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Data Article

^{1}H and ^{13}C-NMR data for novel meroterpenoids isolated from *Arnebia euchroma* (Royle) Johnst

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ABSTRACT

The data presented in this article are associated with the research article entitled "**Meroterpenoids isolated from *Arnebia euchroma* (Royle) Johnst. and their cytotoxic activity in human hepatocellular carcinoma cells**" [1]. The aim of this data was to provide the 1D-NMR spectrum of novel meroterpenoids from *Arnebia euchroma* (Royle) Johnst.

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Specifications table

Subject area	*chemistry*
More specific subject area	*Natural products research*
Type of data	*Figure, Table*
How data was acquired	*^{1}H and ^{13}C-NMR of meroterpenoids*
Data format	*Filtered and Analyzed*
Experimental factors	*First, the Sample were isolated from dichloromethane fraction of the roots of A. Euchroma extracts. Then the samole were dissolved in* DMSO-d_6 *or* CD_3Cl *before NMR test.*
Experimental features	*Nuclear magnetic resonance (NMR) spectra data of meroterpenoids from the roots of A. Euchroma were recorded on a Bruker DPX-400 spectrometer using standard Bruker pulse programs (Bruker, Karlsruhe, Germany). Chemical shifts were shown as δ-values with reference to tetramethylsilane (TMS) as an internal standard.*
Data source location	The herbarium of Key Laboratory for New Drug Research of TCM, Research institute of Tsinghua University in Shenzhen, Shenzhen, China.
Data accessibility	*Data is with this article*
Related research article	Yang Wang, Yuzhen Zhu, Lingyun Xiao, Lanlan Ge, Xin Wu, Weigang Wu, Haoqiang Wan, Keda Zhang, Jiemei L, Boping Zhou, Jun Tian, Xiaobin Zeng. Meroterpenoids isolated from *Arnebia euchroma* (Royle) Johnst. and their cytotoxic activity in human hepatocellular carcinoma cells.Fitoerapia. 131 (2018) 236−244.

Value of the data

- NMR data of meroterpenoids is useful for elucidating their chemical structures.
- NMR data of meroterpenoids is useful for elucidating their chemical analogues.
- This information will allow comparisons across different meroterpinoids from algal species or othernatural sources.

1. Data

In our previous study [1], six previously undescribed naturally occurring meroterpenoids (**2**, **5**–**9**) together with seven known meroterpenoids (**1**, **3**, **4**, **10**–**13**) were isolated from the root plant of *Arnebia euchroma*. The NMR data of meroterpenoids **1**–**5** and **8** suggest they were structure analogue, which contain a bridgehead double bond, which has recently attracted substantial interest in the natural product isolation community in terms of Bredt's law. Six previously undescribed naturally occurring meroterpenoids (**2**, **5**–**9**) were first isolated and identified from *Arnebia euchroma* (Royle) Johnst.

2. Experimental design, materials, and methods

2.1. Study area description

Arnebia euchroma (Royle) Jonst. (family Boraginaceae) is a small genus of annual or perennial herbs, distributed in Asia and the drier regions of Northern Africa [2]. *A. Euchroma* is a traditional Chinese herbal medicine (TCM) recorded in the Pharmacopoeia of China and has been extensively used in China and other countries for the treatment of various diseases [3]. In the current study, a further phytochemical investigation on the $CHCl_3$ extract of the roots of *A. euchroma* led to the isolation and characterization of six (**2**, **5**–**9**) previously undescribed and seven (**1**, **3**–**4**, **10**–**13**) known meroterpenoids. Herein, their structure characterization of these meroterpenoids are identified by various chromatography methods including NMR and MS spectrum.

2.2. Sample collection

The roots of *Arnfebia euchroma* were purchased in Haozhou city, Anhui Province, China.

