Data in brief 27 (2019) 104780

Contents lists available at ScienceDirect

Data in brief

journal homepage: www.elsevier.com/locate/dib

Data Article

NMR and ESIMS data for bisabolane-type sesquiterpenoids

Shinji Ohta [a, *], Yasunori Yuasa [a], Nobuwa Aoki [b], Emi Ohta [a], Tatsuo Nehira [a], Hisashi Ômura [a], Mylene M. Uy [c]

[a] Graduate School of Integrated Sciences for Life, Hiroshima University, 1-7-1 Kagamiyama, Higashi-Hiroshima, 739-8521, Japan
[b] Nagahama Institute of Bio-Science and Technology, 1266 Tamura-cho, Nagahama, Shiga, 526-0829, Japan
[c] Department of Chemistry, Mindanao State University-Iligan Institute of Technology, Iligan City, 9200, Philippines

ARTICLE INFO

Article history:
Received 22 August 2019
Received in revised form 30 October 2019
Accepted 1 November 2019
Available online 11 November 2019

Keywords:
Angelica keiskei
Seed
Bisabolane sesquiterpenoid
NMR
ESIMS

ABSTRACT

The data presented here are related to the research paper entitled "Norbisabolane and bisabolane sesquiterpenoids from the seeds of *Angelica keiskei*" [1]. In this data article, we provide 1D and 2D nuclear magnetic resonance (NMR) spectroscopy and electrospray ionization mass spectrometry (ESIMS) data of three undescribed norbisabolane- and bisabolene-type sesquiterpenoids, ashitabaol B-D isolated from the seeds of *Angelica keiskei*.

© 2019 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

1. Data

The data set presented in this article focuses on characterization of the norbisabolane- and bisabolane-type sesquiterpenoids described in Ref. [1]. The article provides the information on the spectroscopic data of the sesquiterpenoids **1**–**3** isolated from the seeds of *Angelica keiskei* (Fig. 1). The ^{1}H NMR spectra of **1**–**3** are shown in Figs. 2a, 3a and 4a, respectively. The ^{13}C NMR and DEPT spectra of

DOI of original article: https://doi.org/10.1016/j.phytol.2019.08.006.
* Corresponding author.
E-mail address: ohta@hiroshima-u.ac.jp (S. Ohta).

https://doi.org/10.1016/j.dib.2019.104780
2352-3409/© 2019 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

Specifications Table

Subject area	*chemistry*
More specific subject area	*natural products*
Type of data	*Figure*
How data was acquired	*NMR spectroscopy: JEOL A400; ESIMS: Shimadzu LCMS-IT-TOF and Thermo Fisher Scientific LTQ Orbitrap XL.*
Data format	*Raw and analyzed*
Experimental factors	*The undescribed sesquiterpenoids were purified by column chromatography.*
Experimental features	*The isolated compounds were characterized by ESIMS and NMR spectroscopy*
Data source location	*Higashi-Hiroshima, Japan*
Data accessibility	*Data are available with this article*
Related research article	S. Ohta, Y. Yuasa, N. Aoki, E. Ohta, T. Nehira, H. Ômura, M. M. Uy, Norbisabolane and bisabolane sesquiterpenoids from the seeds of *Angelica keiskei, Phytochemistry Letters 33 (2019) 94–101.*

Value of the Data

- The data presents NMR data and ESIMS data of newly isolated sesquiterpenoids and could be used by other researchers.
- The provided information on the spectroscopic data of sesquiterpenoids could be useful for the analysis of spectra and determination of the structure of other sesquiterpenoids.
- This data can serve as a benchmark for other researchers to elucidate the structures of sesquiterpenoids

1–**3** are shown in Figs. 2b, 3b and 4b, respectively. 2D ^{1}H–^{1}H COSY spectra of **1**–**3** are shown in Figs. 2c, 3c and 4c, respectively. 2D NOESY spectra of **1**–**3** are shown in Figs. 2d, 3d and 4d, respectively. 2D ^{1}H–^{13}C heteronuclear single quantum coherence (HSQC) spectra of **1**–**3** are shown in Figs. 2e, 3e and 4e, respectively. 2D ^{1}H–^{13}C heteronuclear multiple-bond correlation (HMBC) spectra of **1**–**3** are shown in Figs. 2f, 3f and 4f, respectively. ESIMS data of **1**–**3** are shown in Figs. 2g, 3g and 4g, respectively. Analyses of the spectra of **1**–**3** are described in the research article [1].

2. Experimental design, materials, and methods

NMR spectra were acquired using a JEOL A400 spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C). ^{1}H and ^{13}C NMR chemical shifts were referenced to residual solvent peaks: δ_H 7.26 (residual $CHCl_3$) and δ_C 77.0 for $CDCl_3$. ESIMS were carried out using a Shimadzu LCMS-IT-TOF mass spectrometer and a Thermo Fisher Scientific LTQ Orbitrap XL mass spectrometer at the Natural Science Center for Basic Research and Development (N-BARD), Hiroshima University.

3. Sesquiterpenoids 1–3

*3.1. (Z)-2-((3R,3aR,7aS)-3-Hydroxy-3,6-dimethyl-3,3a,4,5-tetrahydrobenzofuran-2(7aH)-ylidene) acetaldehyde (ashitabaol B) (**1**)*

1D NMR, 2D NMR, and ESIMS spectra of the compound **1** are shown in Fig. 2a–g.

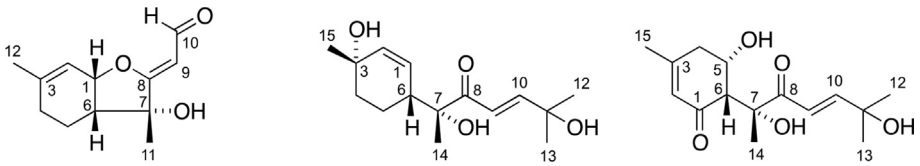


Fig. 1. Structures of norbisabolane- and bisabolane-type sesquiterpenoids isolated from the seeds of *A. keiskei*.

