Data on chemical composition of alkaloids of *Plumula nelumbinis* and antioxidant activity from thirteen habitats in China

Wenyue Tian, Hui Zhi, Chao Yang, Likang Wang, Jiatang Long, Luomin Xiao, Jizheng Liang, Ying Huang, Xi Zheng, Suqing Zhao, Kun Zhang, Junxia Zheng

*Institute of Natural Medicine and Green Chemistry, School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006; PR China
School of Pharmaceutical Science, Guangzhou University of Chinese Medicine, Guangzhou 510006; PR China
Susan Lehman Cullman Laboratory for Cancer Research, Department of Chemical Biology, Ernest Mario School of Pharmacy, Rutgers, The State University of New Jersey, Piscataway, New Jersey 08854, USA
School of Chemistry and Environment Engineering, Wuyi University, Jiangmen 529020; PR China

**Abstract**

*Plumula nelumbinis* is widely consumed as tea for its pharmacological properties, which is related to its chemical composition, so the identification of the major compounds of *P. nelumbinis* is valuable. The data described in this article is supported by the research article entitled “Chemical composition of alkaloids of *Plumula nelumbinis* and their antioxidant activity from different habitats in China” (Tian et al., 2018). Included are the MS-MS Spectrograms of seven alkaloid standards and thirty alkaloids identified in the *P. nelumbinis*, which is based on ultra-performance liquid chromatography electrospray ionization quadrupole time-of-flight mass spectrometry method. Also included are the total alkaloids content and the antioxidant activity of total alkaloid in *P. nelumbinis* from 13 habitats in China, which was accomplished with three different antioxidant assays.

© 2018 The Authors. 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, Biology |
|------------------------------|-------------------|
| More specific subject area   | Natural product chemistry |
| Type of data                 | Table and figures |
| How data was acquired        | Ultra-performance liquid chromatography electrospray ionization quadrupole time-of-flight mass spectrometry (UPLC-ESI-QTOF-MS), UV, Tecan Infinite F200 Pro |
| Data format                  | Raw, Analyzed     |
| Experimental factors         | *Plumula nelumbinis* was extracted three times with 80% EtOH-H2O, dissolved in 0.1% HCl, then loaded on the pretreated D001 cation exchange resin chromatography. The sample was dissolved in MeOH and filtered through a 0.22 μm membrane filter before analysis. |
| Experimental features        | Instrumental testing, the samples were analyzed qualitatively by UPLC-ESI-QTOF-MS. |
| Data source location         | China             |
| Data accessibility           | The data are available with in this article |
| Related research article     | [1] Wenyue Tian, Hui Zhi, Chao Yang, Likang Wang, Jiatang Long, Luomin Xiao, Jizheng Liang, Ying Huang, Xi Zheng, Suqing Zhao, Kun Zhang, Junxia Zheng. Chemical composition of alkaloids of *Plumula nelumbinis* and their antioxidant activity from different habitats in China [J]. *Industrial Crops and Products*, 2018, 125: 537–548. |

Value of the data

- Method and data can be used to identify natural alkaloids by UPLC-ESI-QTOF-MS.
- The chromatographic and mass spectrometric data can be used for comparison with other studies performed on *Plumula nelumbinis*, then serve as a benchmark for other researchers to elucidate the constituents of *P. nelumbinis*.
- The alkaloid contents and the antioxidant activity data will provide a valuable reference for studies comparing the chemical and pharmacological effects of *P. nelumbinis*.

1. Data

The structures and MS-MS spectrograms of seven alkaloid standards is provided in Fig. 1. Data in Fig. 2 presents the MS-MS spectrograms of 30 alkaloids identified in the *Plumula nelumbinis* from Xiangtan, Hunan province. Data in Table 1 includes the total alkaloids content and antioxidant capacity of *P. nelumbinis* obtained from 13 different habitats in China.