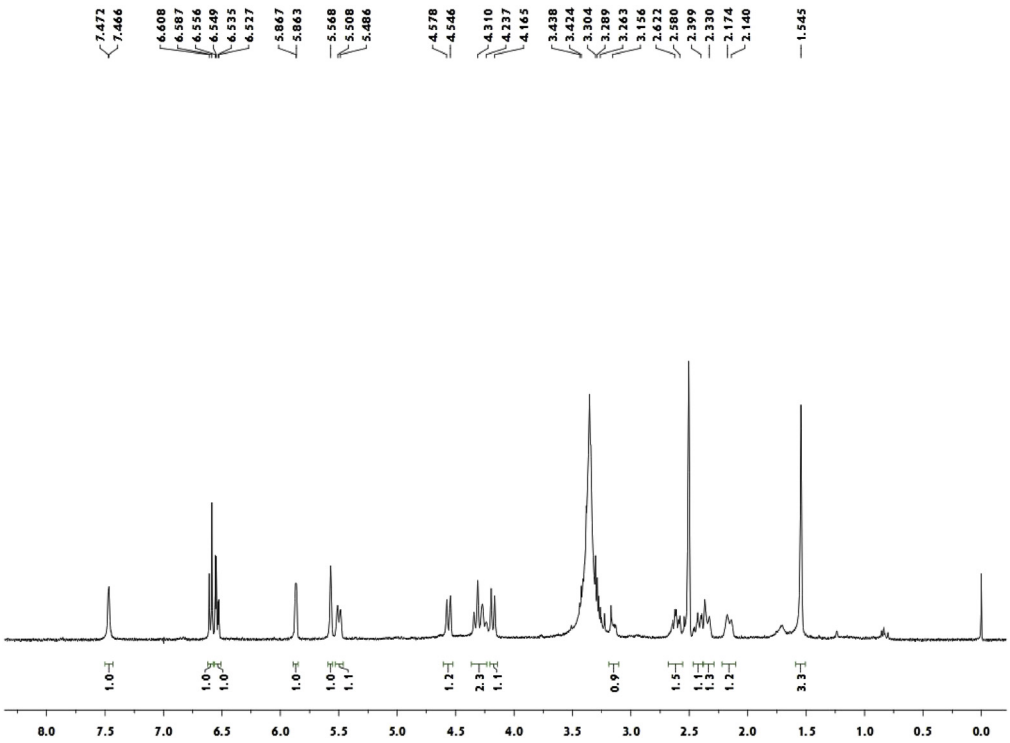

Fig. 1. ^{1}H-NMR spectrum of meroterpenoid **2**.

2.3. ^{1}H and ^{13}C NMR *spectrum* of meroterpenoids (**2**, **5**–**9**)

The dichloromethane-H_2O (1: 1, v/v) extract from the roots of *A. Euchroma* was successively subjected to column chromatography over silica gel, ODS or Sephadex LH-20, and preparative HPLC to afford six previously undescribed meroterpenoids (**2**, **5**–**9**) together with seven known meroterpenoids (**1**, **3**–**4**, **10**–**13**). The known compounds were determined to be 9,17-epoxyarnebinol (**1**) [4], arnebinol B (**3**) [5], arnebinone B (**4**) [6], arnebifuranone (**10**) [7], shikonofuran A (**11**) [8], shikonofuran E (**12**) [8], and arnebinone (**13**) [9], by comparison of their spectral data with literature values.

2.3.1. *Meroterpenoid **2***

Colorless crystals (MeOH–CH_2Cl_2); $[\alpha]_D^{20}$ − 513.4 (c 0.15, CH_2Cl_2); ^{1}H and ^{13}C NMR spectrum see Figs. 1 and 2.

2.3.2. *Meroterpenoid **5***

Red crystal (MeOH–CH_2Cl_2); $[\alpha]_D^{20}$ + 134.3 (c 0.10, MeOH); ^{1}H and ^{13}C NMR spectrum see Figs. 3 and 4.

2.3.3. *Meroterpenoid **6***

White amorphous powder; $[\alpha]_D^{20}$ − 21.4 (c 0.11, MeOH); ^{1}H and ^{13}C NMR spectrum see Figs. 5 and 6.

2.3.4. *Meroterpenoid **7***

Yellow amorphous powder; $[\alpha]_D^{20}$ + 196.7 (c 0.10, MeOH); ^{1}H NMR and ^{13}C NMR spectroscopic data of meroterpenoid **7** see Figs 7 and 8.

