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Examiner's report on the Ph.D. thesis

Examiner: Prof. Vladimír Šindelář, Ph.D.

Applicant: **Mr. Vishwas D. Joshi**

Thesis Title: **Synthesis of novel helquats and their properties**

This thesis describes a multidisciplinary project which is based on the synthesis of new helquats with potential application in fields of nonlinear optics and chemosensing. Large number of new compounds were synthesized and characterized. The synthetic approach is clever as it allows straightforward preparation of many helquat derivatives in gram scale. This appeared to be useful in late stage of the project when the applicant decided to study influence of small structural changes in helquats on their properties.

I was impressed not only by amount of work presented in the thesis, but also by logical concept of the project and the most importantly by exiting results. New compounds were investigated for nonlinear optic applications and for selective recognition of heparin and specific DNA sequences. Some of them performed better than those currently used.

The thesis is written with a good level of English. In some places of the discussion part, I would appreciate more detail description for better understanding (e.g. explanation of fluorescence light-up experiments (page 71) and determination of dissociation constants (page 80). Also several abbreviations are not included in the list in the beginning of the thesis (L-DBT, UFH, LMWH, DAPI) which complicate fluent reading of the text. There are also some formal issues: Title of the thesis I found in the information system of Charles University (Helquats, their synthesis and properties) differs from that one given in the thesis (Synthesis of novel helquats and their properties). In agreement with new requirements for PhD thesis I received only electronic form of the thesis. However, the file I received contains two theses, one following the other.

In conclusion, the thesis as a whole makes good impression. Mr. Vishwas D. Joshi demonstrated creative skills and the presented work meets requirements for PhD thesis. Therefore I am happy to recommend the dissertation work to be suitable for the defense.

I have few specific comments:

1) Applicant should specify in detail his contribution on entire experimental part including the synthesis of new compounds, measurement of nonlinear optical properties and target-specific fluorescence light-up properties.



2) In the conclusion part, applicant stated that more than 500 compounds were synthesized but significantly smaller number of compounds is listed in Experimental section. Please explain.

3) Did you study possible self-association between molecules of helquat derivatives which may influence absorption and emission spectra?

4) Please specify conditions for determination of K_d shown in Table 12 (media, temperature...). How did you calculate K_d for the complexes in which stoichiometry was unclear?

5) Helquats 29, 30, and 33 are very similar structural analogs. Could you discuss (speculate) why only 29 out of these three compounds selectively recognizes AT-rich dsDNA sequences?

Brno, January 10, 2018.

Vladimír Šindelář

