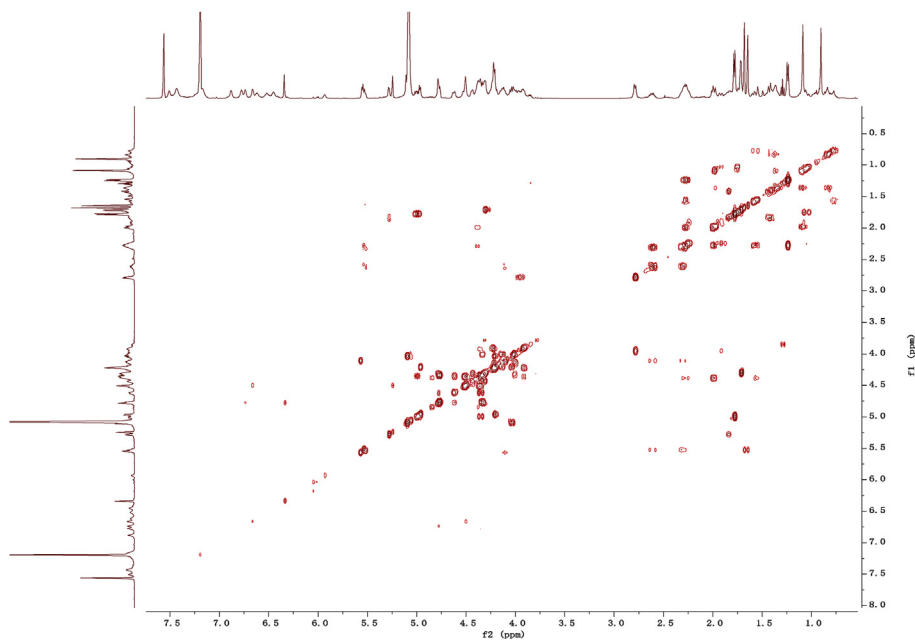


Fig. 23. 2D COSY NMR spectrum in pyridine- d_5 of 3.

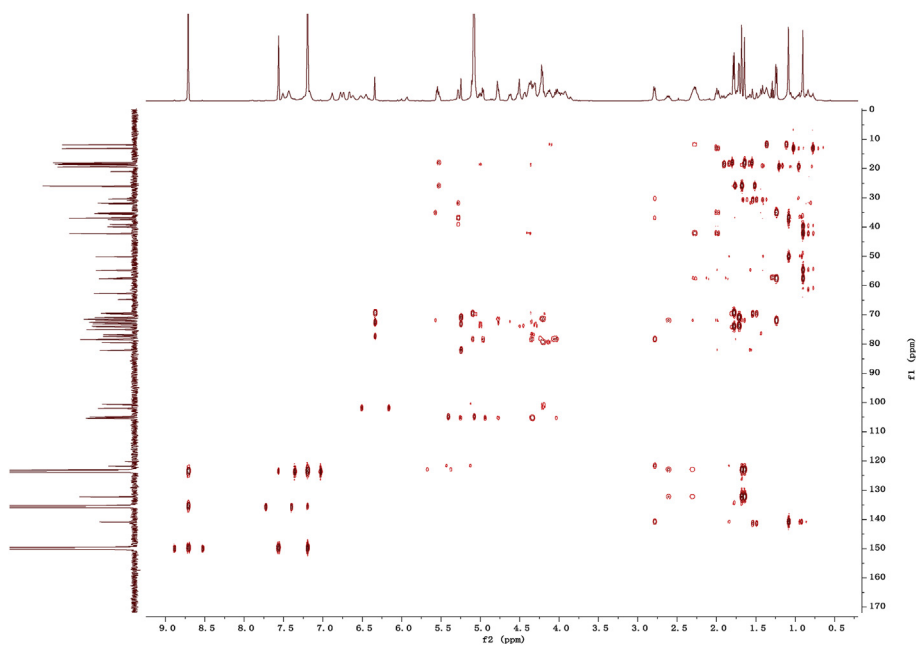


Fig. 24. 2D HMBC NMR spectrum in pyridine- d_5 of 3.

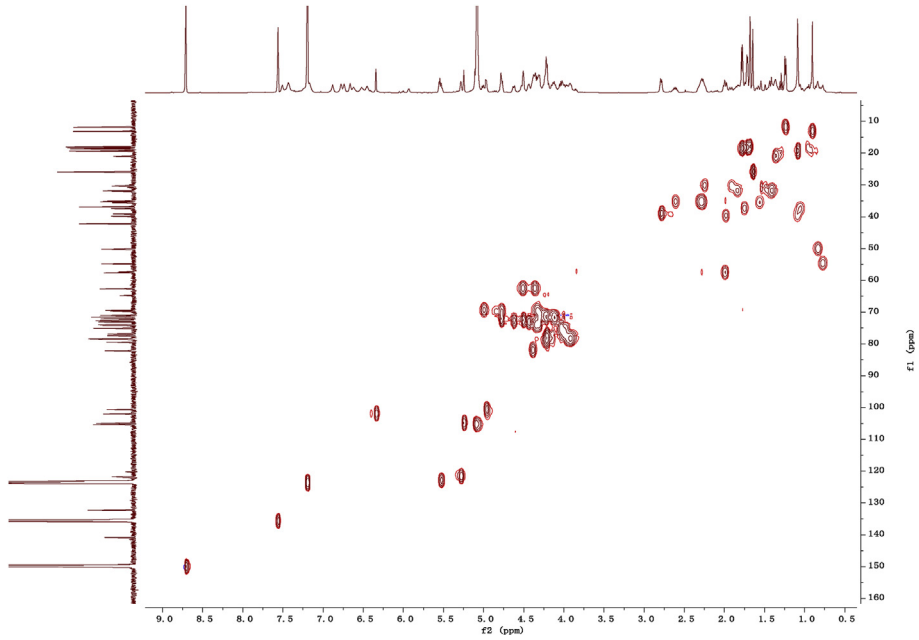


Fig. 25. 2D HSQC NMR spectrum in pyridine- d_5 of 3.

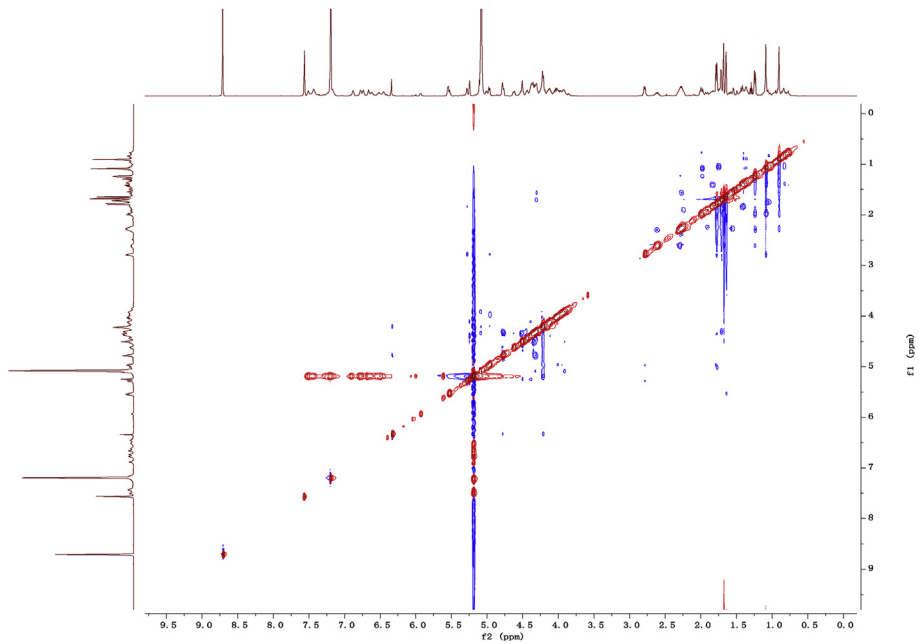


Fig. 26. 2D ROESY NMR spectrum in pyridine- d_5 of 3.

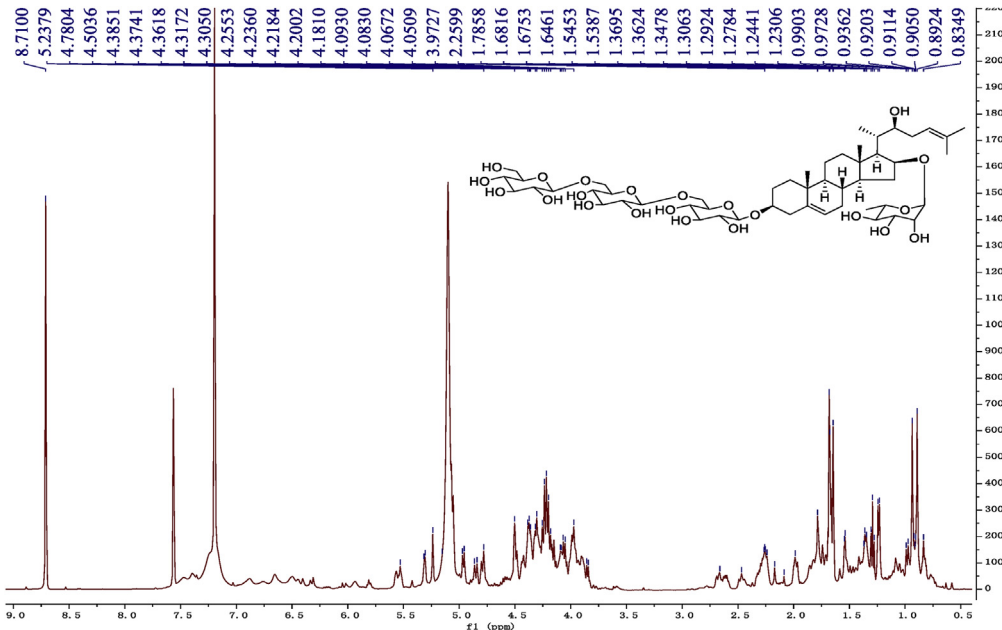


Fig. 27. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 4.