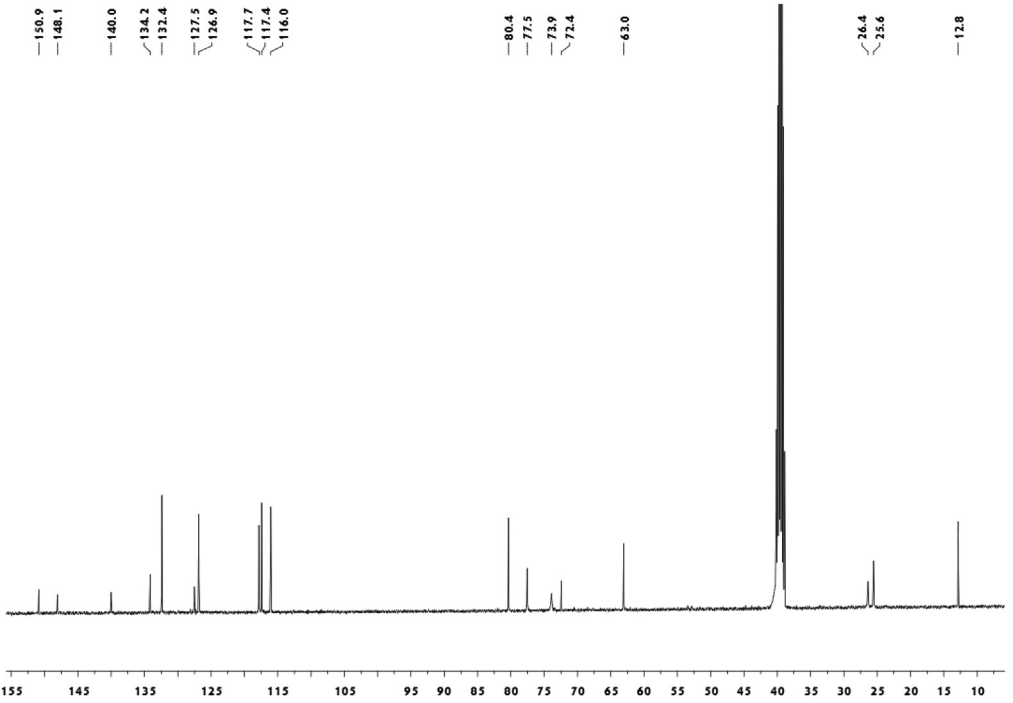

Fig. 2. ^{13}C-NMR spectrum of meroterpenoid **2**.

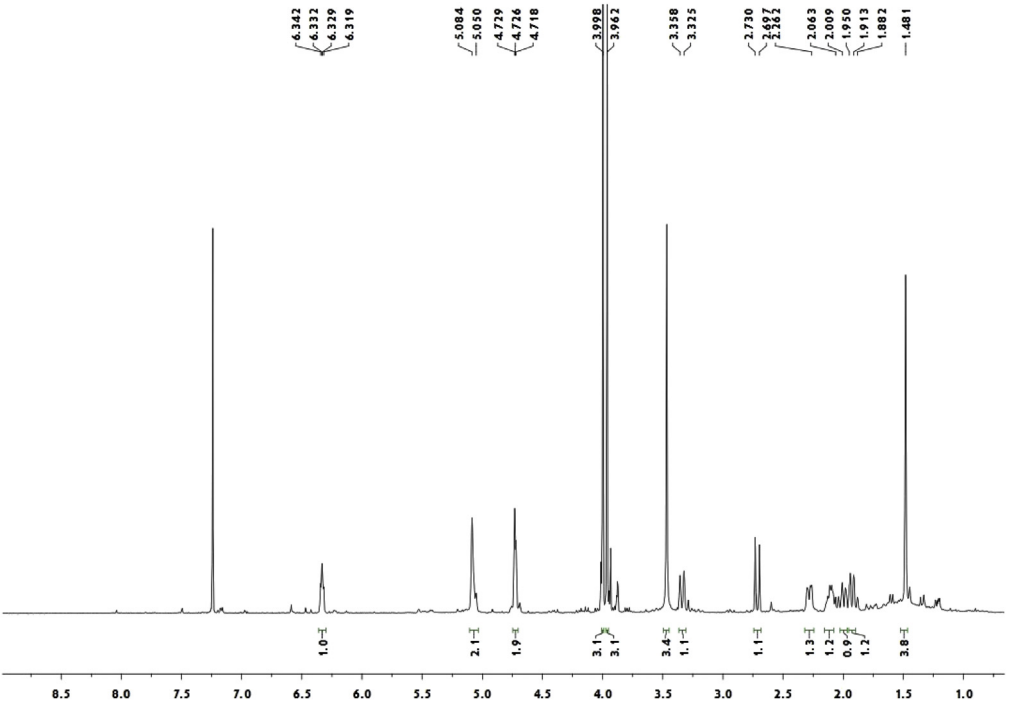

Fig. 3. ^{1}H-NMR spectrum of meroterpenoid **5**.