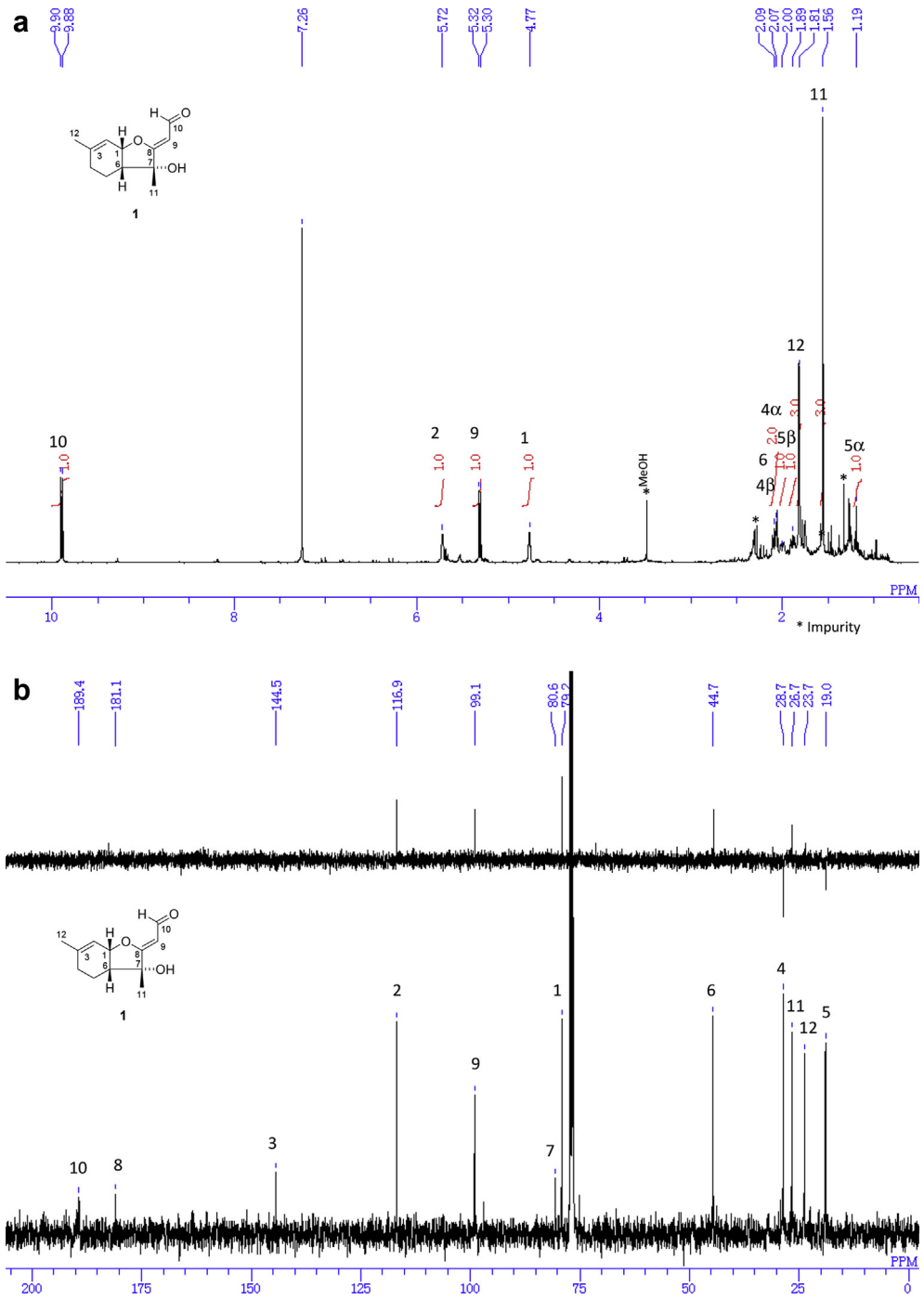
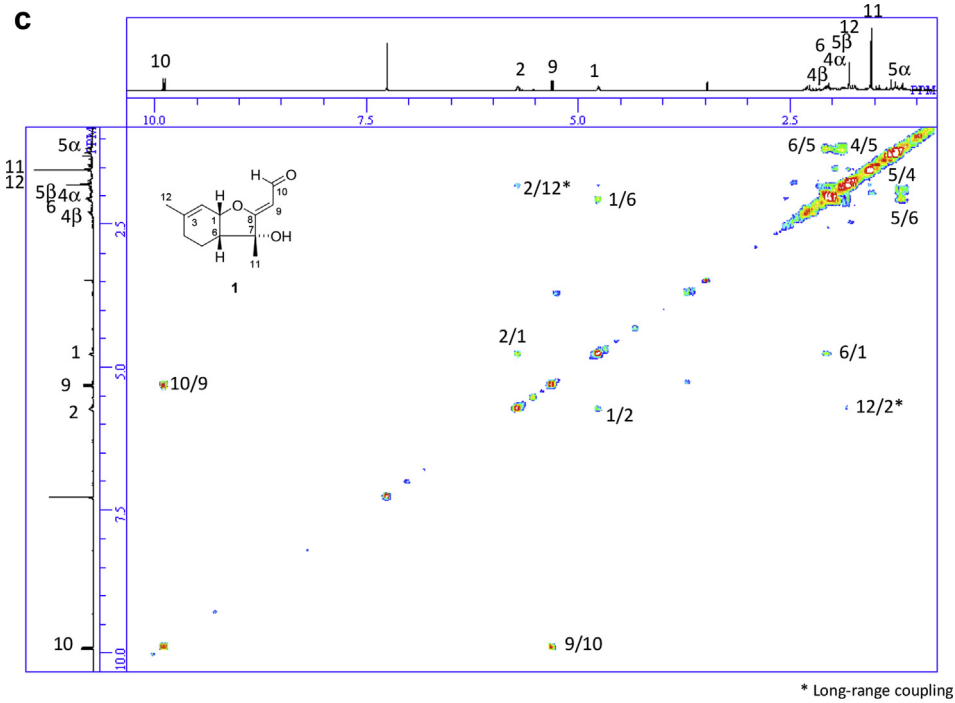


Fig. 2. **a**. ^{1}H NMR (400 MHz, $CDCl_3$) of **1**, **b**. ^{13}C NMR and DEPT (100 MHz, $CDCl_3$) of **1**, **c**. ^{1}H−^{1}H COSY of **1**, **d**. NOESY of **1**, **e**. HSQC of **1**, **f**. HMBC of **1**, **g**. (+)ESIMS of **1**.