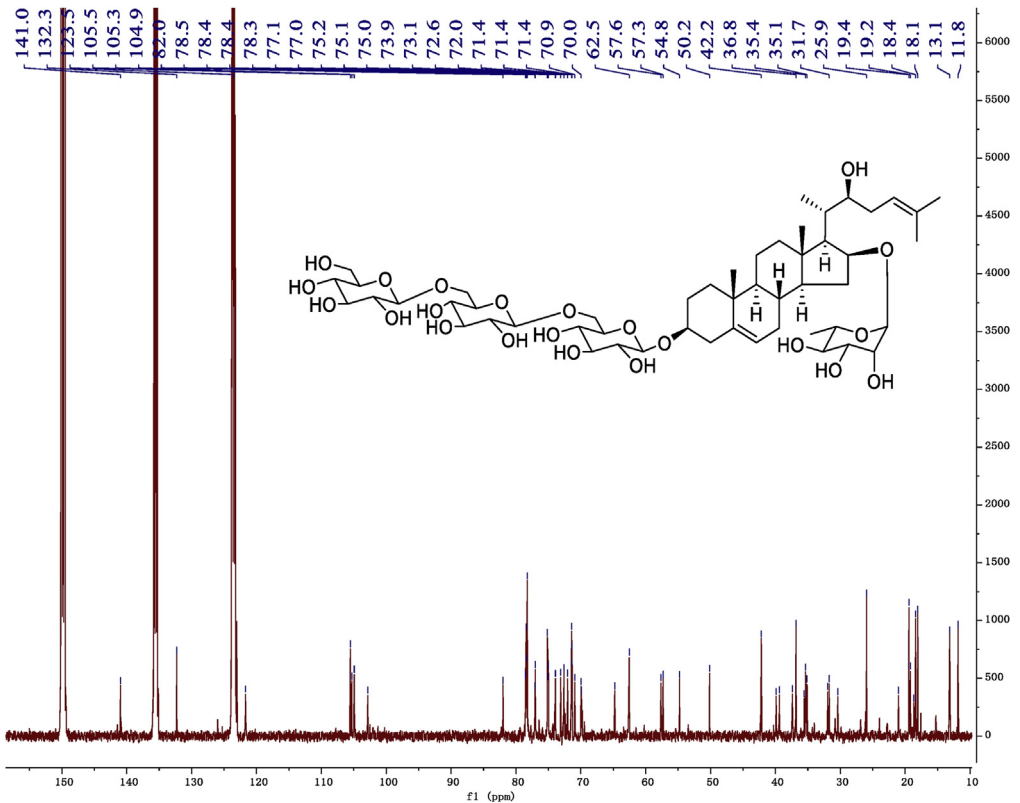


Fig. 28. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 4.

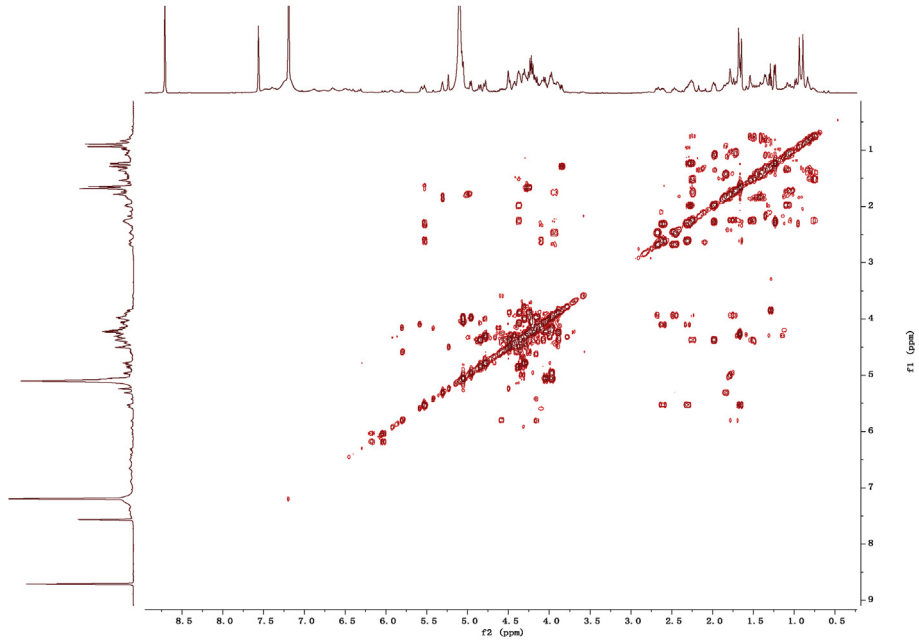


Fig. 29. 2D COSY NMR spectrum in pyridine- d_5 of 4.

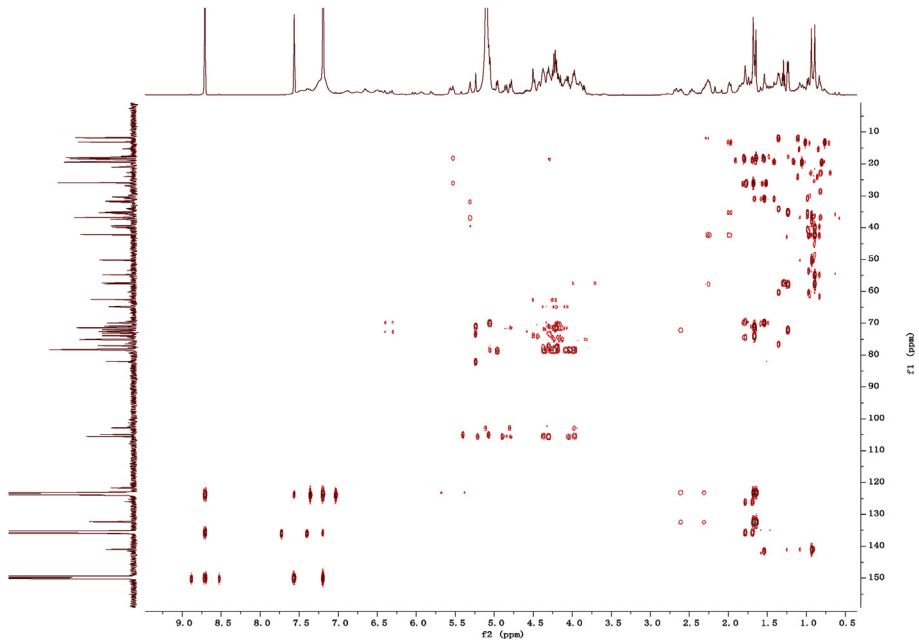


Fig. 30. 2D HMBC NMR spectrum in pyridine- d_5 of 4.

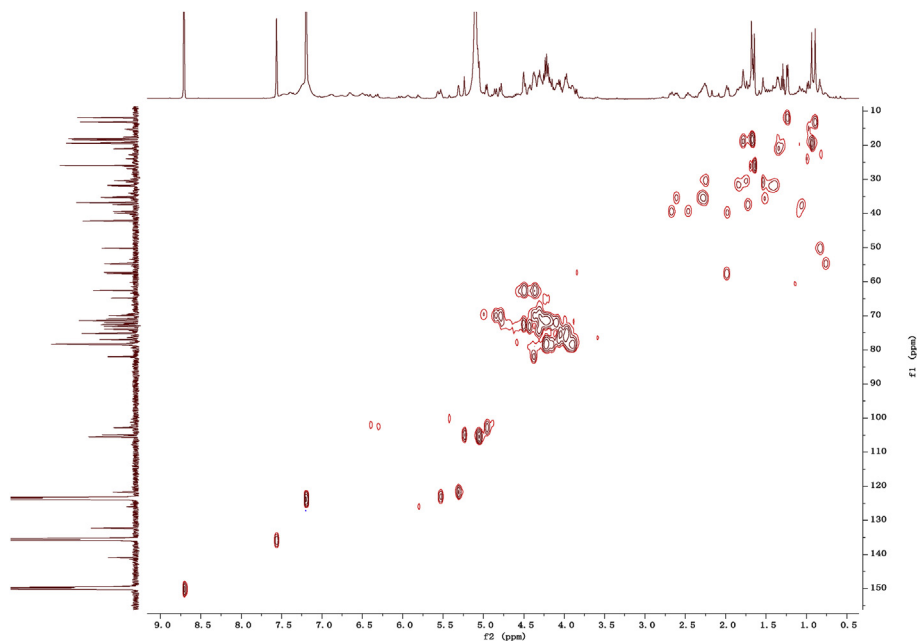


Fig. 31. 2D HSQC NMR spectrum in pyridine- d_5 of 4.

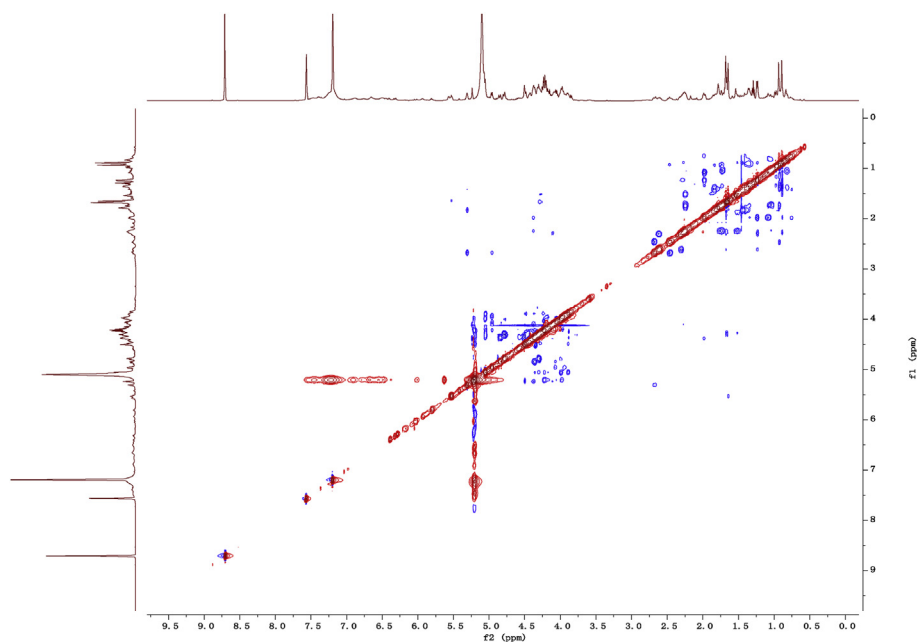


Fig. 32. 2D ROESY NMR spectrum in pyridine- d_5 of 4.