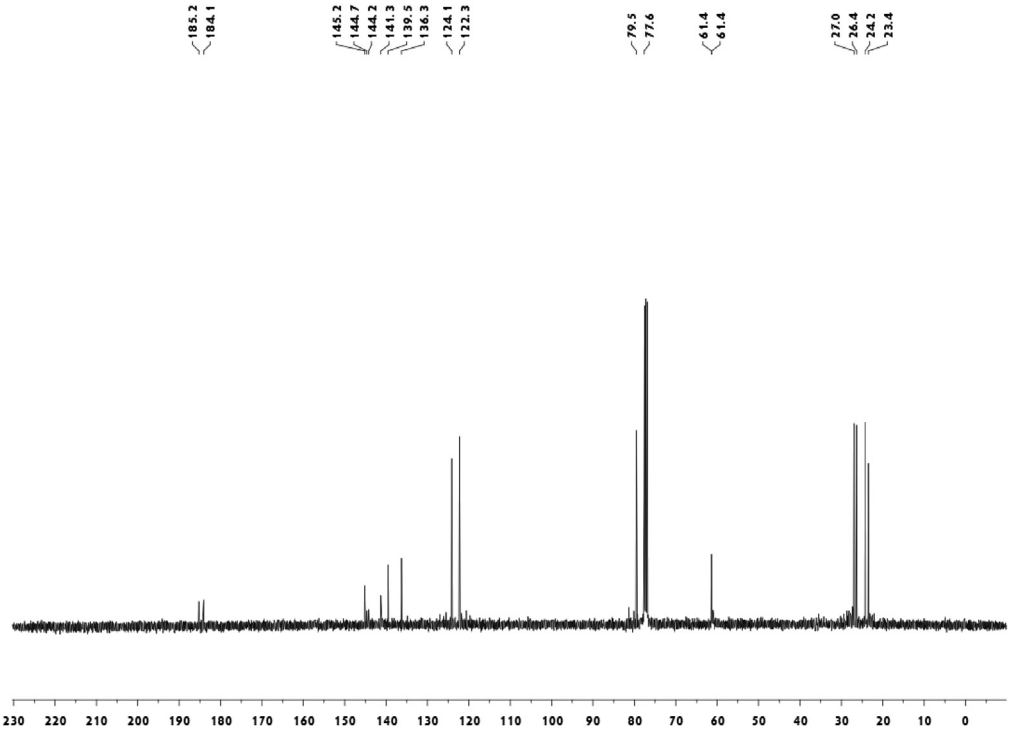

Fig. 4. ^{13}C-NMR spectrum of meroterpenoid **5**.

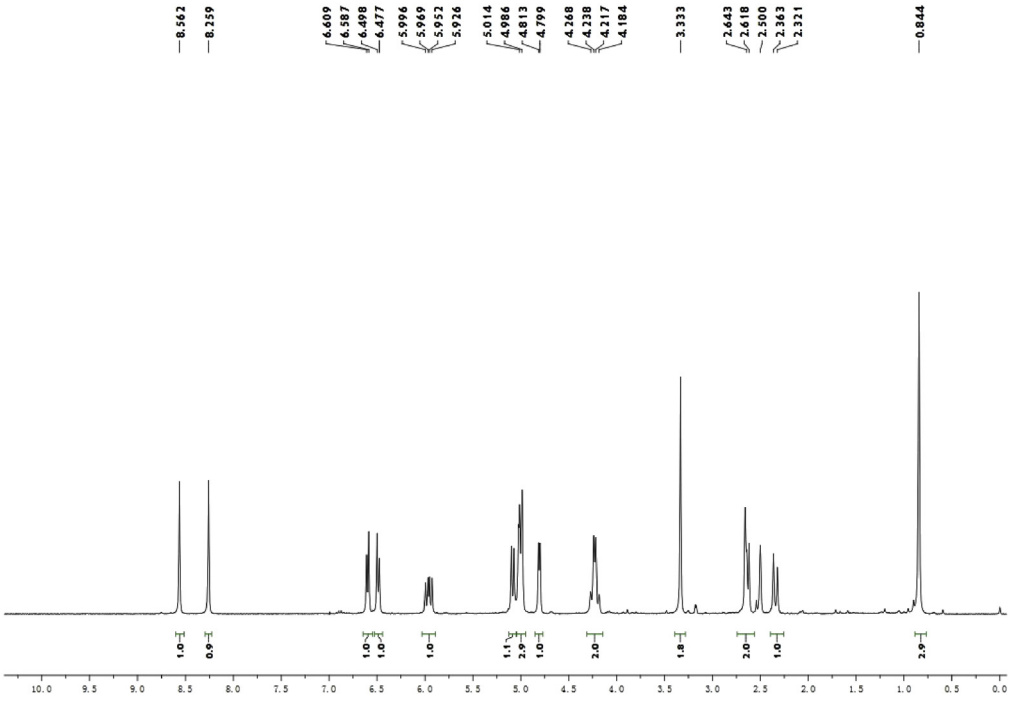

Fig. 5. ^{1}H-NMR spectrum of meroterpenoid **6**.