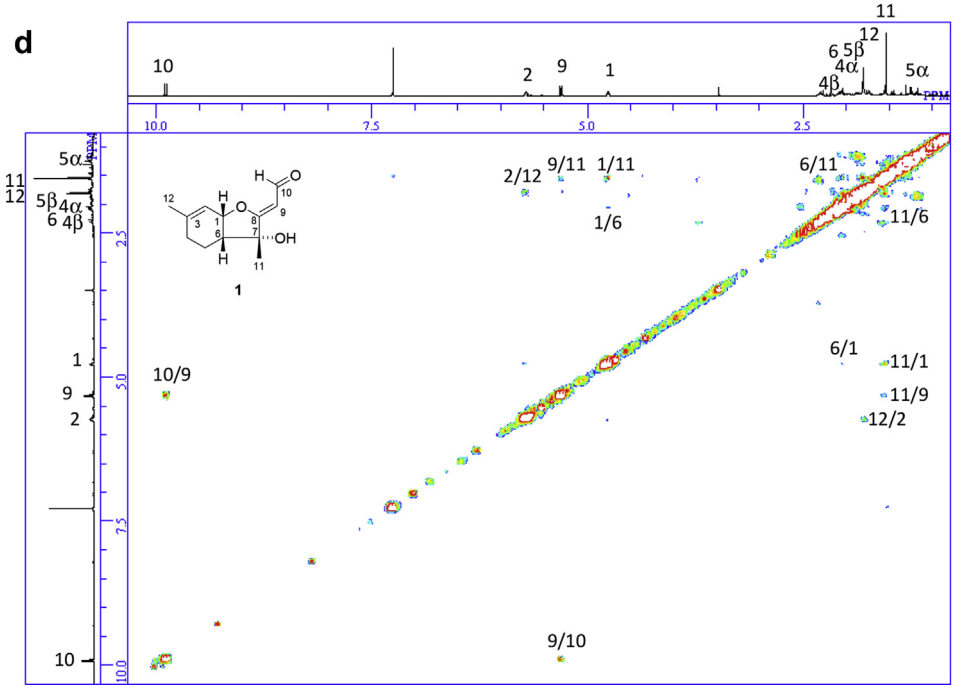


Fig. 2. (*continued*).

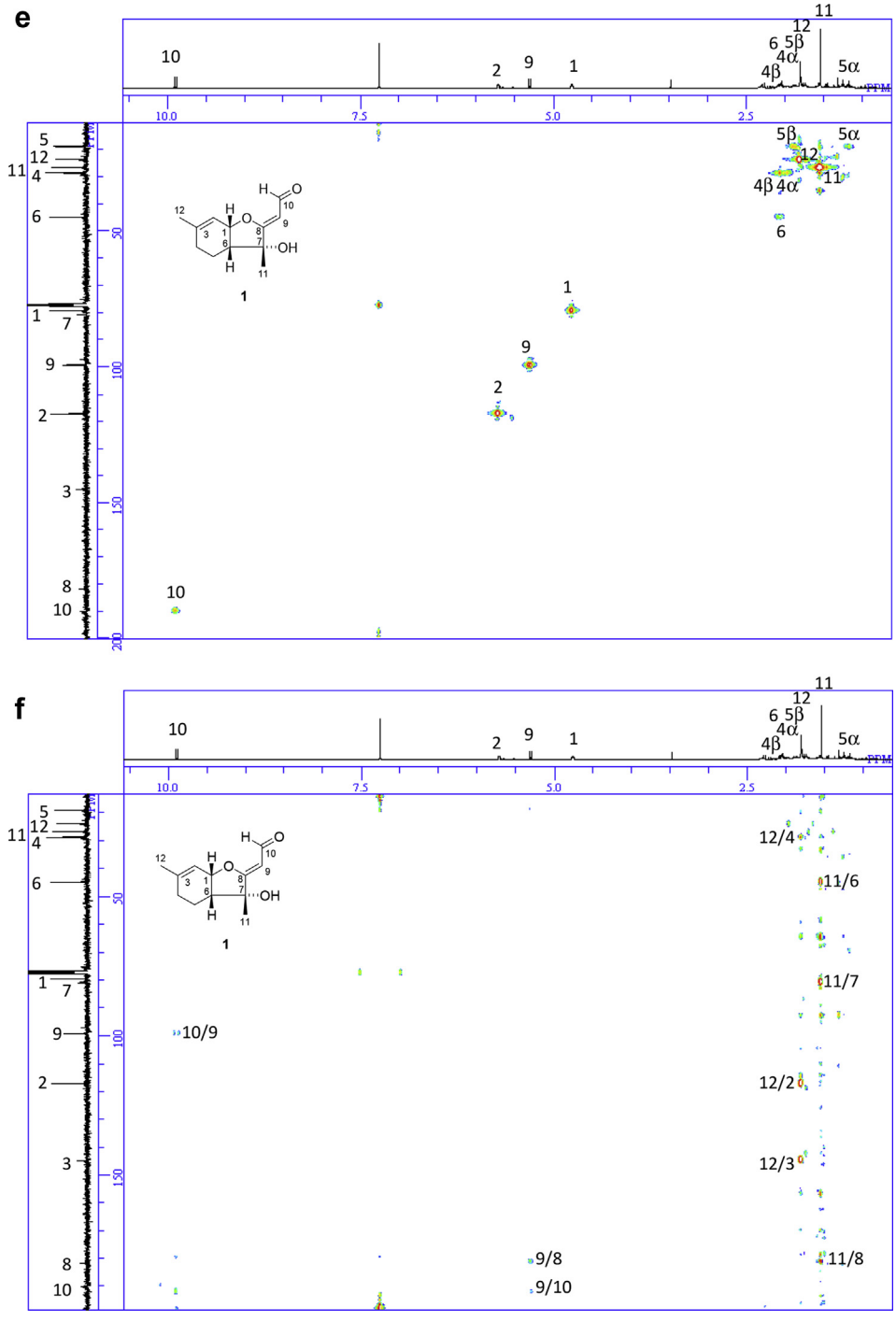


Fig. 2. (*continued*).