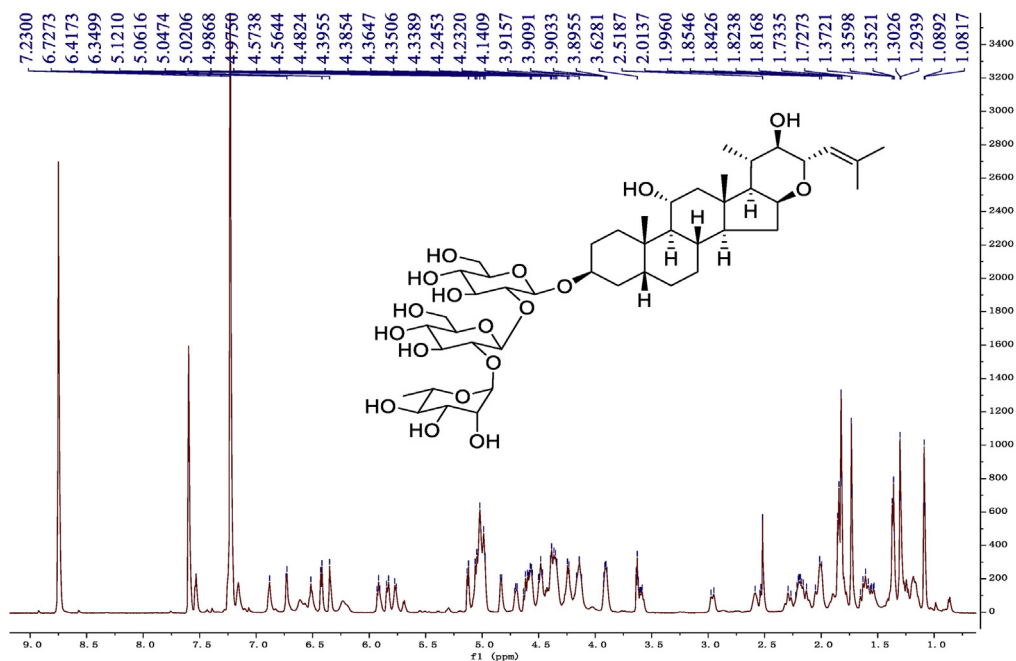


Fig. 33. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 5.

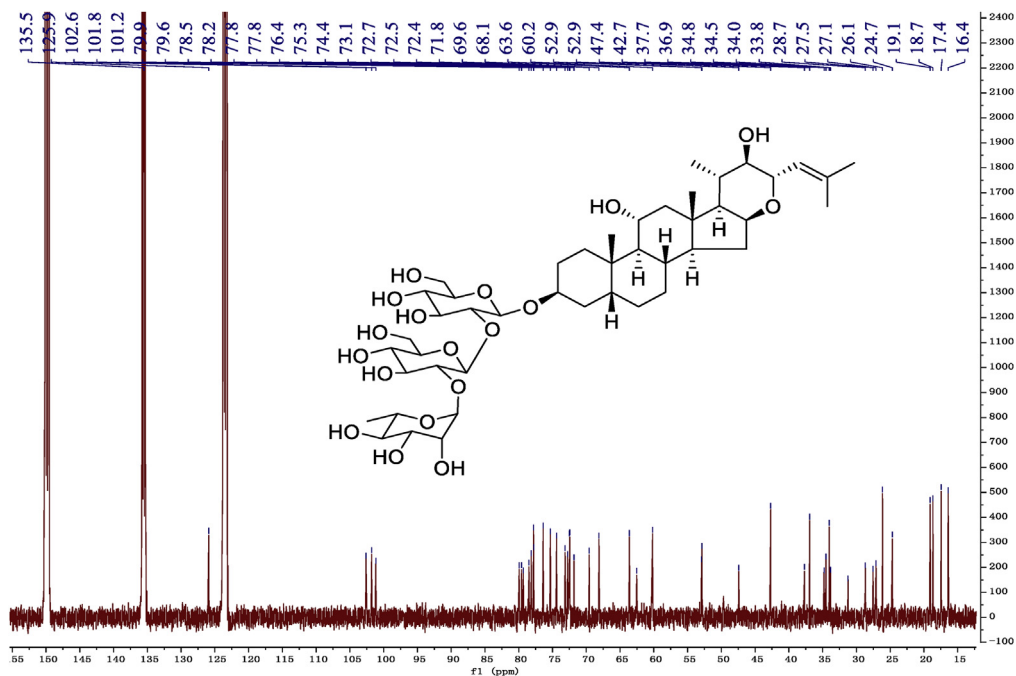


Fig. 34. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 5.

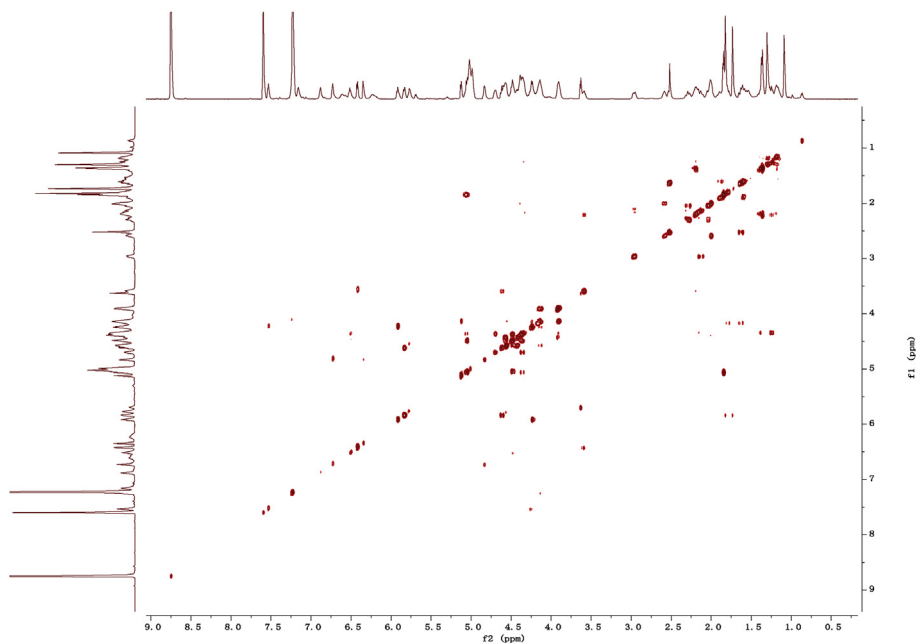


Fig. 35. 2D COSY NMR spectrum in pyridine-*d*₅ of 5.

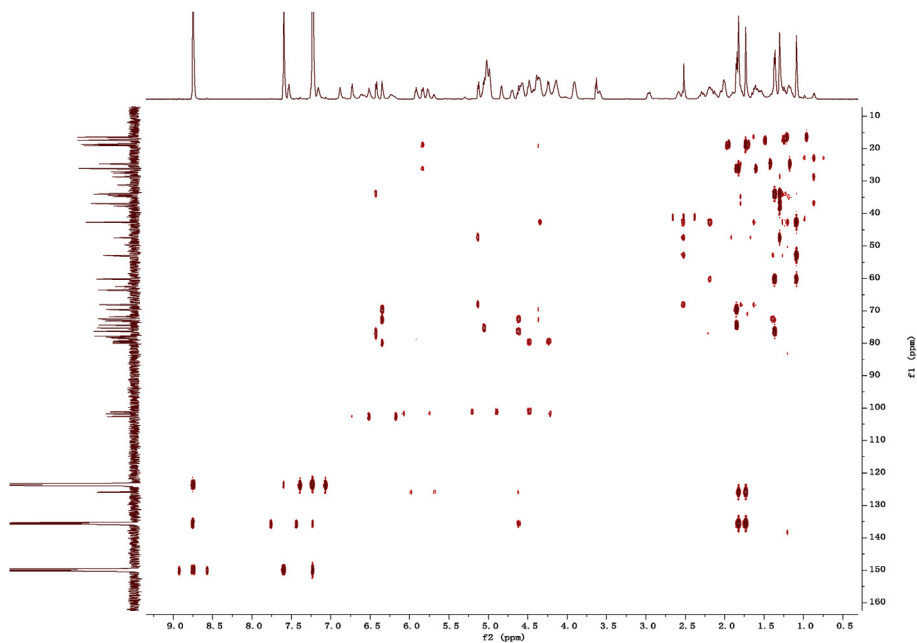


Fig. 36. 2D HMBC NMR spectrum in pyridine-*d*₅ of 5.

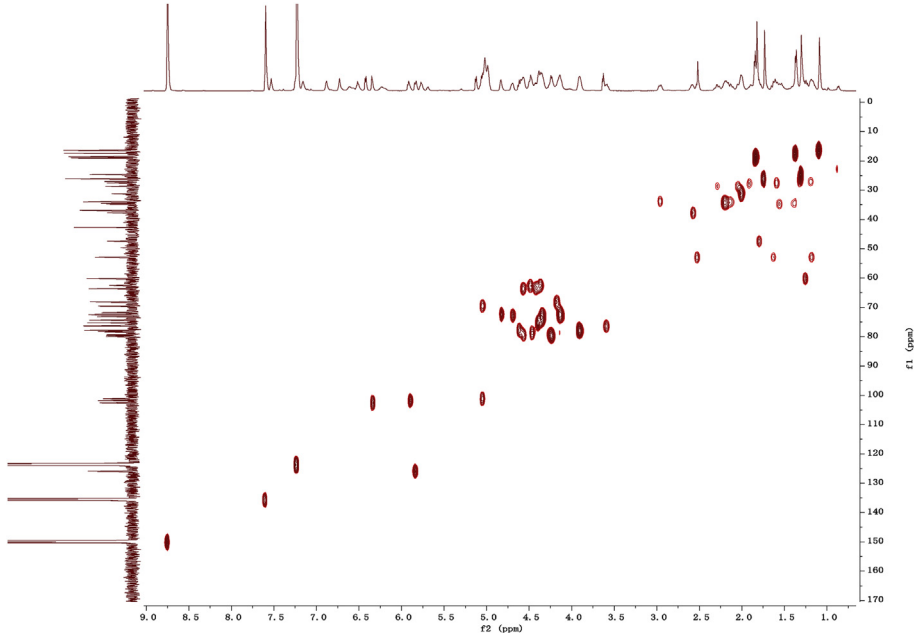


Fig. 37. 2D HSQC NMR spectrum in pyridine- d_5 of 5.

