

Information on Doctoral thesis of Fellows Dao Thi Nhung

1. Full name: Dao Thị Nhung
2. Sex: Female
3. Date of birth: March 12, 1983
4. Place of birth: Bac Ninh
5. Admission decision number: 5429/SĐH dated October 30, 2008 by President of Vietnam National University, HaNoi
6. Changes in academic process: None
7. Official thesis title: "Synthesis and properties of 5-Isothiocyanatoaryl-1,3,4-oxadiazol-2-thiol
8. Major: Organic Chemistry
9. Code: 62 44 27 01
10. Supervisors: Assoc.Prof.Dr.Sc. Luu Van Boi
11. Summary of the new findings of the thesis

Have been improved the new, high efficiency and environmentally friendly method for thiocarbamylation of aminobenzohidrazide by tetramethylthiuram disulphide for synthesis of 3-[4-(or 5)-(5-mercapto-1,3,4-oxadiazol-2-yl)phenyl]-1,1-dimethylthioure derivatives, including 5 new substances.

Have been developed the optimum conditions for the decomposition of 3-[4-(or 5)-(5-mercapto-1,3,4-oxadiazol-2-yl)phenyl]-1,1-dimethylthioure derivatives into 5-[(4 or 5)-(isothiocyanatophenyl)-1,3,4-oxadiazol-2-thiol by mineral acid in which have 5 new substances.

By condensation of isothiocyanates with N-nucleophile agents, have been synthesized 76 organic compounds of thiosemicarbazides, thioureas, thiazolines, thiadiazol-2-thiols, quinazolines and thiohydantoins, including 70 new substances;

Have been used microwave-assisted method for synthesis of organic compounds. The results showed that the microwave-assisted method not only improved the yields, but also allowed significantly shorten the reaction time from 18-70 times compared with conventional methods.

Have been determined structures of all synthesized substances by modern physico-chemical methods (IR-, NMR-, MS). By ¹H-NMR method, have been detected and successfully explained the appearance of two rotational isomers of thiohydantoin derivatives XIg- XVIIg is due to methyl group attached in aryl ring is at *ortho position* towards the thiohydantoin heterocycle.

Have been tested the biological activity of the prepared compounds. The results showed that the compounds contained thiadiazol VIa,g and thioure IXa-d,f,g possessing high antifungal activity, the thioure VIIc, IXc and quinazolin Xc resistant 4 to 6 microorganisms.

12. Paratical applicability, if any:

This study showed that thiocarbamoylation of containing-amine benzohydrazides is one of the best ways affording compounds with two functional groups namely thiol group and isothiocyanate group. The presence of these two groups in one molecule of obtained compounds could not only intensify ability of bioactive but also increase chemical transformation. Therefore, some potential substances applied in pharmaceutical chemistry could be prepared easily by this way.

13. Further research directions, if any:

In this study, have been transformed of NCS group. Further studies will focus on transformation of SH group to make « pseudonucleoside» derivatives used for inhibiting the growth of cancer cells and anti-HIV type I.

14. Thesis-related publications:

[1]. Dao Thi Nhung, Luu Van Boi (2010), "Synthesis and properties of 5-(4-isothiocyanatophenyl)-1,3,4-oxadiazol-2 thiol", *Journal of Chemistry* 48 (4B), pp. 46-51.

[2]. Dao Thi Nhung, Luu Van Boi (2010), "Contribution to synthesis of 5-isothiocyanate-2-(5-mercapto-1,3,4-oxadiazol-2-yl)phenol and its derivatives", *Journal of Chemistry* 48 (4B), pp. 52-56.

[3]. Dao Thi Nhung, Luu Van Boi (2012), "Preparation and properties of 5-(4-isothiocyanato-2-bromphenyl)-1,3,4-oxadiazol-2-thiol", *Journal of Chemistry* 50 (1), pp. 19-24.

[4]. Dao Thi Nhung, Luu Van Boi (2012), "Synthesis and transformation of 4-isothiocyanato-2-(5-mercapto-1,3,4-oxadiazol-2-yl)phenol", accepted paper, *Journal of Science*, Vietnam National University, Natural Sciences and Technology.

[5]. Dao Thi Nhung, Luu Van Boi (2012), "Preparation and properties of 5-(3-isothiocyanato-4-methylphenyl)-1,3,4-oxadiazol-2-thiol", accepted paper, *Journal of Science*, Vietnam National University, Natural Sciences and Technology.