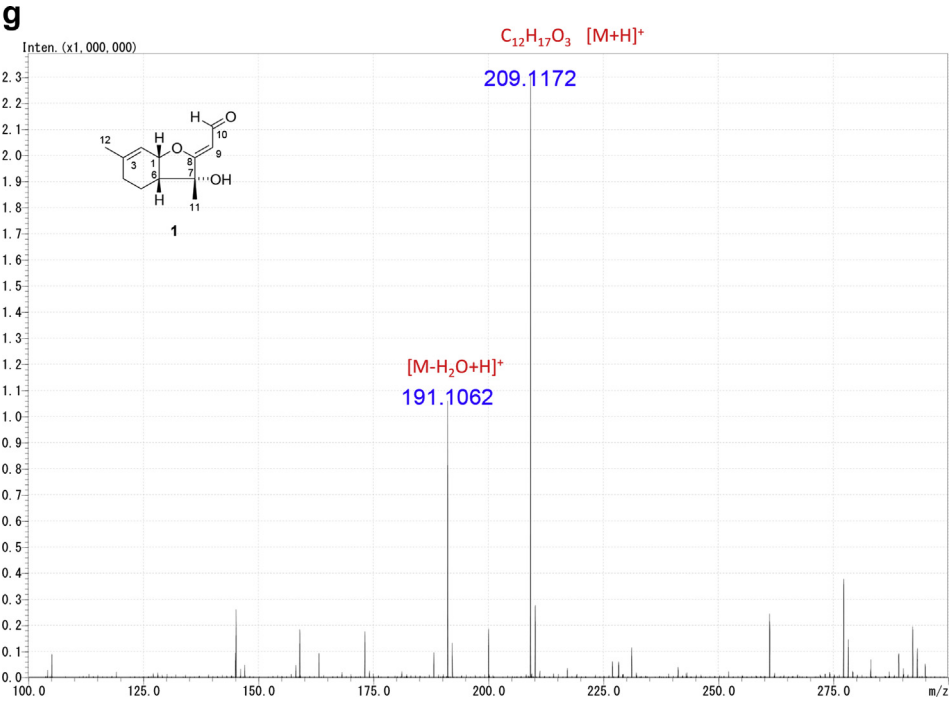


Fig. 2. (*continued*).

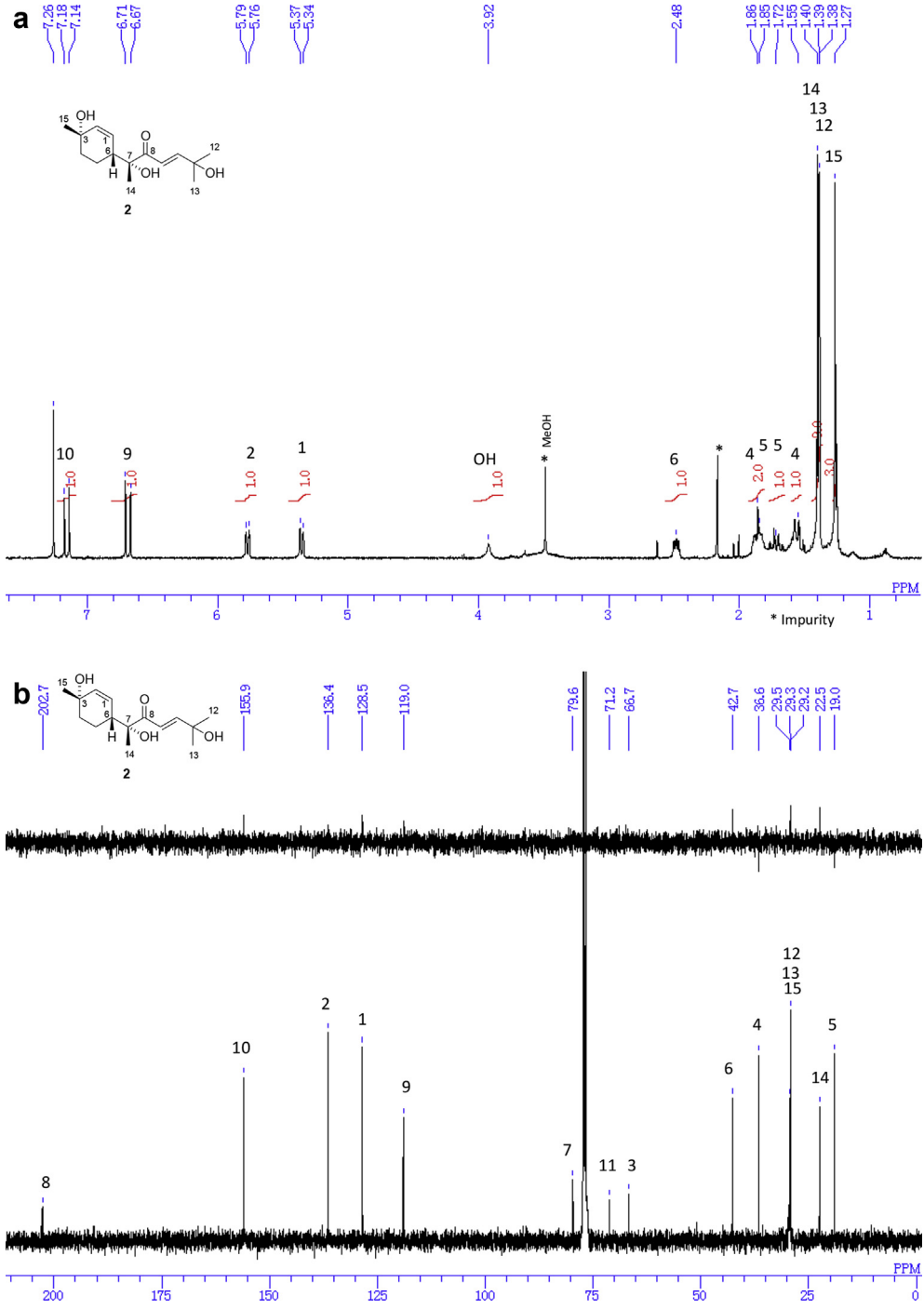
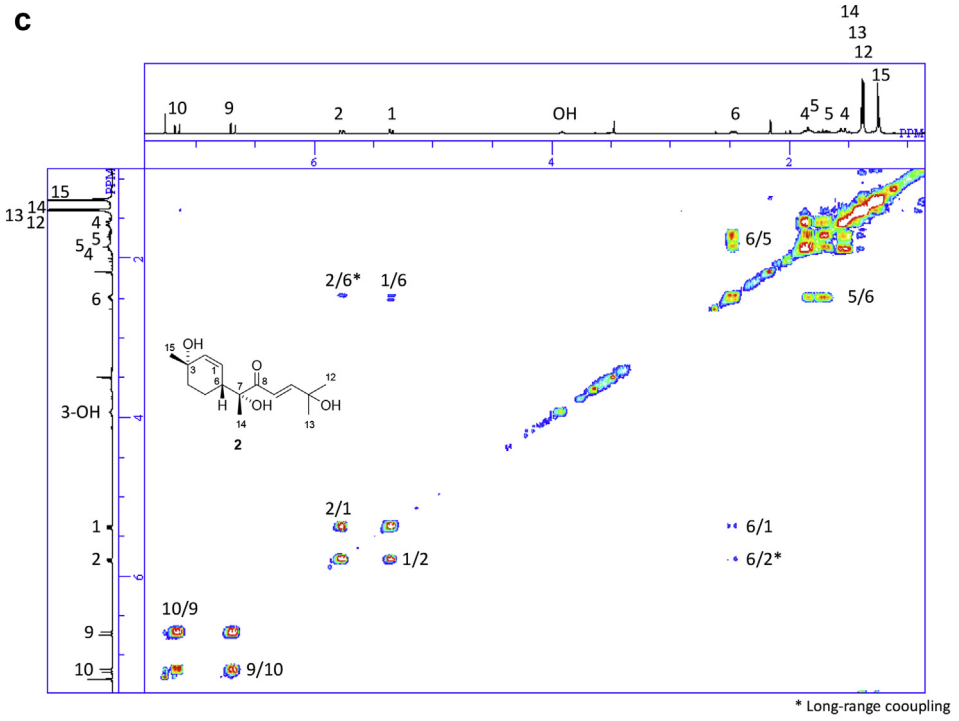