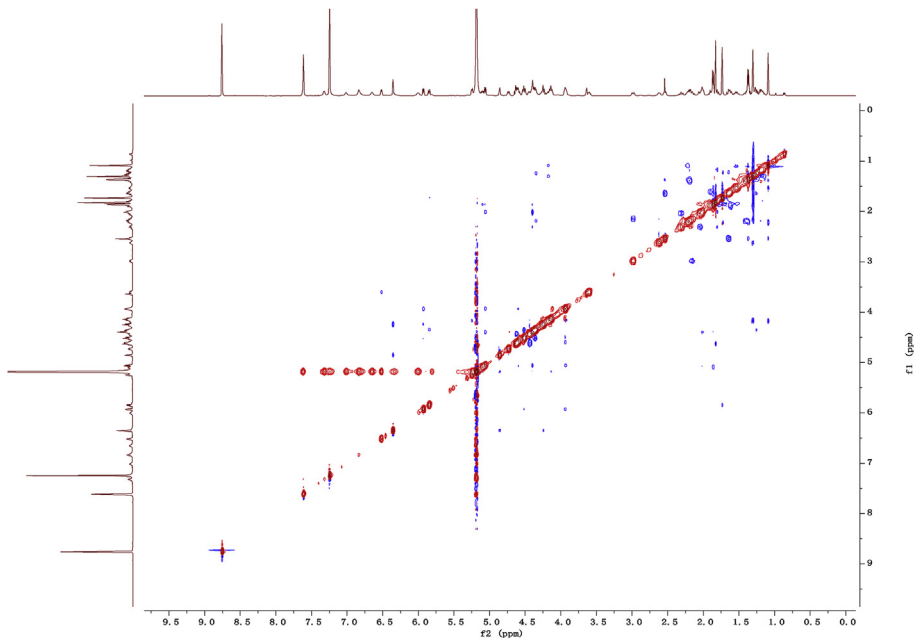


Fig. 38. 2D ROESY NMR spectrum in pyridine- d_5 of 5.

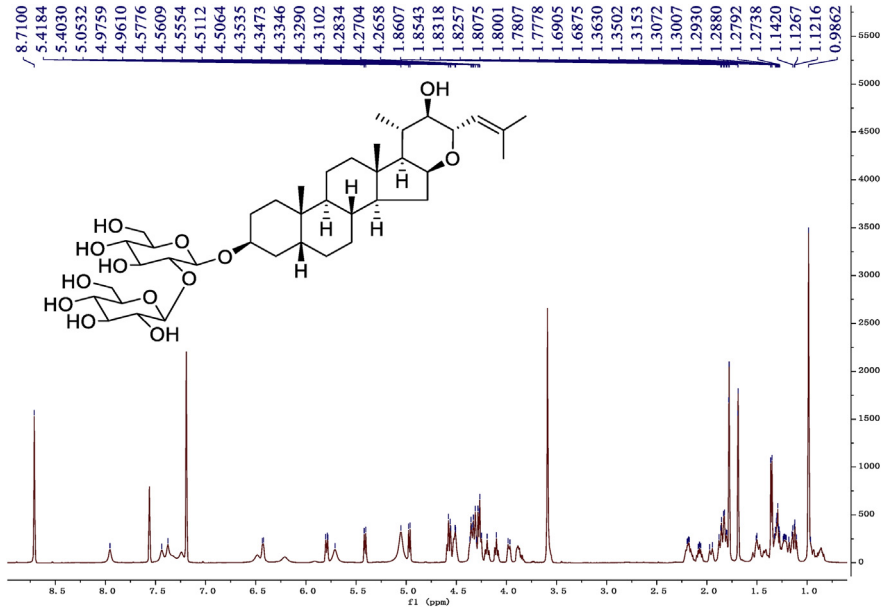


Fig. 39. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 6.

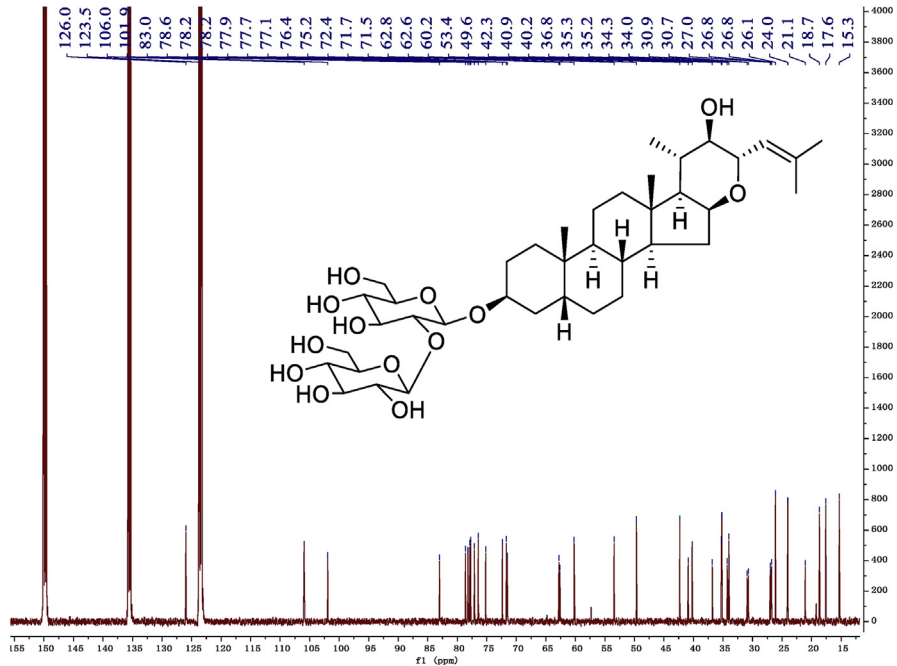


Fig. 40. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 6.

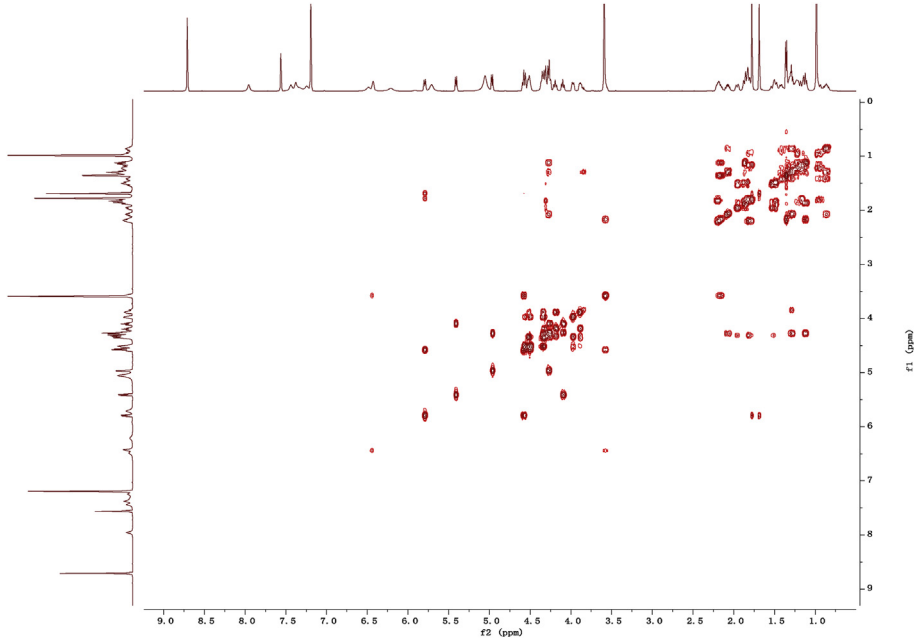


Fig. 41. 2D COSY NMR spectrum in pyridine-*d*₅ of 6.

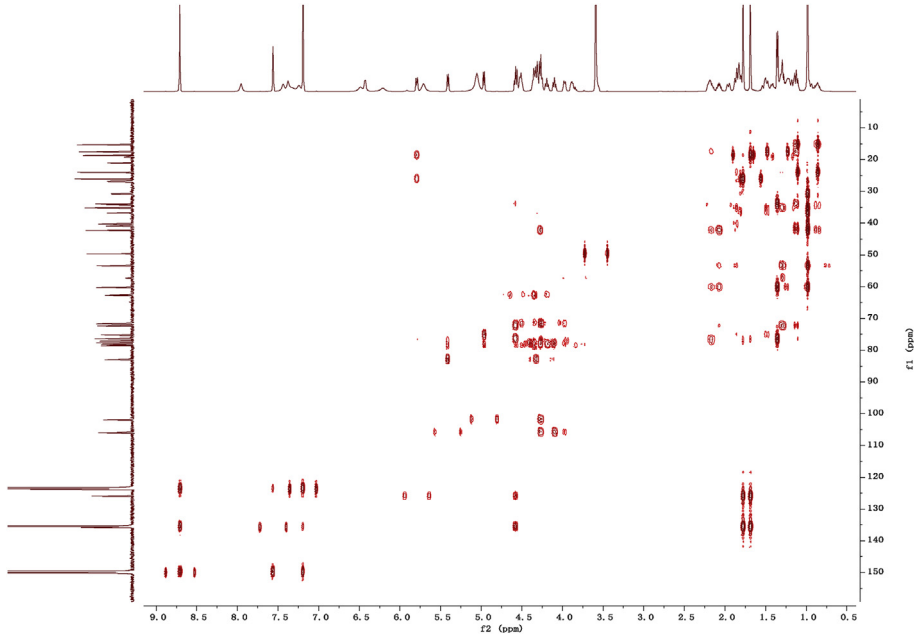


Fig. 42. 2D HMBC NMR spectrum in pyridine-*d*₅ of 6.

