

Department of Chemistry

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A standpoint of supervisor regarding PhD Theses "Adamantane based multitopic guests and their binding properties" by Shantanu Ganesh Kulkarni

Shantanu Kulkarni has participated on research in my group for four years, since 2012. As title of his theses indicates, his work was aimed at preparation of guest molecules with multiple binding sites and studies of their binding properties towards suitable hosts, namely cucurbiturils (CBs) and cyclodextrins (CDs). Considering the number of binding sites based on adamantane moiety, the guests of his interest can be divided into three families, tetratopic, tritopic and ditopic (actually with one additional site of lower affinity). The main purpose of working on such guest molecules was to prepare and describe new suitable components for complex supramolecular assemblies such as hydrogels or vesicles.

The structure of submitted document reflects aims mentioned above. Theoretical part provides information regarding structure of cucurbituril and cyclodextrin hosts and some basic properties of adamantane itself and its derivatives. Large space is dedicated to presentation of application of supramolecular systems based on CBs and CDs. Discussion part is divided into three parts as synthetic approaches and binding properties (if applicable) of tetratopic, tritopic and ditopic guests are given.

Shantanu did not succeed in one area, namely in preparation of tetratopic guests. However, I must state that he paid a lot of effort in these syntheses and this failure should be attributed rather to unbiased circumstances than to his deficiency in lab skills or whatever else. On the other hand, his work on tritopic guest was successfully finished and results were already published in scientific journal. In final chapter regarding ditopic guests, some new interesting findings are described. Particularly, supramolecular properties and behaviors of stilbene guests were described in details and presently supported by molecular dynamics simulations (not included in Thesis). These results are prepared for publication.

Based on his previous experiences, Shantanu developed and improved his skills in organic synthesis and supramolecular binding studies. He has demonstrated excellent theoretical knowledge in organic synthesis, very good practical skills in the laboratory, and very good analytical skills in interpreting spectral data and presenting results. Shantanu has been able to analyze scientific problems, propose solutions and perform experiments autonomously.

Last but not least, as open, kind, friendly, and enthusiastic person, acting always in a civil manner Shantanu was very pleasant co-worker.

In my opinion, submitted PhD Thesis meets all requirements and therefore I support acceptance of the Thesis for the defence.

In Zlín, 23-09-2016