Fig. 3. **a**. ^{1}H NMR (400 MHz, $CDCl_3$) of **2**, **b**. ^{13}C NMR and DEPT (100 MHz, $CDCl_3$) of **2**, **c**. $^{1}H-^{1}H$ COSY of **2**, **d**. NOESY of **2**, **e**. HSQC of **2**, **f**. HMBC of **2**, **g**. (+)ESIMS of **2**.



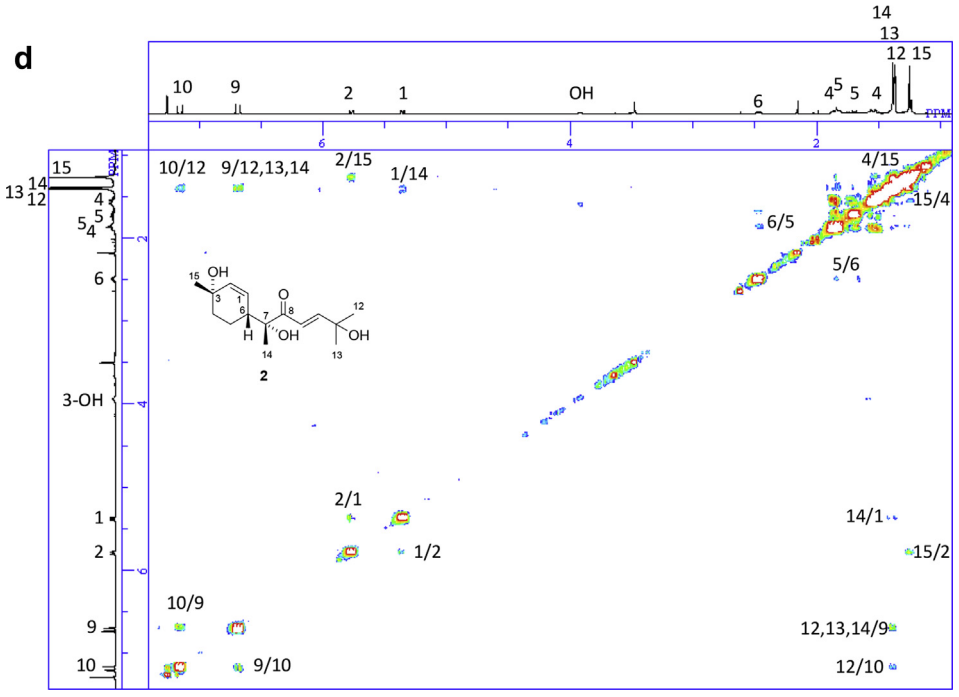


Fig. 3. (*continued*).