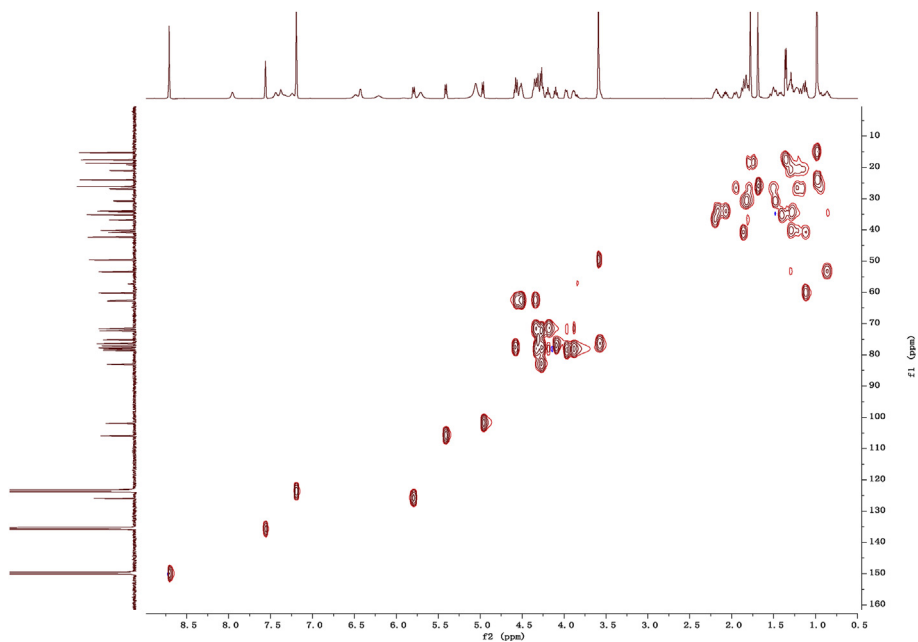


Fig. 43. 2D HSQC NMR spectrum in pyridine-*d*₅ of 6.

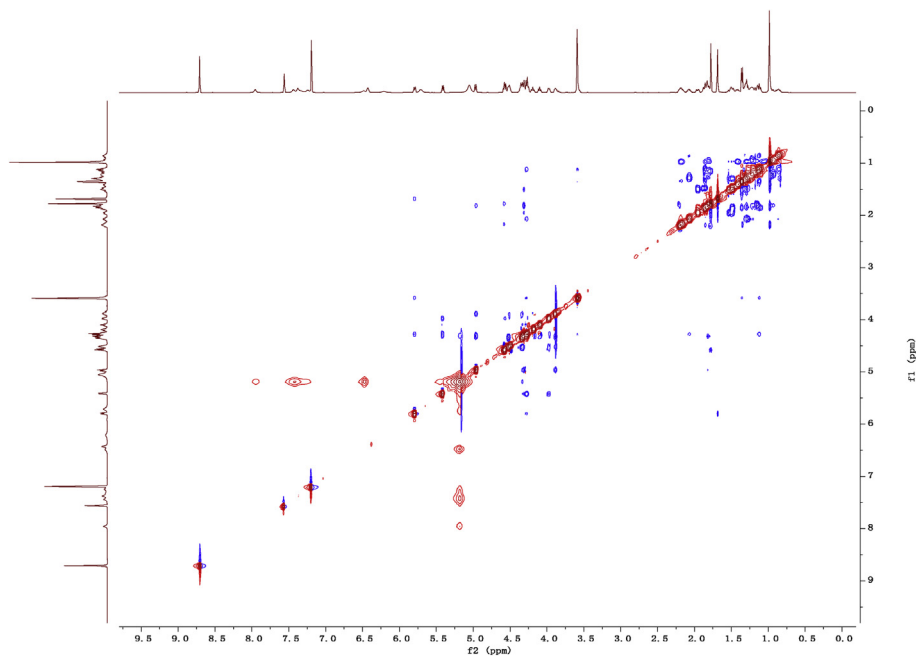


Fig. 44. 2D ROESY NMR spectrum in pyridine-*d*₅ of 6.

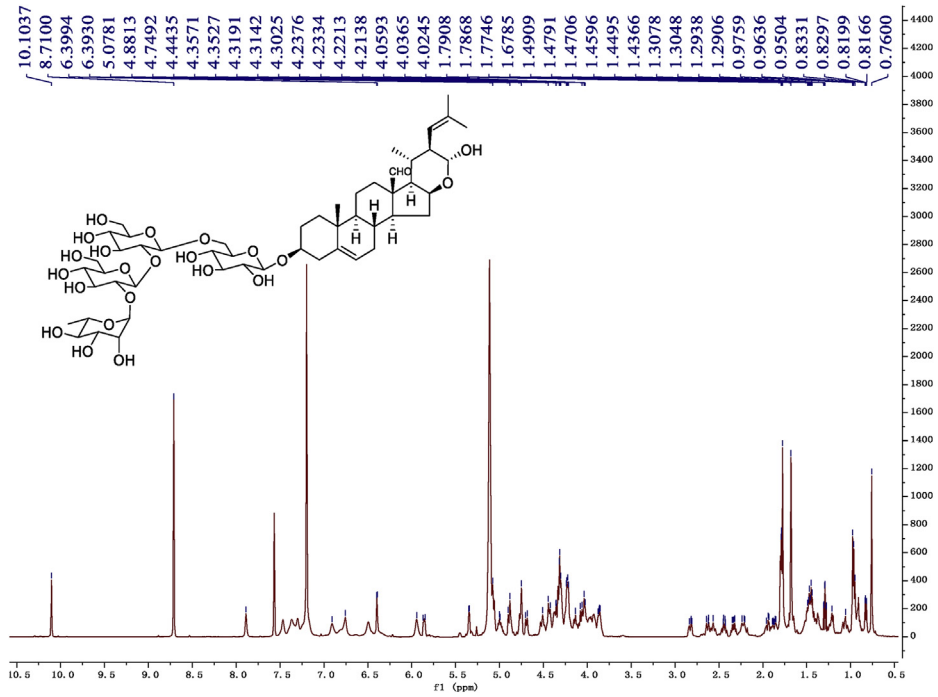


Fig. 45. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 7.

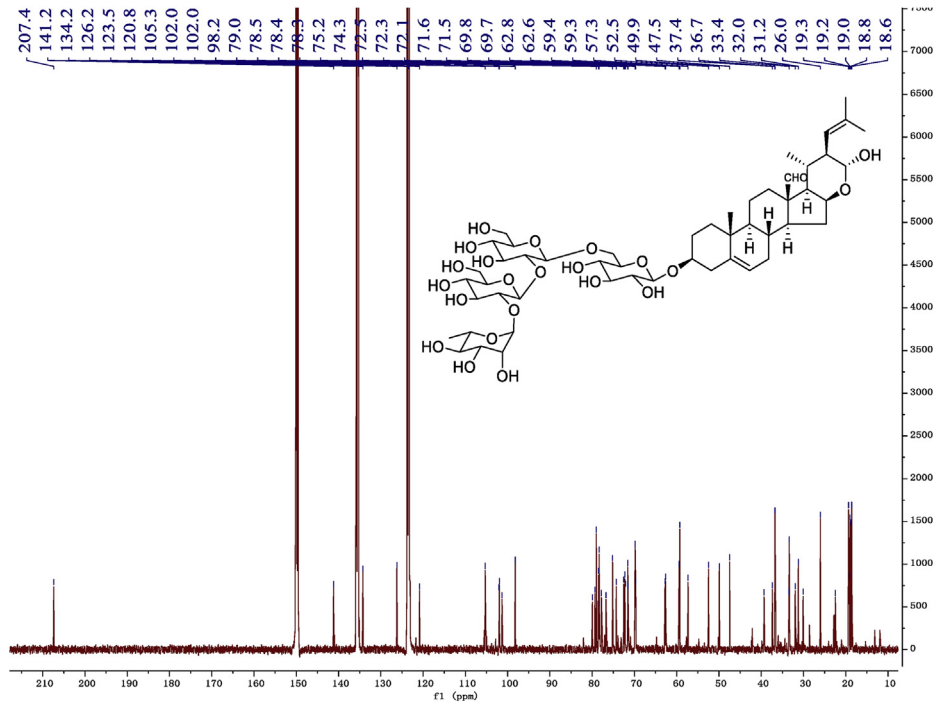


Fig. 46. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 7.

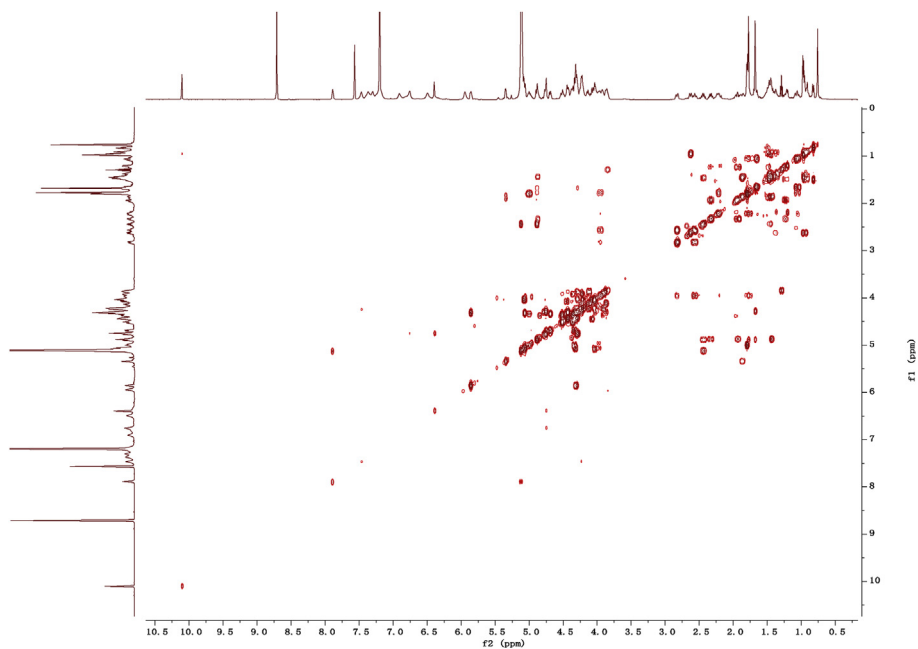


Fig. 47. 2D COSY NMR spectrum in pyridine-*d*₅ of 7.