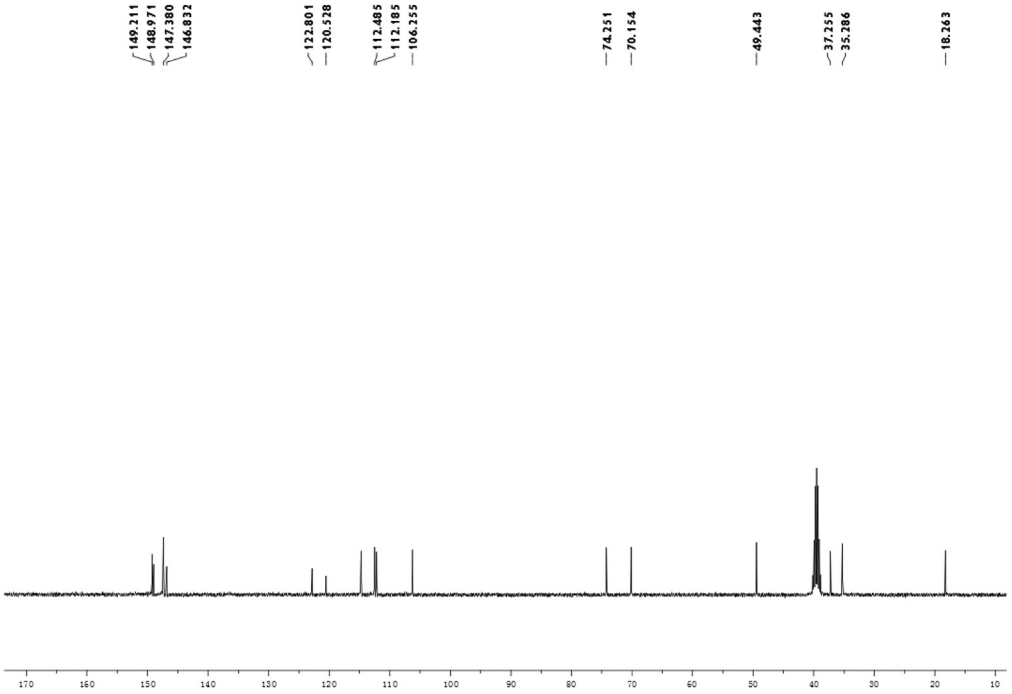

Fig. 6. ^{13}C-NMR spectrum of meroterpenoid **6**.

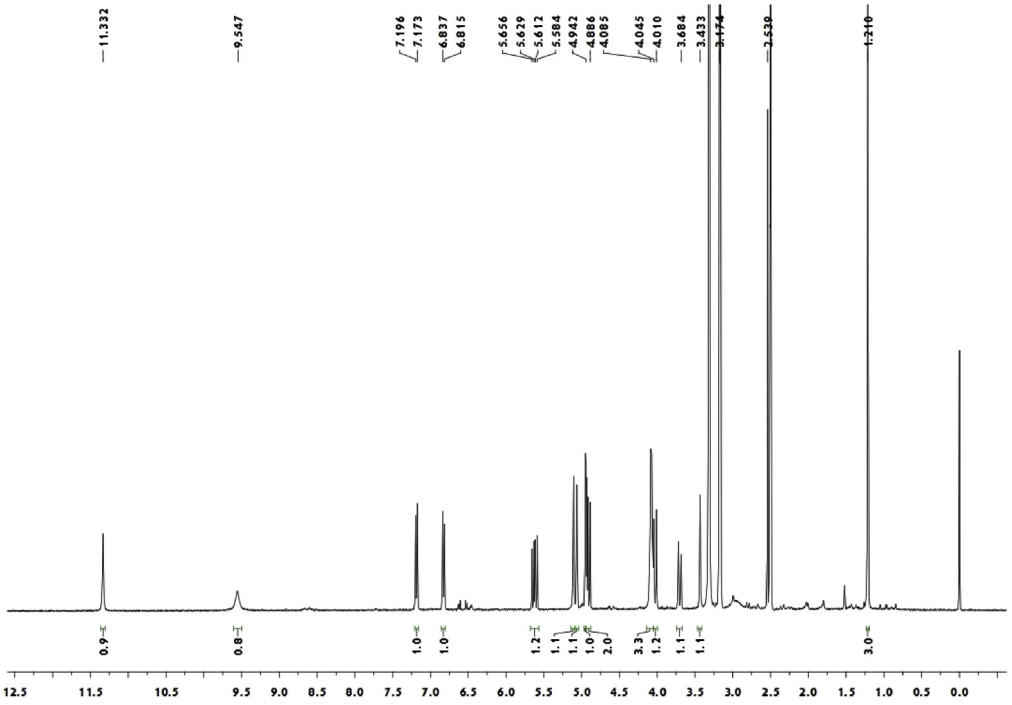

Fig. 7. ^{1}H-NMR spectrum of meroterpenoid **7**.