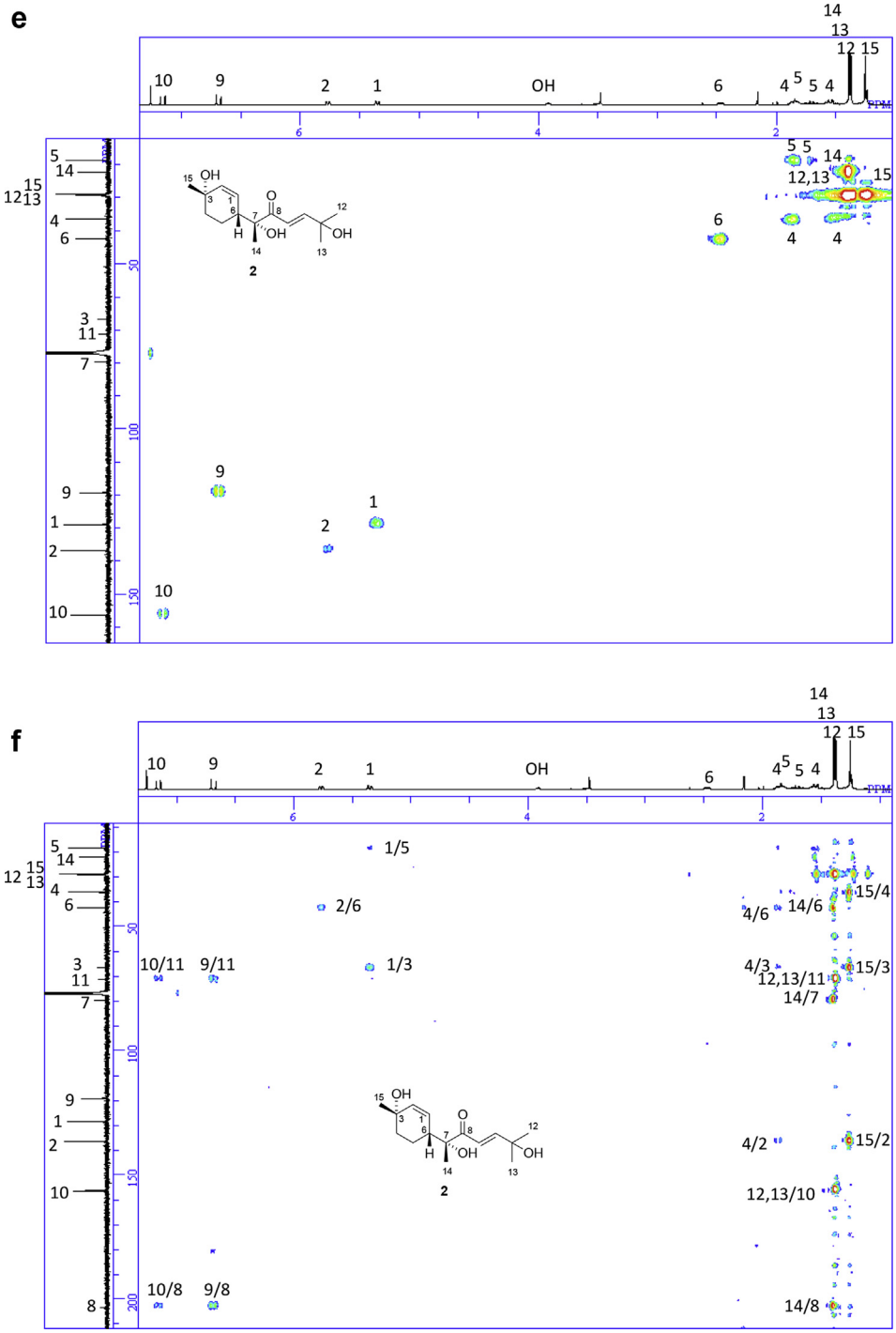


Fig. 3. (*continued*).

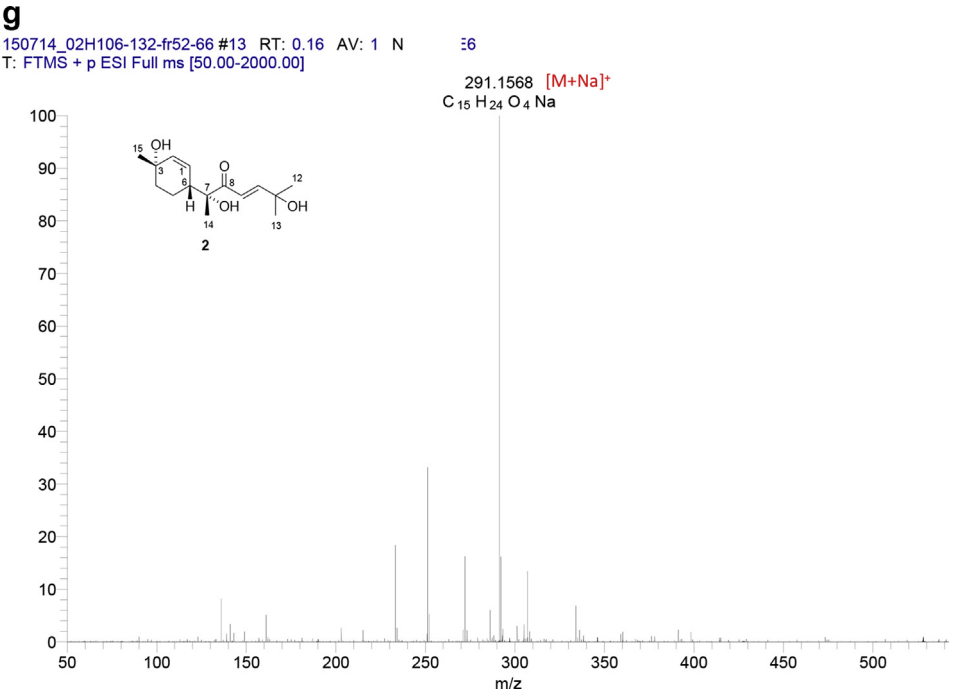


Fig. 3. (*continued*).

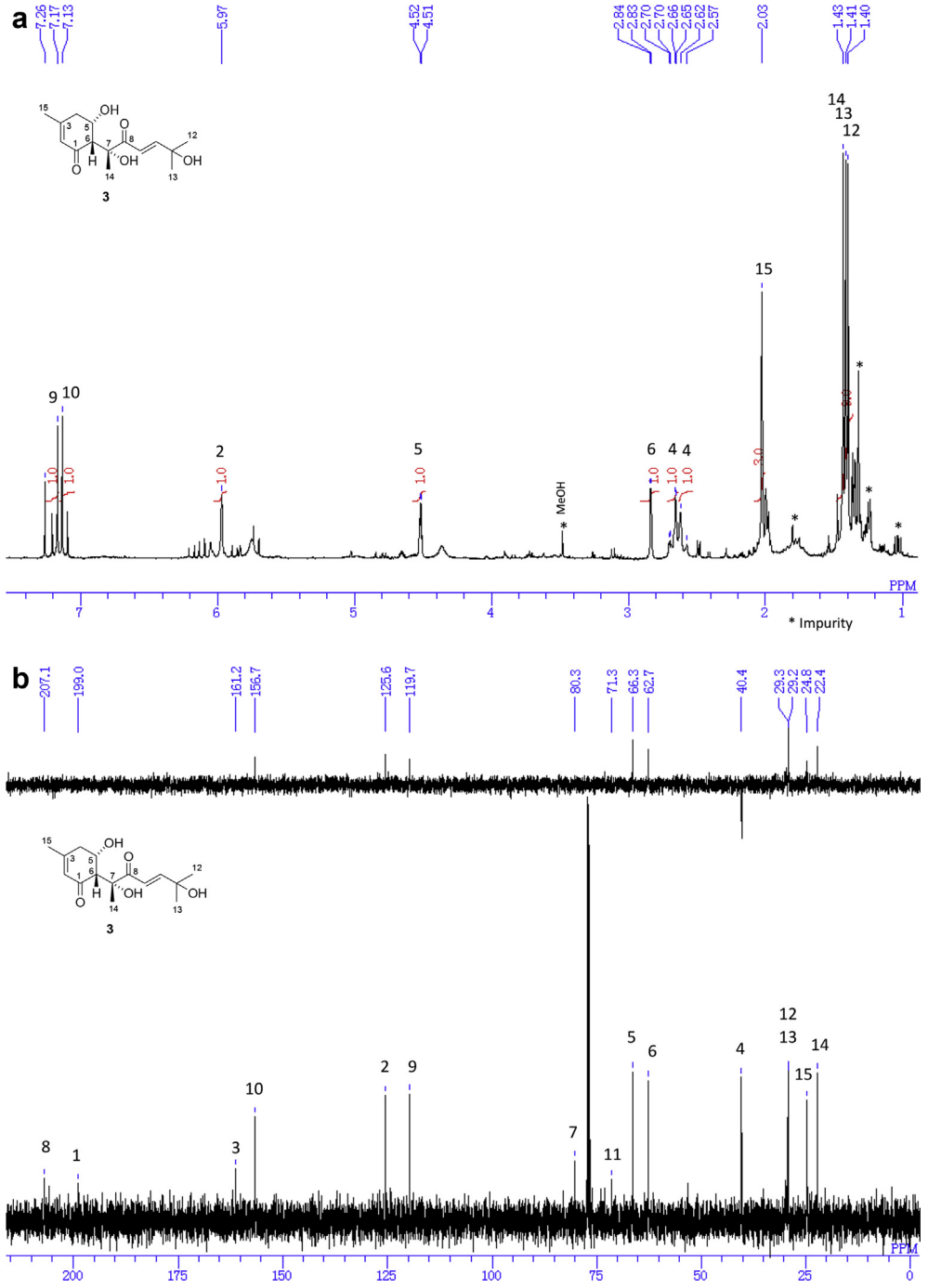
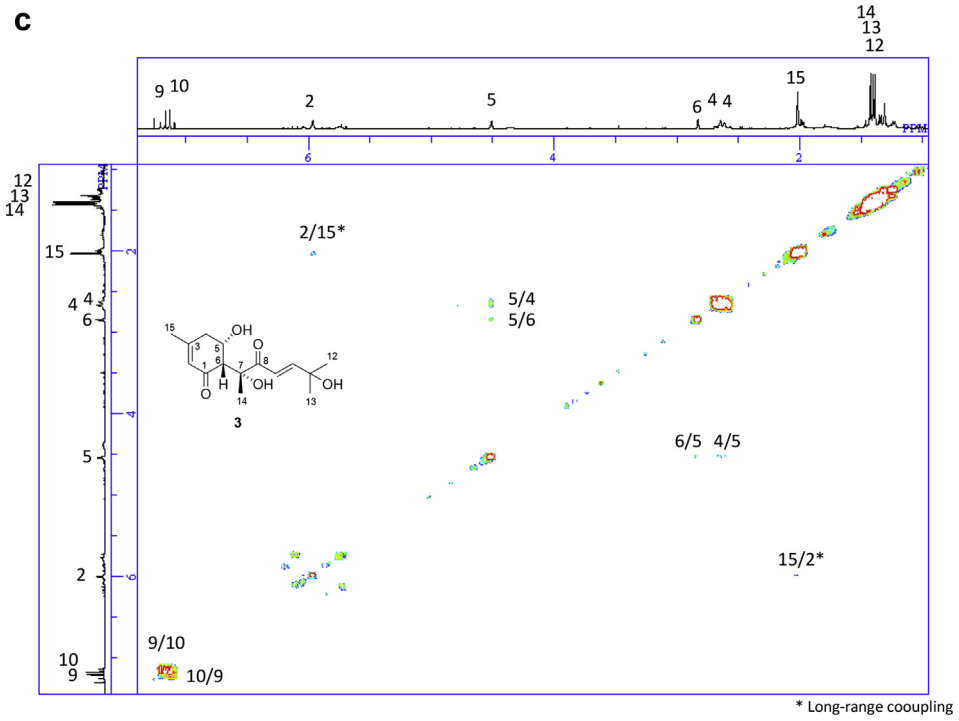