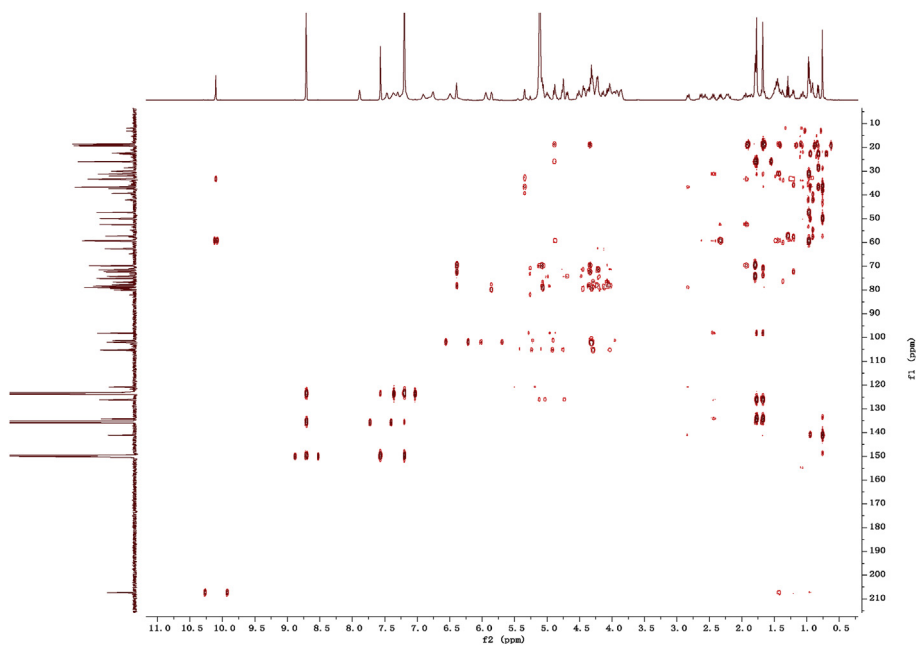


Fig. 48. 2D HMBC NMR spectrum in pyridine-*d*₅ of 7.

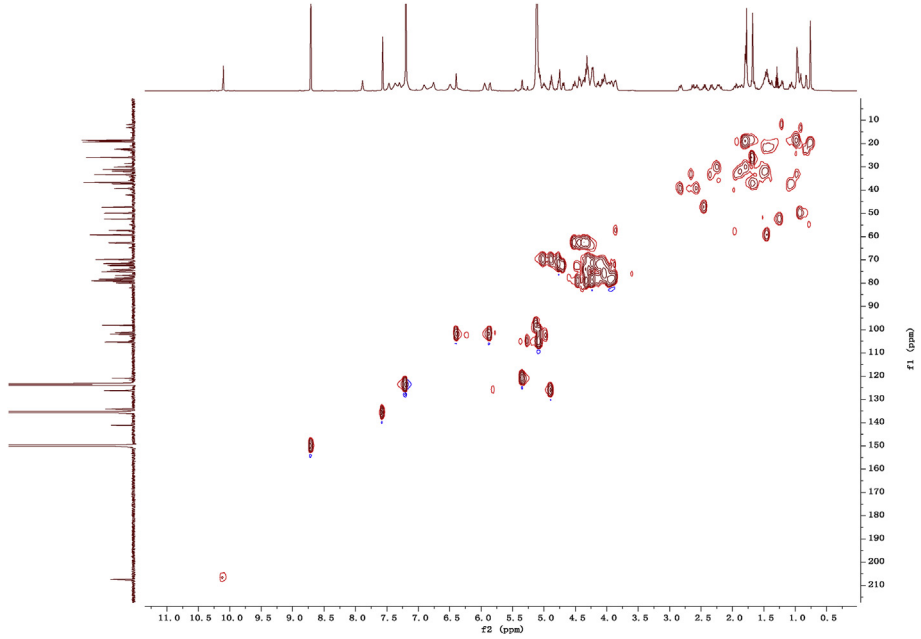


Fig. 49. 2D HSQC NMR spectrum in pyridine- d_5 of 7.

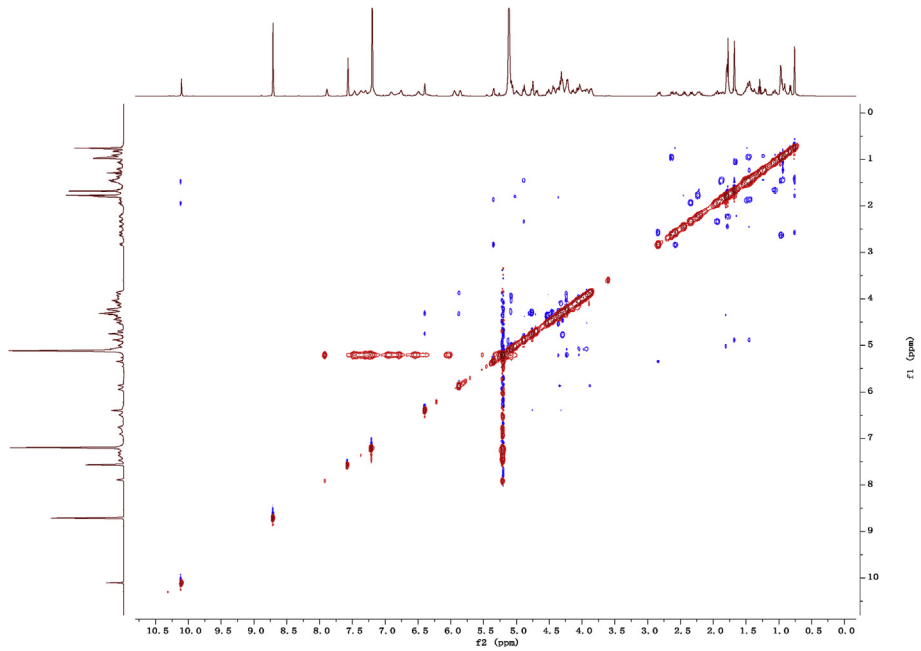


Fig. 50. 2D ROESY NMR spectrum in pyridine- d_5 of 7.

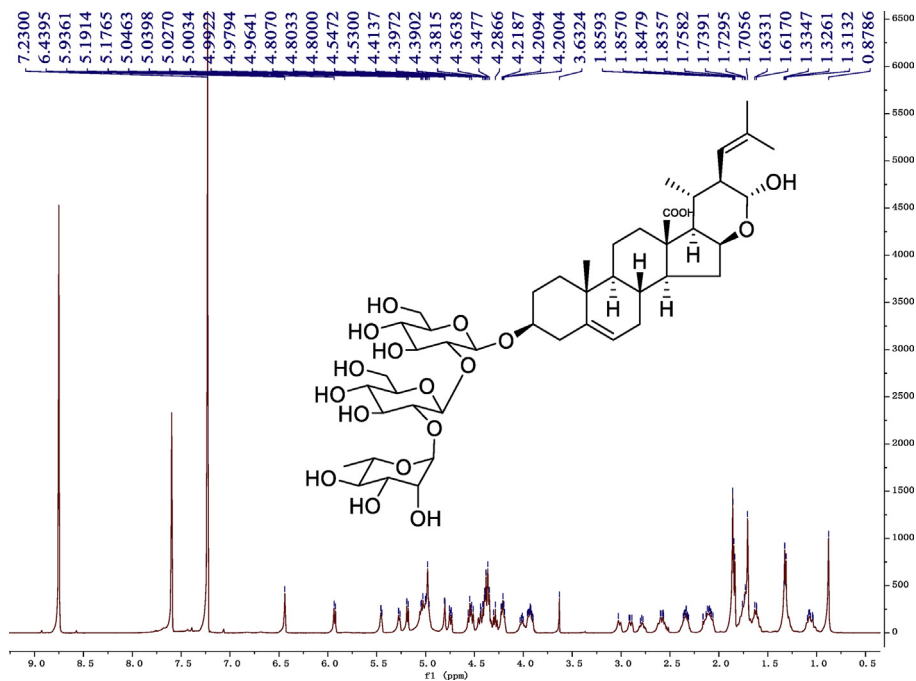


Fig. 51. $^1\text{H-NMR}$ (500 MHz) spectrum in pyridine- d_5 of 8.

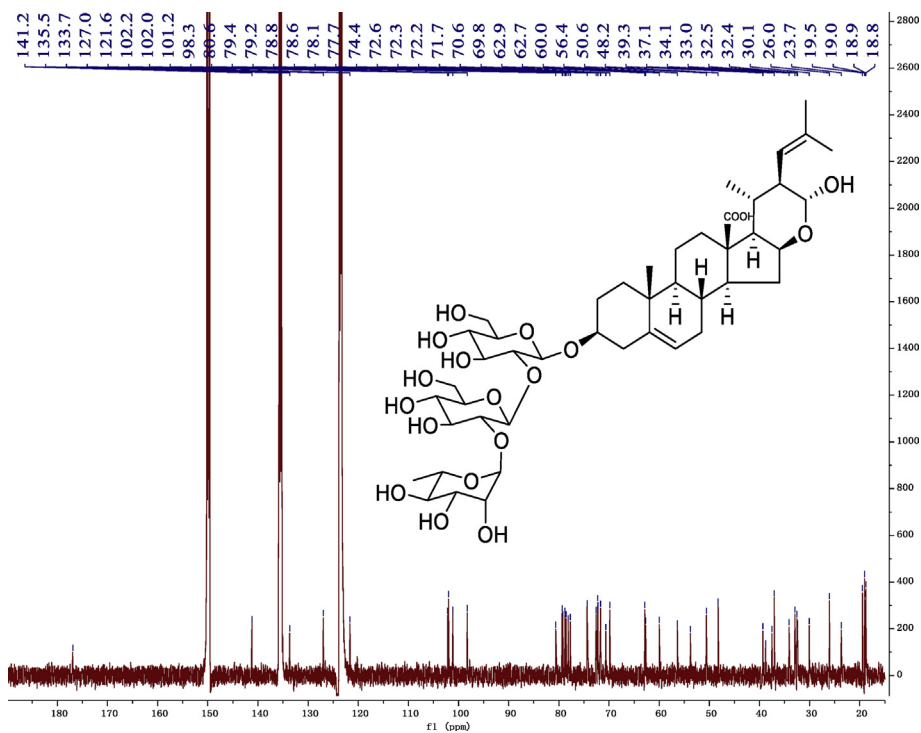


Fig. 52. $^{13}\text{C-NMR}$ (125 MHz) spectrum in pyridine- d_5 of 8.