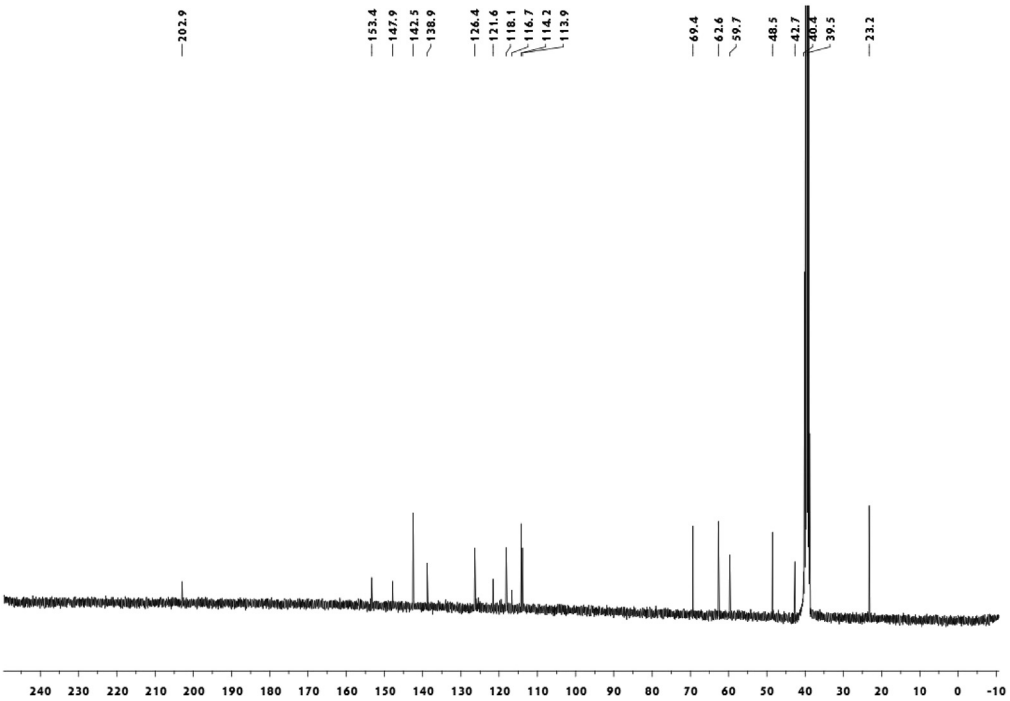

Fig. 8. ^{13}C-NMR spectrum of meroterpenoid **7**.