2. Experimental design, materials, and methods

2.1. Chemicals and materials

*The P. nelumbinis* samples were collected from 13 different habitats in China, during August, 2017. Nuciferine, pronuciferine, liensinine, isoliensinine, neferine, arnepavine and norcoclaurine were obtained from Junmu Biotechnology Co. Ltd (Guangzhou, China). 2,2'-Azobis(2-amidinopropane dihydrochloride), 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid, L-ascorbic acid, sodium fluorescein, 2,4,6-tri(2-pyridyl)-s-triazine and 2,2-diphenyl-1-picrylhydrazyl were purchased from the Sigma-Aldrich Chemical Co. Ltd (Saint Louis, MO, USA). Methanol, acetonitrile (all chromatographic grade) were purchased from Swedish Oceanpak Co. And the formic acid (chromatographic grade) were added to all solutions.
grade) were purchased from the Fine Chemical Co. Ltd (Tianjin, PR China). Ultrapure water was purified using a Milli-Q Advantage A10 system (Millipore, Billerica, MA, USA). And the detailed description of chemicals and materials has been described in Ref. [1].

2.2. Extraction and isolation

Dried *P. nelumbinis* was extracted three time with 80% EtOH-H₂O, and the ethonal extract isolated by D001 cation exchange resin chromatography, as washed with water and 95% ethanol (included 1% ammonia) in turn, the 95% ethanol/ammonia wash fraction contains the bulk of the alkaloids, which was stored at −20°C after freeze-drying. The detail procedures were described in Ref. [1].

2.3. UPLC-ESI-QTOF-MS parameter

Identification of the samples were carried out using a Shimadzu Prominence UPLC system (Nexera UHPLC LC-30A, Kyoto, Japan) equipped with a A triple TOF™ 5600+ mass spectrometer (AB Sciex, Foster City, CA). And the detail parameter setting of LC system and mass spectrometric detection were selected as described in Ref. [1]. Briefly, the analysis was carried out using a Waters Acquity UPLC BEH C₁₈ column (2.1 mm × 100 mm, 1.7 μm) and the mobile phase of acetonitrile (containing 0.1% formic acid)-water (containing 0.1% formic acid) at a flow rate of 0.3 mL/min with the column temperature kept at 40 °C and the

---

[S1. Liensinine](#)  [S2. Isoliensinine](#)

[S3. Neferine](#)  [S4. Nuciferine](#)

[S5. Norcoclaurine](#)  [S6. Pronuciferine](#)

[S7. Armepavine](#)

---

**Fig. 1.** The structures and MS-MS Spectrograms of seven alkaloid standards. (S: standard).
injection volume of 3 µL. And the mass spectrometric detector was operated in the positive ESI mode and was equipped with a DuoSpray™ source (AB Sciex, Foster City, CA).

2.4. Total alkaloid content

The total alkaloid content of *P. nelumbinis* was determined using the acid dye colorimetric method according to the methods in Ref. [1]. In which, neferine was used as a reference compound.

Fig. 2. The MS-MS Spectrograms of 30 alkaloids detected in the *Plumula nelumbinis* from Xiangtan, Hunan province. (P: peak).
2.5. Antioxidant activity of total alkaloids

In this study, three different chemical methods, like the DPPH, ORAC and FRAP assays were used to evaluate the antioxidant activity of the total alkaloids which from different habitats. The free radical-scavenging activity of the total alkaloids of *P. nelumbinis* was determined with a DPPH test according to the methods in Ref. [1]. The ORAC assay was completed in accordance with the previously described according to the methods in Ref. [1].
The Ferric reducing antioxidant power assay of *P. nelumbinis* were determined according to the methods in Ref. [1].

Acknowledgments

This study was supported by a research grant from the National Natural Science Foundation of China (No. 81573294, 81773593), the Excellent Young Teachers Program of Guangdong Provincial Colleges and Universities (YQ 2015061), the Pearl River S&T Nova Program of Guangzhou...
(201610010100), Science and Technology Program of Guangzhou (201707010414), Key platform and characteristic innovation project of Guangdong Education Department (21615428).

Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.004.

Reference

[1] Wenyue Tian, Hui Zhi, Chao Yang, Likang Wang, Jiatang Long, Luomin Xiao, Jizheng Liang, Ying Huang, Xi Zheng, Suqing Zhao, Kun Zhang, Junxia Zheng, Chemical composition of alkaloids of Plumula nelumbinis and their antioxidant activity from different habitats in China, Ind. Crop. Prod. 125 (2018) 537–548.