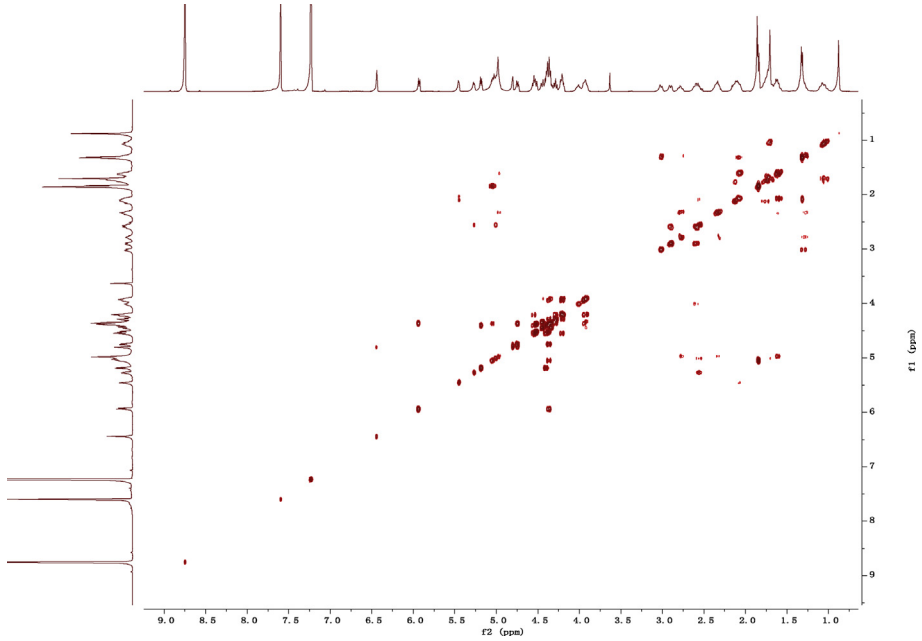


Fig. 53. 2D COSY NMR spectrum in pyridine-*d*₅ of 8.

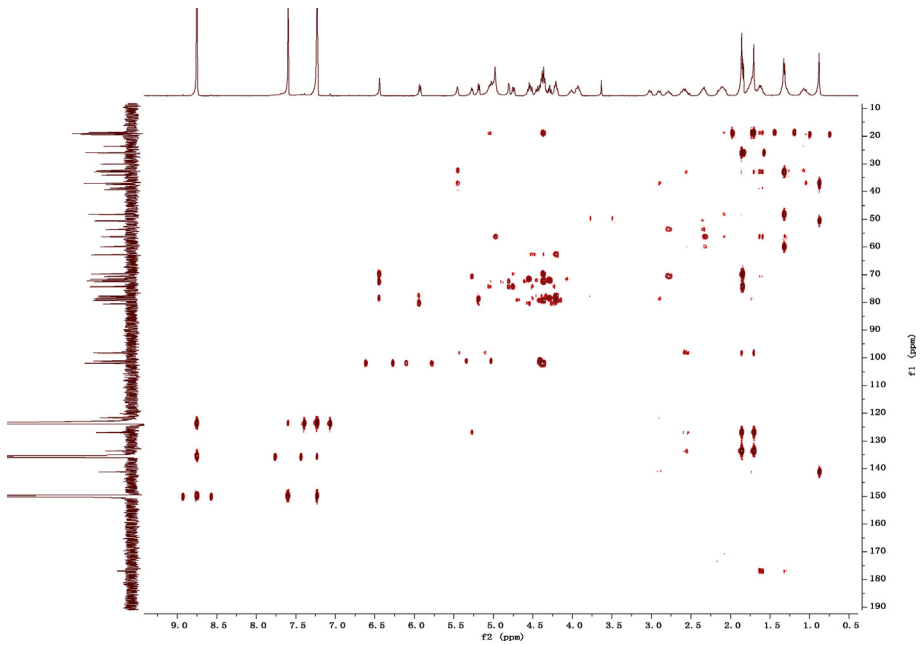


Fig. 54. 2D HMBC NMR spectrum in pyridine-*d*₅ of 8.

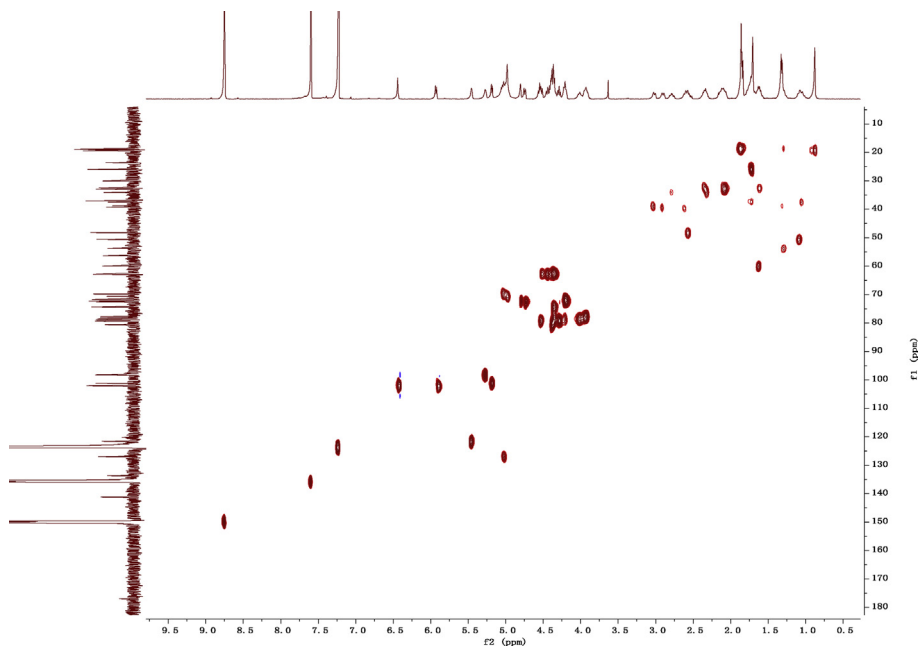


Fig. 55. 2D HSQC NMR spectrum in pyridine- d_5 of **8**.

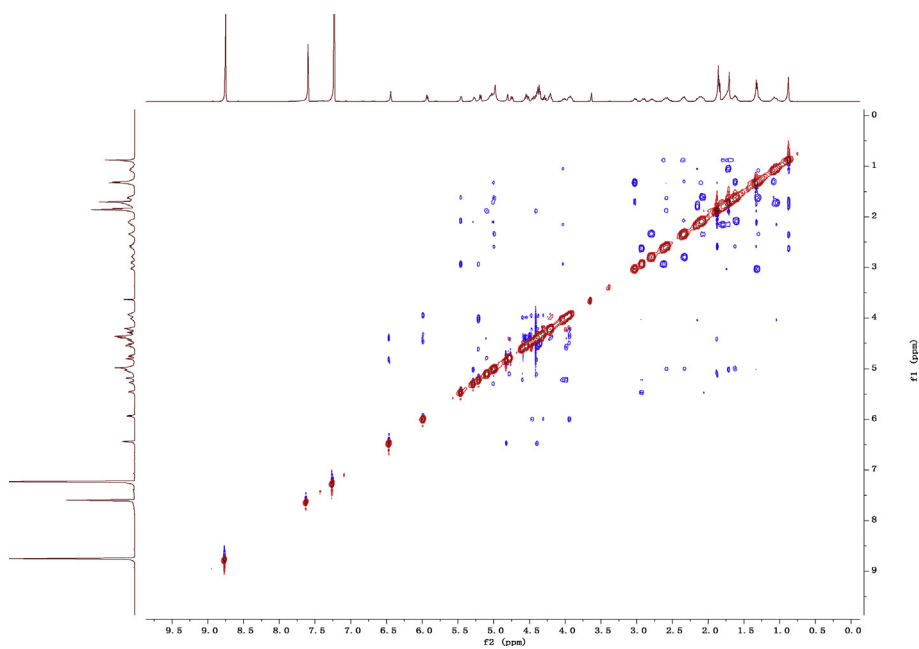


Fig. 56. 2D ROESY NMR spectrum in pyridine- d_5 of **8**.

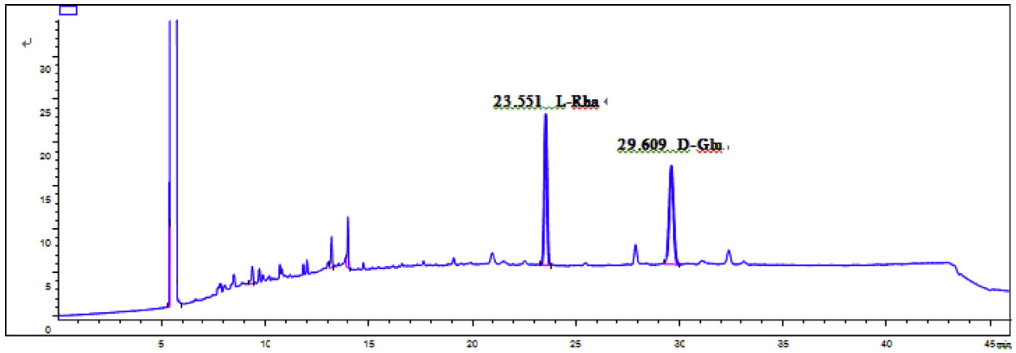


Fig. 57. GC analysis spectra of 1.

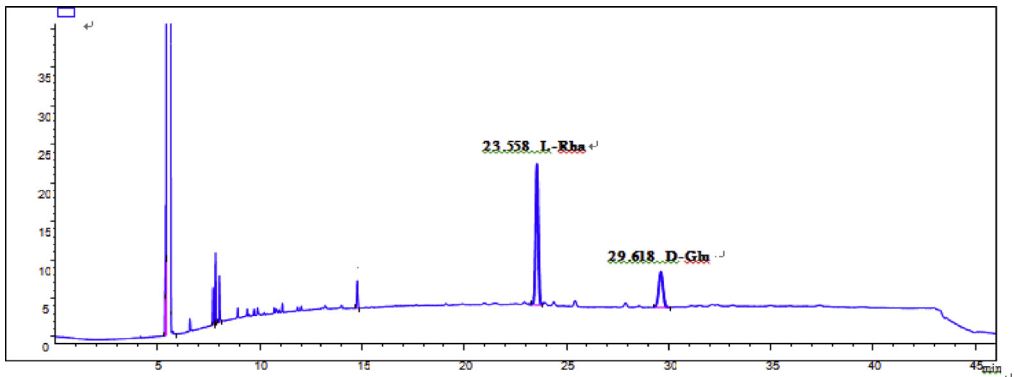


Fig. 58. GC analysis spectra of 2.

