

## Information on Doctoral thesis of Fellows Duong Ngoc Toan

1. Full name: Duong Ngoc Toan
2. Sex: Male
3. Date of birth: 02 November 1983
4. Place of birth: Thai Nguyen
5. Admission decision number: 3201/QĐ-SĐH. Dated: November, 08<sup>th</sup>, 2010. Issued by the President of Vietnam National University, Hanoi.
6. Changes in academic process: None
7. Official thesis title: Study synthesis and metabolism of  $\alpha,\beta$ -unsaturated ketones derived from acetyl coumarin and acetylchromone.
8. Major: Organic Chemistry
9. Code: 62 44 01 14
10. Supervisors: Prof. Doc. Nguyễn Minh Thảo
11. Summary of the new findings of the thesis
  - $\alpha,\beta$ - Unsaturated ketones and their converted products (117 compounds, in which 96 haven't been documented) have been synthesized from *o*-hydroxyacetophenone, resoxinol,  $\beta$ -naphthol.
  - The decomposition of the chromone ring in basic condition has been detected when attempting to prepare  $\alpha,\beta$ -unsaturated ketones from 3-acetyl-2-methylchromone.
  - Five 3-pyrazoline derivatives have been successfully prepared from  $\alpha,\beta$ -unsaturated ketones of 3-aryl-1-(4-methylcoumarin-3-yl)prop-2-enon.
  - Fourteen benzothiazepine derivatives have been successfully prepared from  $\alpha,\beta$ -unsaturated ketones of 3-aryl-1-(2-hydroxyphenyl)prop-2-enon, and 3-aryl-1-(5-hydroxy-4-methylcoumarin-6-yl)prop-2-enon.
  - The structures of 96 new compounds have been determined by IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, HSQC, HMBC, and mass spectroscopies.
  - Conducted test and antibacterial activity of 37 antifungal compounds synthesized, that they are active against strains of *Gr* (-) and yeast. Test conducted cytotoxic activity of 18 cancer compounds and identified nine compounds have cytotoxic effects, including 5 compounds show cytotoxic activity relatively well with cancer cells carcinoma (KB), the 5 test active compounds with liver cancer cell line (HepG2) we also see relatively good activity. Especially M<sub>2</sub> compounds (compounds pyrimidine) show activity caused toxic cell carcinoma lines with IC<sub>50</sub> values at concentrations 4.64  $\mu$ g/ml, T<sub>12</sub> compounds (compounds benzothiazepin) show activity caused toxic cell carcinoma lines with IC<sub>50</sub> values at concentrations 6.0  $\mu$ g/ml, activated cytotoxic liver cancer

cell lines with  $IC_{50}$  values in 4.25 concentration  $\mu\text{g/ml}$ ,  $T_5$  compounds (compounds benzothiazepin) show activity caused toxic cell carcinoma lines with  $IC_{50}$  values at concentrations 5.53  $\mu\text{g/ml}$ , activated cytotoxic liver cancer cell lines with  $IC_{50}$  values in 8.0 concentration  $\mu\text{g/ml}$ .

12. Paratical applicability, if any:

- It comes from the acetylcoumarin and acetylchromone to synthesize  $\alpha,\beta$ -unsaturated ketone, which will be transformed into heterocyclic compounds pyrazolines, pyrimidines, benzodiazepines and benzothiazepines have you as bioactive antibacterial, and antifungal activity cytotoxic properties of cancer for good results.

- Researchers can deploy applications in the search for compounds active against cancer, thus generating new compounds with pharmaceutical quarter.

13. Further research directions, if any: Metabolism  $\alpha,\beta$ -unsaturated ketones into derivatives of isoxazolines, pyrimidin-2-thiones,...

14. Thesis-related publications:

[1] Nguyen Minh Thao, Duong Ngoc Toan, Nguyen Van Nam, Nguyen Ngoc Thanh, Nguyen Thi Bao Yen (2011), "Stydy, synthesis and metabolism of some  $\alpha,\beta$ -unsaturated ketones derived from 3-acetyl-2-methylchromone", *Journal of Chemistry*, Vol. 49 (2ABC), pp. 656-664.

[2] Duong Ngoc Toan, Nguyen Thi Minh Thu, Nguyen Minh Thao, Ta Van Dai (2013), "Synthesis of some 2-aryl-4-(2'-hydroxyphenyl)-1,5-benzothiazepines", *Journal of Chemistry*, Vol. 51 (2ABC), pp. 292-295.

[3] Duong Ngoc Toan, Le Van Thuan, Nguyen Minh Thao (2012), "Synthesis of some  $\alpha,\beta$ -unsaturated ketones from 3-acetyl-2-methylbenzo[f]chromone", *Journal of Chemistry*, Vol. 50 (2), pp. 239-244.

[4] Duong Ngoc Toan, Ngo Thi Van, Chu Anh Van, Nguyen Thi Minh Thu, Nguyen Minh Thao (2012), "Synthesis of some  $\alpha,\beta$ -unsaturated ketones from 3-acetyl-4-methylbenzo[f]coumarin", *Journal of Chemistry*, Vol. 50 (4A), pp. 110-114.

[5] Duong Ngoc Toan, Nguyen Hong Huan, Nguyen Minh Thao, Nguyen Thi Minh Thu (2013), "Synthesis of some 2-aryl-4-(5'-hydroxy-4'-methylcoumarin-6'-yl)-1,5-benzothiazepines", *Journal of Chemistry*, Vol. 51 (4), pp. 438-442.

[6] Duong Ngoc Toan, Nguyen Minh Thao (2012), "Synthesis of some 2-aryl-4-(2'-hydroxyphenyl)-2,3-dihydro-1H-1,5-benzodiazepines", *Journal of Chemistry*, Vol. 50 (3), pp. 357-361.

[7] Duong Ngoc Toan, Nguyen Minh Thao (2012), "Synthesis of some 2-aryl-4-(4'-methylcoumarin-3'-yl)-2,3-dihydro-1H-1,5-benzodiazepines", *Journal of Chemistry*, Vol. 50 (4A), pp. 100-104.

[8] Duong Ngoc Toan, Nguyen Minh Thao (2012), "Synthesis of some 2-amino-6-aryl-4-(5-hydroxy-4-methylcoumarin-6-yl)pyrimidines", *Journal of Chemistry*, Vol. 50 (4A), pp. 105-109.

[9] Duong Ngoc Toan, Nguyen Minh Thao (2012), "Synthesis of some 5-aryl-3-(2-hydroxyphenyl)-1-(4-nitrophenyl)pyrazolines", *Journal of Chemistry*, Vol. 50 (4), pp. 444-448.

[10] Duong Ngoc Toan, Nguyen Minh Thao, Nguyen Thi Minh Thu, Nguyen Ngoc Thanh (2013), "Synthesis of some 5-aryl-3-(4-methylcoumarin-3-yl)-1-(4-nitrophenyl)-3-pyrazolines", *Journal of Chemistry*, Vol. 51 (1), pp. 91-95.

[11] Duong Ngoc Toan, Nguyen Minh Thao, Nguyen Hong Huan (2012), "Study on synthesis and biological activities of some 2-aryl-4-(5'-hydroxy-4'-methylcoumarin-6'-yl)-2,3-dihydro-1H-1,5-benzodiazepines", *Journal of Chemistry*, Vol. 50 (5A), pp. 131-135.