Fig. 4. **a**. ^{1}H NMR (400 MHz, $CDCl_3$) of **3**, **b**. ^{13}C NMR and DEPT (100 MHz, $CDCl_3$) of **3**, **c**. ^{1}H−^{1}H COSY of **3**, **d**. NOESY of **3**, **e**. HSQC of **3**, **f**. HMBC of **3**, **g**. (+)ESIMS of **3**.



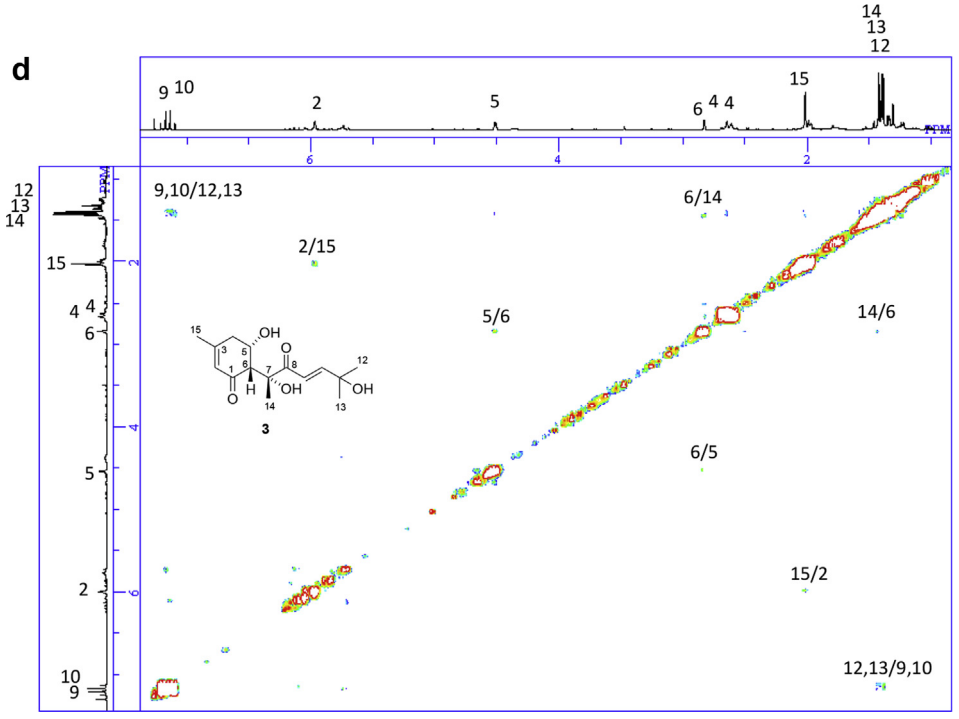


Fig. 4. (*continued*).