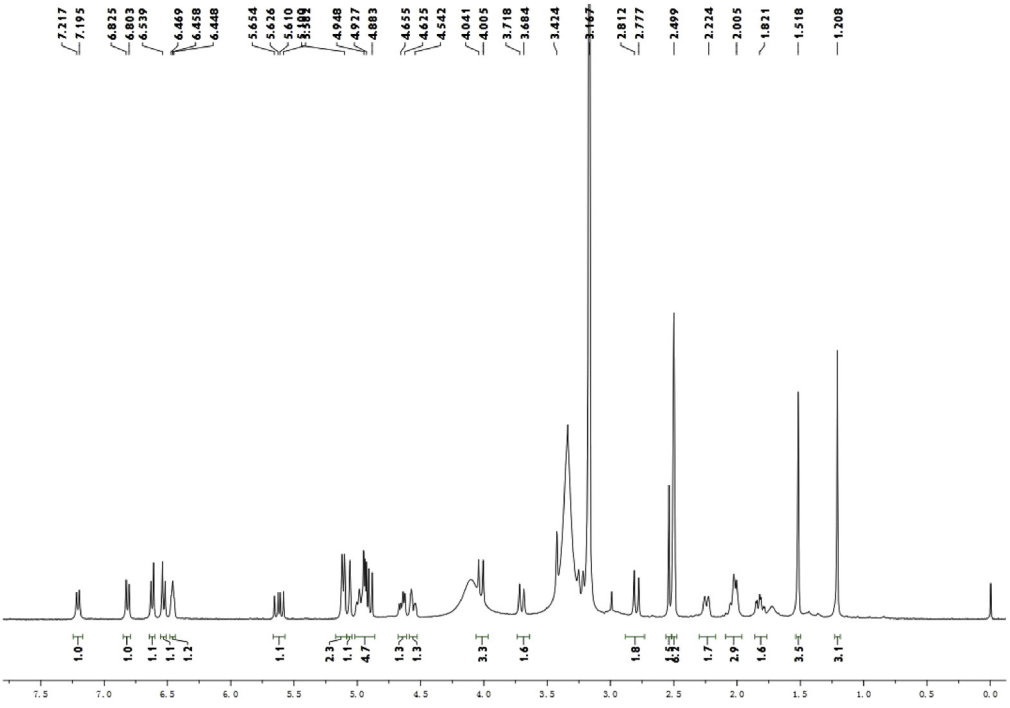

Fig. 9. ^{1}H-NMR spectrum of meroterpenoid **8**.

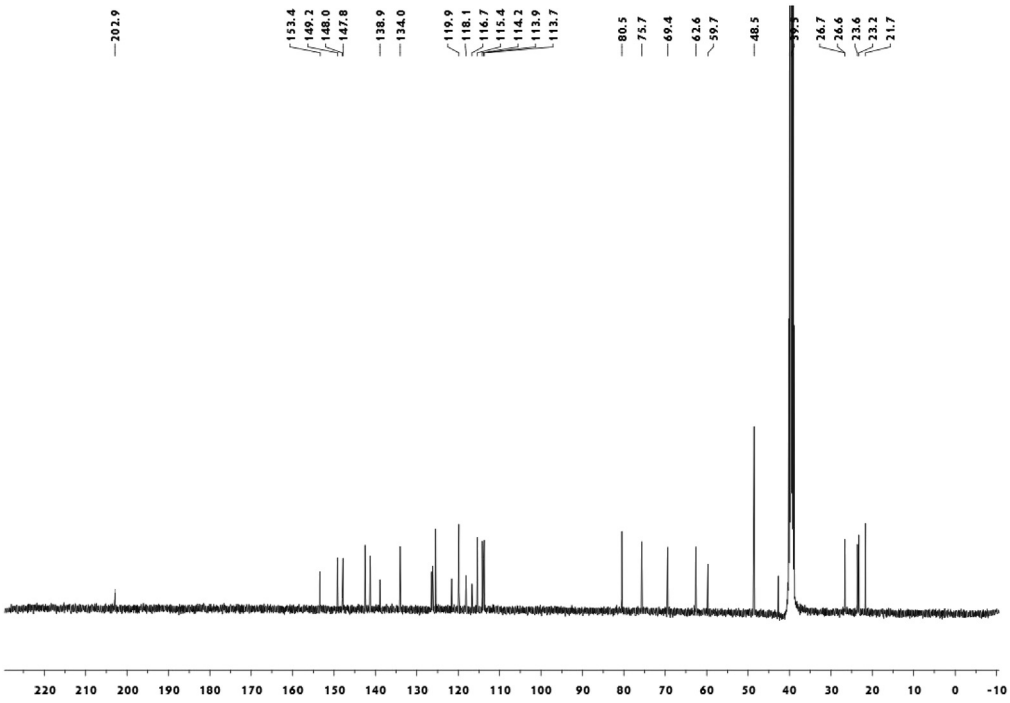

Fig. 10. ^{13}C-NMR spectrum of meroterpenoid **8**.