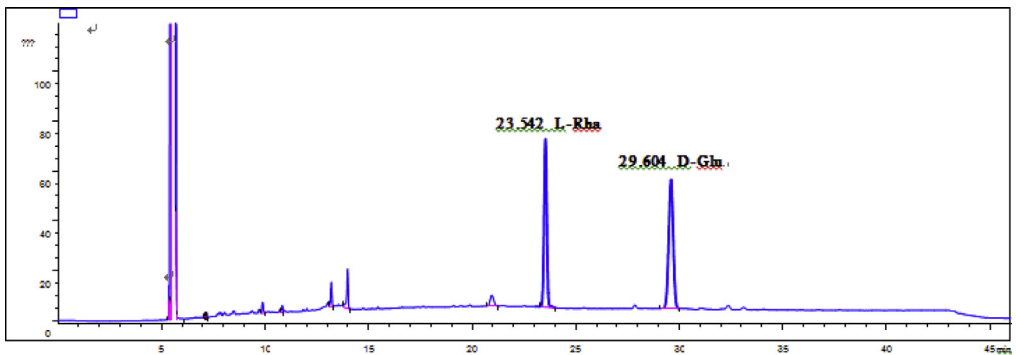


Fig. 59. GC analysis spectra of 3.

2.2. NMR analysis

Cholestane glycosides were dissolved in C5D5N, respectively. Next, NMR spectra of these glycosides were acquired using a Bruker AV-III-500 spectrometer or a Bruker-600 NMR spectrometer for ^1H -NMR (500MHz or 600MHz) or for ^{13}C -NMR (125MHz or 150MHz) at 25 °C.

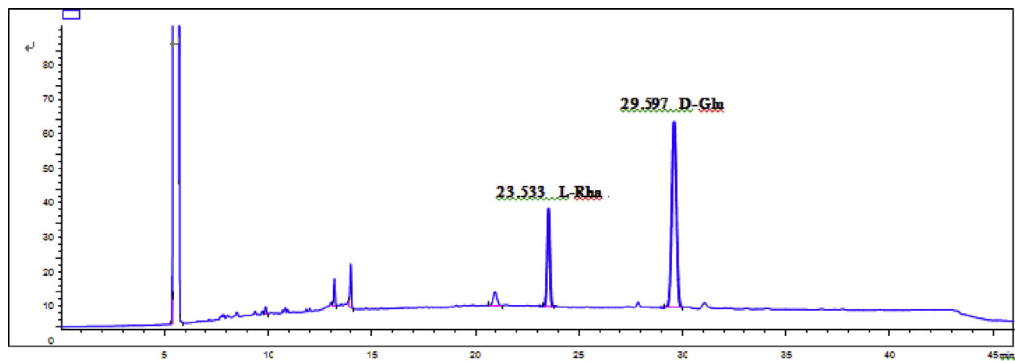


Fig. 60. GC analysis spectra of 4.

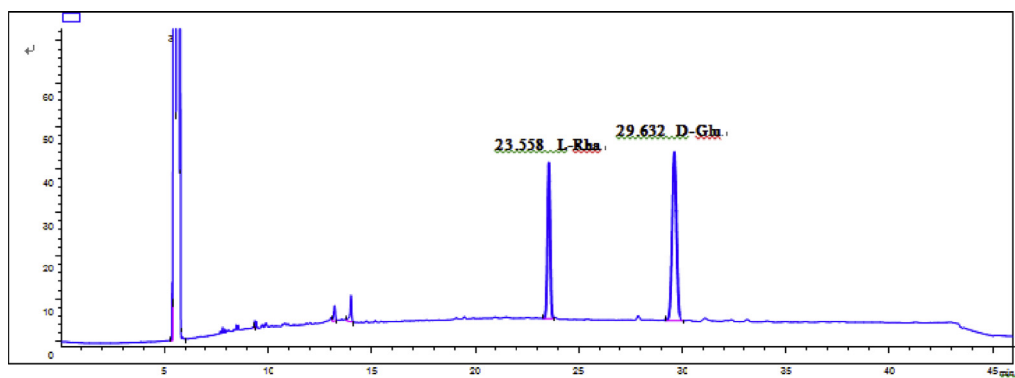


Fig. 61. GC analysis spectra of 5.

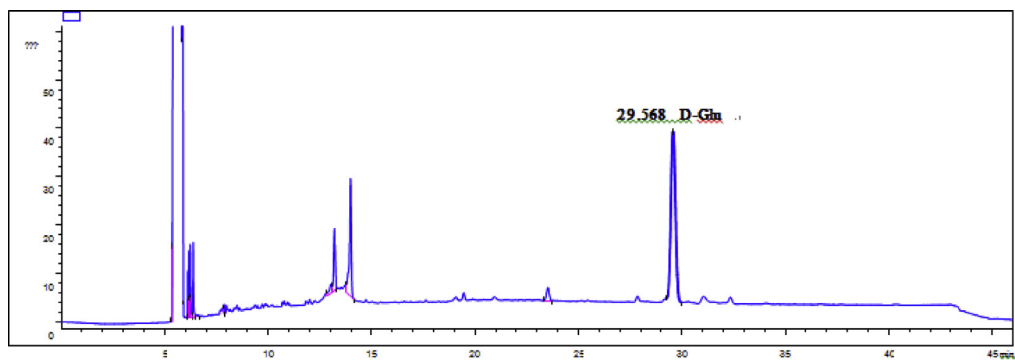


Fig. 62. GC analysis spectra of 6.

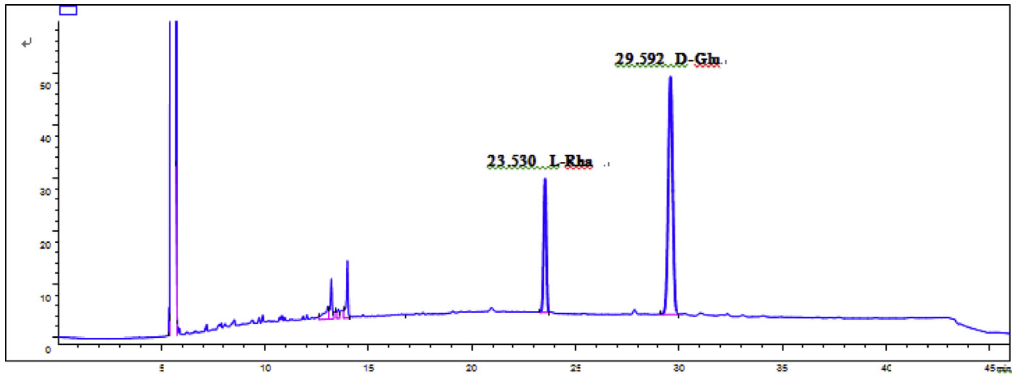


Fig. 63. GC analysis spectra of 7.

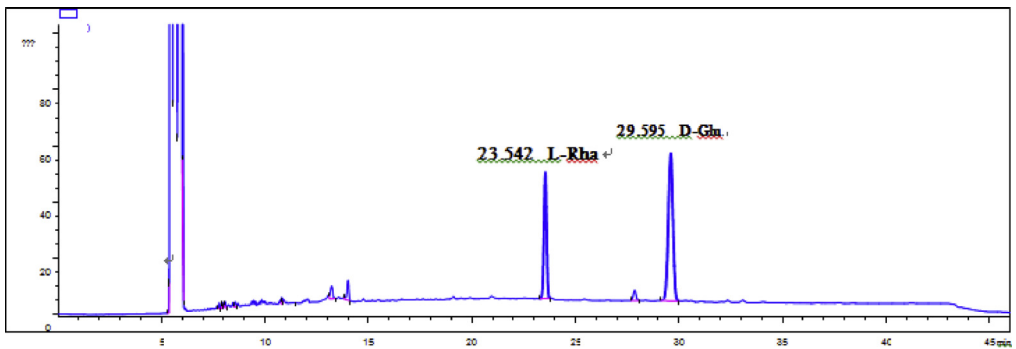


Fig. 64. GC analysis spectra of 8.

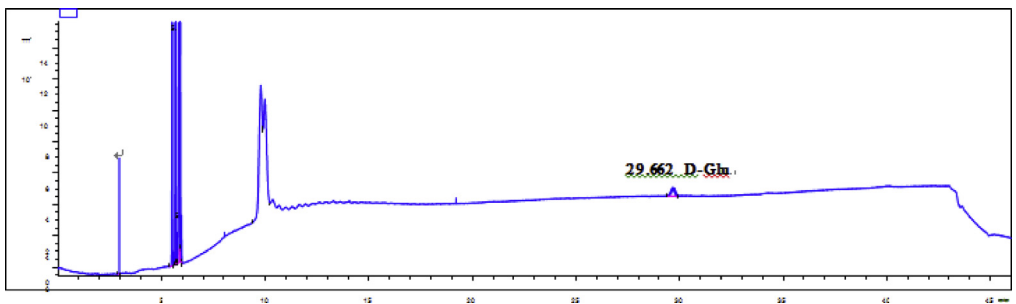


Fig. 65. GC analysis spectra of D-Glucose.

2.3. GC analysis

The absolute configuration determination of sugar moieties was achieved by GC analysis in Agilent 7890 system equipped with a flame ionization detector (FID) for analysis. A non-polar HP-5 (60 m × 0.25 mm, with a 0.25 μm film) capillary column was applied to separate compounds.

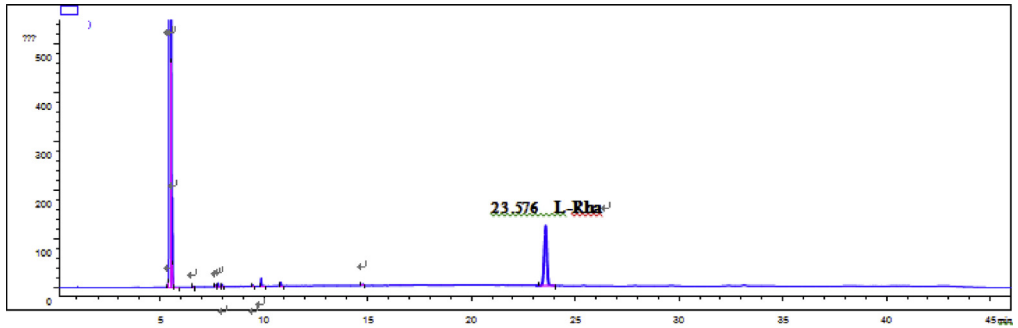


Fig. 66. GC analysis spectra of L-rhamnose.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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