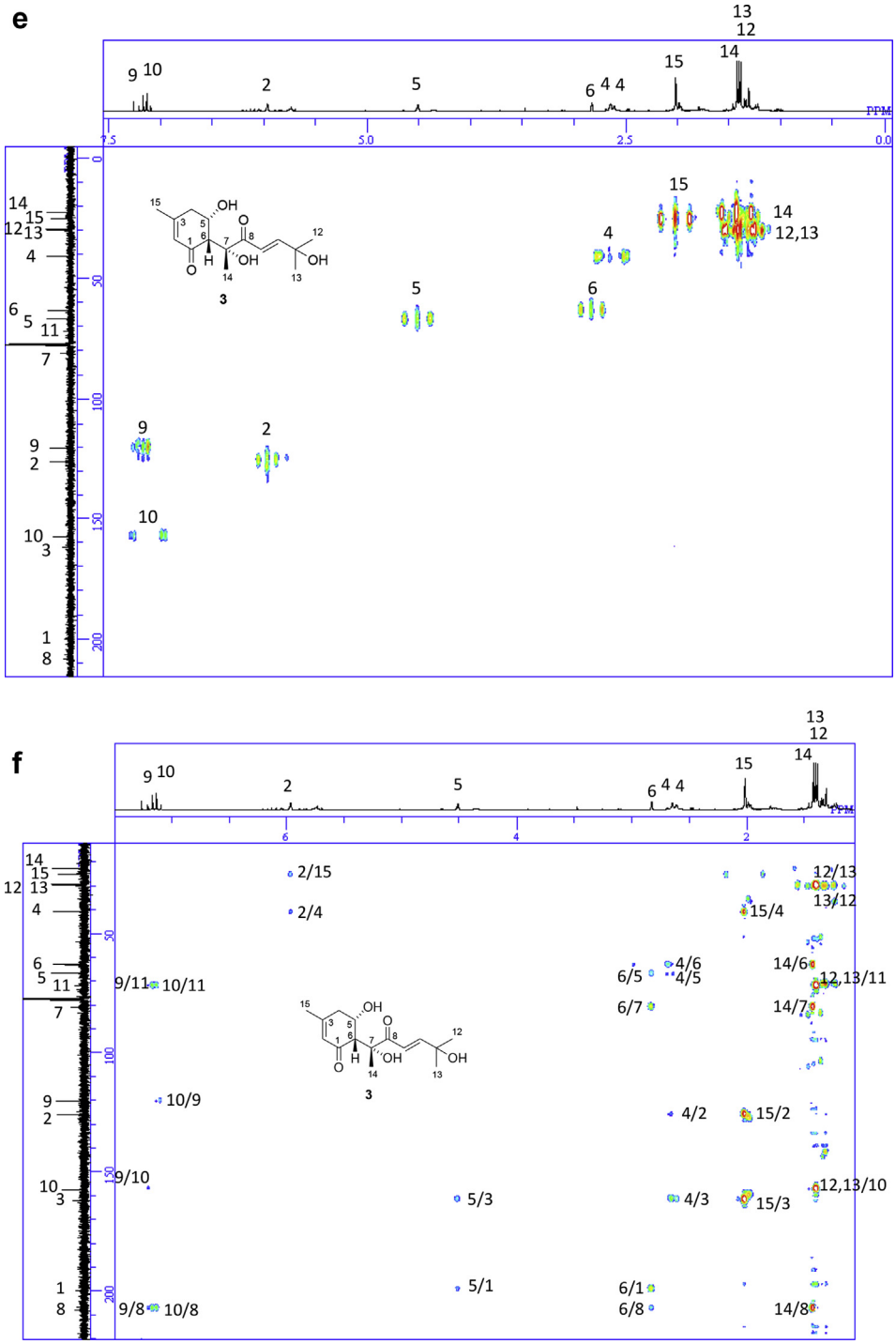


Fig. 4. (*continued*).

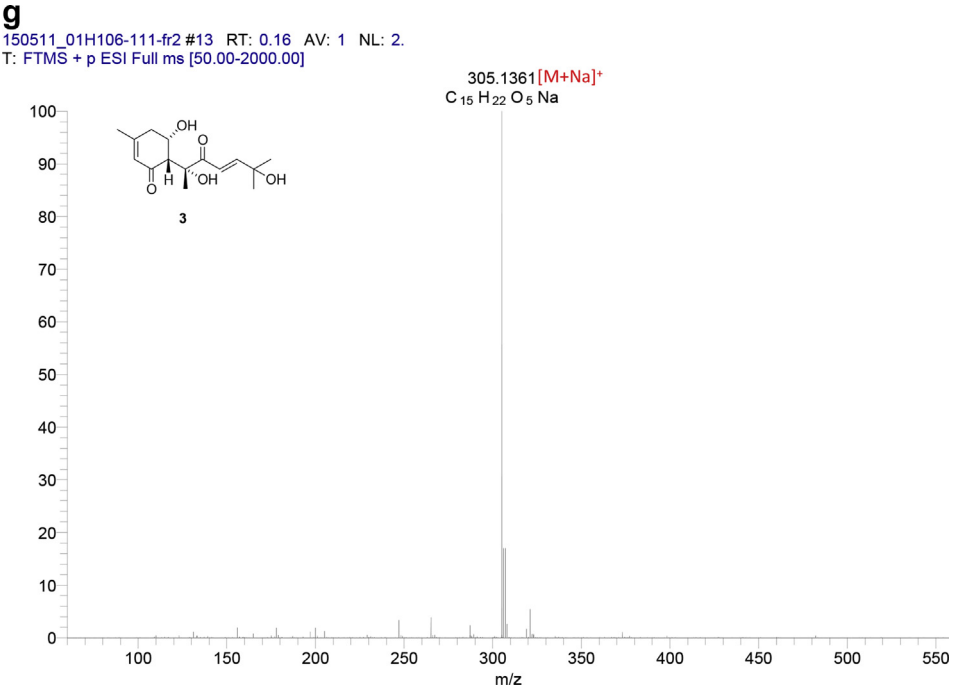


Fig. 4. (*continued*).

*3.2. (E)-2,6-Dihydroxy-2-(4-hydroxy-4-methylcyclohex-2-en-1-yl)-6-methylhept-4-en-3-one (ashitabaol C) (**2**)*

1D NMR, 2D NMR, and ESIMS spectra of the compound **2** are shown in Fig. 3a–g.

*3.3. (5S,6R)-6-((R,E)-2,6-Dihydroxy-6-methyl-3-oxohept-4-en-2-yl)-5-hydroxy-3-methylcyclohex-2-enone (ashitabaol D) (**3**)*

1D NMR, 2D NMR, and ESIMS spectra of the compound **3** are shown in Fig. 4a–g.

Acknowledgments

This work was supported in part by JSPS KAKENHI Grant Number 18K05335.

Conflict of Interest

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.

References

[1] S. Ohta, Y. Yuasa, N. Aoki, E. Ohta, T. Nehira, H. Ômura, M.M. Uy, Norbisabolane and bisabolane sesquiterpenoids from the seeds of *Angelica keiskei*, Phytochemistry Lett. 33 (2019) 94–101.