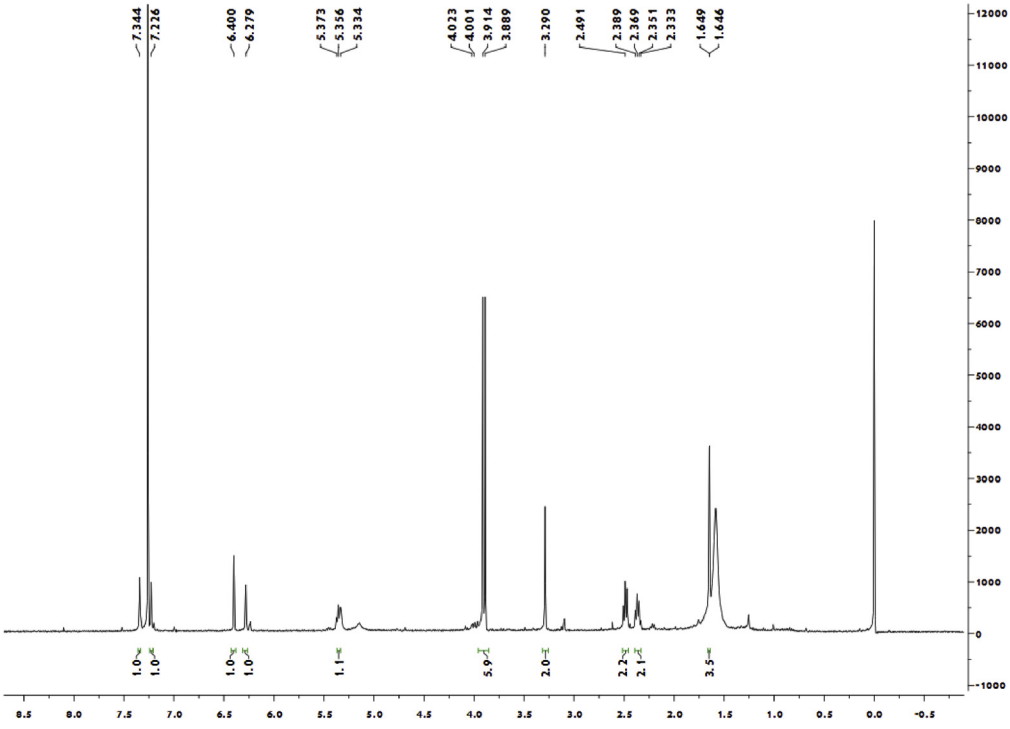

Fig. 11. ^{1}H-NMR spectrum of meroterpenoid **9**.

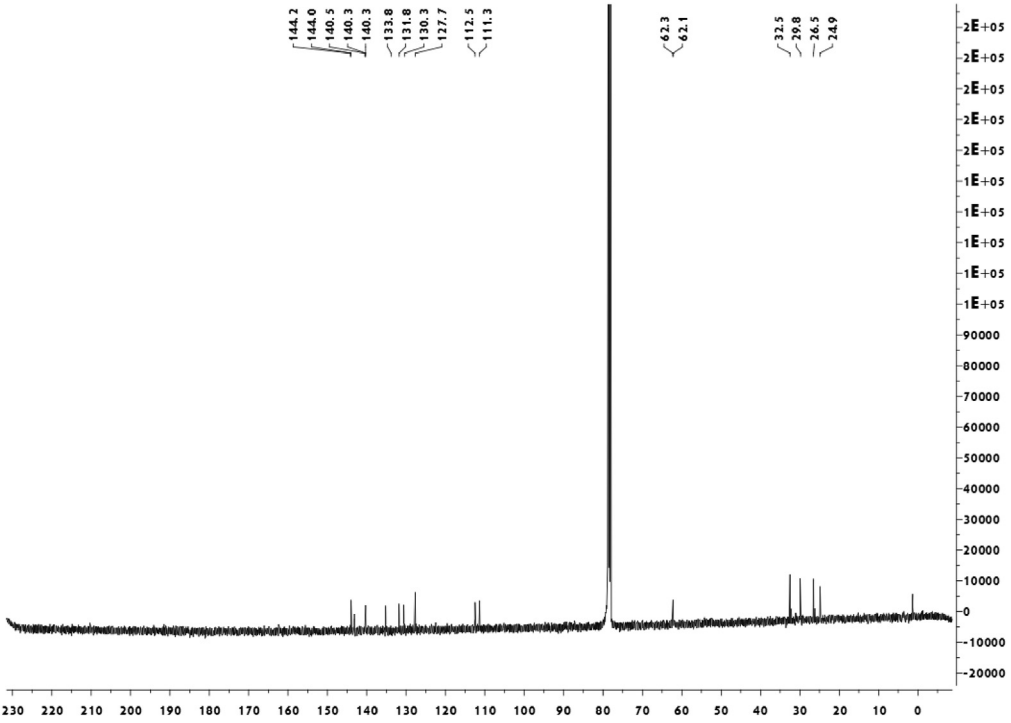

Fig. 12. ^{13}C-NMR spectrum of meroterpenoid **9**.

*2.3.5. Meroterpenoid **8***

Red amorphous powder; $[\alpha]_D^{20}$ + 432.1 (c 0.10, MeOH); ^{1}H NMR and ^{13}C NMR spectroscopic data of meroterpenoid **8** see Figs. 9 and 10.

*2.3.6. Meroterpenoid **9***

Red amorphous powder; ^{1}H NMR and ^{13}C NMR spectroscopic data of meroterpenoid **9** see Figs. 11 and 12.

Acknowledgments

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Transparency document

Transparency document associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2019.103908.

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