



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student : KAUSTAV BANERJEE

Roll Number : 166122042

Programme of Study : Ph.D.

Thesis Title: SYNTHESSES OF BIOACTIVE ORGANOSELENIUM COMPOUNDS AND EVALUATION OF THEIR ANTI-CANCER AND ANTIOXIDANT ACTIVITIES

Name of Thesis Supervisor(s) : DR. KRISHNA PADA BHABAK

Thesis Submitted to the Department/ Center : DEPARTMENT OF CHEMISTRY

Date of completion of Thesis Viva-Voce Exam : 19.11.2021

Key words for description of Thesis Work : ORGANOSELENIUM, ANTIOXIDANT, ANTI-CANCER.

SHORT ABSTRACT

The thesis described above deals with the synthesis of novel organoselenocyanates and evaluation of their activity as antioxidants and anti-proliferative agents. As an introduction to the thesis in Chapter 1, a general background on cancer and carcinogenesis leading to cancer development, preventive and treatment options is provided. Relevant literature evidences of important organoselenium compounds as potential chemopreventive/therapeutic agents are also discussed here. Following the literature, a series of benzylic selenocyanates have been developed in Chapter 2 which are inspired from previously known benzyl selenocyanates such as *p*-XSC, having promising chemopreventive properties. The compound bearing three selenocyanate functionalities was identified as the most effective compound against MDA-MB-231 cells and also MCF-7 and T-47D cells while being relatively less toxic to normal cells. Furthermore, the same compound arrested the cancer cells at S phase of the cell cycle, inhibited cellular migration, and showed favourable drug-like properties suggesting that increasing the number of selenocyanate functionalities in a single molecule enhances the anti-proliferative activity of the compound against triple-negative cancer cells. Chapter 3 describes synthesis of additional substituted benzyl selenocyanates as well as 1,2,3-triazole and 2,4-thiazolidine-1,3-dione-containing selenocyanates which also showed significant anti-cancer activities. Compounds bearing 1,2,3-triazole moiety, displayed prominent cytotoxicity against both MDA-MB-231 cells and normal HEK-293 cells, therefore showing lesser selectivity towards cancer cells. Contrastingly, 4-nitrobenzyl selenocyanate showed higher selectivity towards MDA-MB-231 cells. The same compound was found to be responsible for S-phase cell-cycle arrest and downregulation of anti-apoptotic, cell survival and anti-inflammatory proteins such as bcl-2, survivin

and COX-2 respectively. Chapter 4 reports development of benzimidazole- and imidazole-based ionic selenocyanates and the corresponding selenazolium and selenazinium selenocyanates and evaluation of their antioxidant activities. Finally, Chapter 5 reports synthesis of additional set of benzimidazole-based selenazolium and selenazinium selenocyanates having a 4-substituted phenyl moiety and a newer class of C2-phenyl substituted benzimidazole-based open chain ionic and neutral selenocyanates. The compounds developed in chapters 4 and 5 were evaluated for their anti-cancer activities similar to as reported in chapter 2; 4-NO₂-substituted benzimidazole-based neutral selenocyanate was identified as the best compound against MDA-MB-231 cells.

