## SUPPLEMENTARY MATERIAL

Markhasphingolipid A, new phytosphingolipid from the leaves of *Markhamia stipulata* var. *canaense* V.S. Dang

Trong Nghia Ngo<sup>a,h</sup>, Nu Dan Phuong Nguyen<sup>c,d</sup>, Ngoc Thien Ly Nguyen<sup>e</sup>, Nguyen Kim Tuyen Pham<sup>c</sup>, Nhat Minh Phan<sup>b</sup>, Trong Dat Bui<sup>b</sup>, Van Son Dang<sup>f</sup>, Cong Luan Tran<sup>a,g</sup>, Dinh Tri Mai<sup>a,b</sup>, Tan Phat Nguyen<sup>a,b</sup>\*

<sup>a</sup>Graduate University of Science and Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Viet Nam
<sup>b</sup>Institute of Chemical Technology, Vietnam Academy of Science and Technology, 01 Mac Dinh Chi, Ho Chi Minh city, Viet Nam
<sup>c</sup>Sai Gon University, 273 An Duong Vuong, Ho Chi Minh City, Viet Nam
<sup>d</sup>Tran Phu High School, Binh Phuoc Province, Viet Nam
<sup>e</sup>Tan Hiep High School, Kien Giang Province, Viet Nam
<sup>f</sup>Institute of Tropical Biology, Vietnam Academy of Science and Technology, 85 Tran Quoc Toan, Ho Chi Minh city, Viet Nam
<sup>g</sup>Tay Do University, 68 Lo Hau Thanh My, Can Tho city, Viet Nam
<sup>h</sup>Kien Giang University, 320A QL 61, Kien Giang city, Viet Nam

Corresponding author. Tel.: +84 916.360.751 Email: ntphat@ict.vast.vn

## Markhasphingolipid A, new phytosphingolipid from the leaves of *Markhamia stipulata* var. *canaense* V.S. Dang

From the leaves of *Markhamia stipulata* var. *canaense* V.S. Dang, one new phytosphingolipid, named markhasphingolipid A (**6**), together with five known compounds, 4',7-*O*-dimethylapigenin (**1**), narigenin (**2**), tectoquinone (**3**), mollic acid (**4**), 1-hexadecanoyl-*sn*-glycerol (**5**) were classified by various chromatographic methods. Their structures were designated by IR, UV, HR-ESI-MS, HR-ESI-MS/MS and NMR experiments. All compounds were recognized for the first time from this species. The cytotoxicity of all *n*-hexane fractions and isolated compounds (**5** & **6**) against three human cancer cell lines (HeLa, HepG2, and MCF-7) were evaluated by SRB assay. All *n*-hexane fractions expressed cytotoxic effect on three tested cancer cell lines (at the concentration of 100  $\mu$ g/mL, percent of cytotoxicity ranged from 55.81 to 95.83%) as well as compound **5** (IC<sub>50</sub> ranged from 48.51 to 63.30  $\mu$ M) whereas fraction H.I and compound **6** did not show activity.

**Keywords:** *Markhamia stipulata*; Bignoniaceae; Markhasphingolipid A; cytotoxic activity.

## List of supporting information

Figure S1. Chemical structures and selected COSY, HMBC correlations of 1.

Figure S2. Important fragmentation of compound 1.

Figure S3. <sup>1</sup>H-NMR spectrum (500 MHz) of compound **1** in Methanol- $d_4$ .

Figure S4. <sup>13</sup>C-NMR spectrum (125 MHz) of compound **1** in Methanol- $d_4$ .

Figure S5. DEPT spectrum of compound 1 in Methanol- $d_4$ .

Figure S6. COSY spectrum of compound 1 in Methanol- $d_4$ .

Figure S7. HSQC spectrum of compound **1** in Methanol- $d_4$ .

Figure S8. HMBC spectrum of compound 1 in Methanol- $d_4$ .

Figure S9. IR spectrum of compound 1.

Figure S10. UV-VIS spectrum of compound 1.

Figure S11. HR-ESI-MS (positive) spectrum of compound 1.

Figure S12. HR-ESI-MS (nagative) spectrum of compound 1.

Figure S13. HR-ESI-MS/MS (positive) spectrum of compound 1.

Figure S14. HR-ESI-MS/MS (positive, extended) of compound 1.

Figure S15. HR-ESI-MS/MS (nagative) spectrum of compound 1.

Figure S16. HR-ESI-MS/MS (nagative, extended) spectrum of compound 1.



Figure S2. Important fragmentation of compound 1.









Figure S8. HMBC spectrum of compound 1 in Methanol- $d_4$ .



Figure S10. UV-VIS spectrum of compound 1.



Figure S13. HR-ESI-MS/MS (positive) spectrum of compound 1.



Figure S14. HR-ESI-MS/MS (positive, extended) spectrum of compound 1.



Figure S16. HR-ESI-MS/MS (nagative, extended) spectrum of compound 1.