SUMMARY OF DISSERTATION

Name of Doctoral candidate: Hoang Thi Dieu Huong

Dissertation title: "Study on chemical constituents and biological activities of *Elsholtzia penduliflora* W. W. Smith"

Speciality: Medicinal Materials - Traditional Pharmacy

Code of specciality: 9720206

Name of academic advisors:

1. Assoc. Prof. Dr. Do Thi Ha
2. Dr. Le Thi Kim Van

Name of academic institute: National Institute of Medicinal Materials

Summary of the dissertation

1. Objectives

- Chemical constituents: To determine the content and main constituents of essential oil from *Elsholtzia penduliflora* W. W. Smith; To identify groups of compounds; To isolate pure compounds from the extract and identify their chemical structure.

- Biological activities: To evaluate anti-imflammatory effect and anti-cancer effects *in vitro* of ethanol, fractional extracts and isolated compounds from *Elsholtzia penduliflora* W. W. Smith.

2. Methods

2.1. Chemical study:

- Essential oils are quantified by steam distillation. The main constituents of essential oils were determined by GC-MS.

- Qualitative method: to identify groups of compounds by characteristic chemical reactions.

- Extraction and isolation of chemical constituents:
  + Chemical contents have been extracted and fracted with ethanol 80% and *n*-hexane, dichloromethan and EtOAc at temperature room.
  + Compounds were isolated in open chromatography column, using station phases silica gel (0,04 - 0,063 mm, Merck), YMC RP-18 (30-50 μm, Fuji Silysia Chemical Ltd.), Sephadex LH20, Diaion HP-20. Determination the similar fractions by using TLC.

+ Structural elucidation of isolated compounds: Chemical structures were identified base on spectroscopy analysis: ESI-MS, HR-EI-MS, 1D-NMR, 2D-NMR, and comparison with the published data. Determination of sugar configuration by hydrolysis method.

2.2. Biological study:

- The anti-inflammatory effect *in vitro* were evaluated base on the inhibition of PGE_2 production by ELISA method and the mRNA expression of COX-2 on RAW 264.7 cells by RT-PCR.

- The cytotoxic activity were evaluated on 4 human cancer cell lines (A549, MCF-7, HepG2, K562) by the MTT method to determine the IC_{50} value.

3. Results and Conclusion

3.1. Chemical constituents:

- The content of essential oil from *Elsholtzia penduliflora* W. W. Smith was determined: in Sin Ho (0.87%), Sa Pa (0.85%) and Bat Xat (0.88%). The main constituent of them was 1,8-cineole (57.73 – 74.42%).

- Identified groups of compounds presented in *Elsholtzia penduliflora* W. W. Smith including: Flavonoid, saponin, triterpenoide, fat, phytosterol, coumarin, amino acid, reducing sugar and anthranoide.

- Structure of 23 compounds isolated from *Elsholtzia penduliflora* W. W. Smith were identified, in which:

- ✓ 7 new saponin triterpenoides named Pendulosid A-G.
- ✓ 11 compounds were isolated from genus *Elsholtzia* Willd. for the first time: Sericoside, 2*α*,3*α*,19*α*,24-tetrahydroxyolean-12-en-28-oic acid 28-*O*-*β*-D-glucopyranoside, kaji-ichigoside F1, rosamultin, officinoterpenoside B, pruvuloside B, 24-hydroxytormentic acid ester glucoside, niga-ichigoside F1, thymoquinol 5-*O*-*β*-D-glucopyranoside, thymoquinol 2-*O*-*β*-D-glucopyranoside and foliachinenoside A1.
- ✓ 5 known compounds: Acid *trans*-cinnamic, acid hyptadienic, tectochrysin, *β*-sitosterol and daucosterol.

3.2. Biological activities:

- *Anti-imflammatory effect in vitro:* The ethylacetate fraction (20 µg/mL) and compounds pendulosid E, pendulosid C, rosamultin (3 µM) inhibited PGE_2 production and reduced mRNA expression of COX-2 enzyme on RAW 264.7 cells.

- *Cytotoxic activity against four human cancer cell lines in vitro:*

+ The IC_{50} values of ethylacetate fraction were 16.86 µg/mL (A549 cell line), 22.67 µg/mL (MCF-7 cell line), 29.49 µg/mL (HepG2 cell line) and 29.20 µg/mL (K562 cell line).

+ The IC_{50} values of sericoside were 7.725 µM (A549 cell line), 12.65 µM (MCF-7 cell line), 16.91 µM (HepG2 cell line) and 13.10 µM (K562 cell line).

+ The IC_{50} values of penduloside C were 7.846 µM (A549 cell line), 10.79 µM (MCF-7 cell line), 12.52 µM (HepG2 cell line) and 12.49 µM (K562 cell line).

+ The IC_{50} values of penduloside G were 4.882 µM (A549 cell line), 5.406 µM (MCF-7 cell line), 6.333 µM (HepG2 cell line) and 7.350 µM (K562 cell line).

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ACADEMIC ADVISORS		**DOCTORAL CANDIDATE**
Assoc. Prof. Dr. Do Thi Ha	**Dr. Le Thi Kim Van**	**Hoang Thi Dieu Huong**