



Přírodovědecká
fakulta
Faculty
of Science

Jihočeská univerzita
v Českých Budějovicích
University of South Bohemia
in České Budějovice

OPPONENT'S REVIEW ON BACHELOR THESIS

Name of the student: Marco Halbeisen

Thesis title: Modelling of tick-borne encephalitis virus (TBEV) proteins and their complexes

Supervisor: doc. Mgr. Roman Tůma, Ph.D.

Referee: Mgr. Libor Hejduk

Referee's affiliation: Department of Chemistry FSc USB

	Point scale ¹	Points
(1) FORMAL REQUIREMENTS		
Extent of the thesis (for bachelor theses min. 18 pages, for masters theses min. 25 pages), balanced length of the thesis parts (recommended length of the theoretical part is max. 1/3 of the total length), logical structure of the thesis	0-3	3
Quality of the theoretical part (review) (number and relevancy of the references, recency of the references)	0-3	3
Accuracy in citing of the references (presence of uncited sources, uniform style of the references, use of correct journal titles and abbreviations)	0-3	3
Graphic layout of the text and of the figures/tables	0-3	2
Quality of the annotation	0-3	3
Language and stylistics, complying with the valid terminology	0-3	3
Accuracy and completeness of figures/tables legends (clarity without reading the rest of the text, explanation of the symbols and labeling, indication of the units)	0-3	3
Formal requirements – points in total		20
(2) PRACTICAL REQUIREMENTS		
Clarity and fulfillment of the aims	0-3	3
Ability to understand the results, their interpretation, and clarity of the results, discussion, and conclusions	0-3	3
Discussion quality – interpretation of the results and their discussion with the literature (absence of discussion with the literature is not acceptable)	0-3	3
Logic in the course of the experimental work	0-3	3
Completeness of the description of the used techniques	0-3	3

¹ Mark as: 0-unsatisfactory, 1-satisfactory, 2-average, 3-excellent.

Experimental difficulty of the thesis, independence in experimental work	0-3	3
Quality of experimental data presentation	0-3	3
The use of up-to-date techniques	0-3	3
Contribution of the thesis to the knowledge in the field and possibility to publish the results (after eventual supplementary experiments)	0-3	3
Practical requirements – points in total		27
POINTS IN TOTAL (MAX/AWARDED)	48	47

Comments of the reviewer on the student and the thesis:

Student Marco Halbeisen presented a well-made thesis, which is a nice example of modern approach in structural biochemistry integrating computational and experimental methods for studying biomacromolecules. Student mastered various computational methods including modelling, docking, molecular dynamics simulation, experimental laboratory methods of production of recombinant protein, and its usage in assays. The thesis indicates quantity of work, which was done especially in the computational part, which cannot be described in the text. The topic is briefly but adequately introduced, methods are well described and results are clearly explained and discussed. In a nutshell, I did not find any procedural mistakes in the experimental part.

The thesis is well written and properly structured with adequate length of each part. Concerning the formal requirements, I did not find any serious mistakes, which can influence the final evaluation. However, there are several formal mistakes, which may be missed during the final proofreading of the thesis. Author mainly forgot about page numbers, which can complicate orientation in the thesis. Other mistakes mentioned in points:

- *Ixodes ricinus* at the first page is not written in italics
- methyltransferase abbreviation is explained when used the second time
- sometime missing dots and spacers
- repeated numbering of sections, examples: 3.1.3.5 or 3.2.2 or 4.3 or skipped from 1.2 to 1.4.

The layout of Table 2 is a little bit irritating: table legend is interrupted and divided into two pages after two lines of text and table column “L539A forward” is divided into two pages. Also numbering of figures and tables is sometime chaotic: Figure 4 in section 1.2.2 is mentioned before Figure 2 in section 1.4. In section 3.1.2, the mentioned table should be number 3, not 4 and tables mentioned as the appendix tables number 2 and 3 were numbered in the appendix as tables 6 and 7. In the methodology part, 3.2.8 Enzymatic phosphate assay the plate loading is described with formal (proofreading missed) mistakes in numbers and units, which do not correspond to the manual of the assay kit. This will be mentioned in the questions.

Despite the several formal mistakes, which did not influence thesis evaluation, I recommend this thesis for the defense.

Suggestions and questions, to which the student has to answer during the defense.
Mistakes, which the students should avoid in the future:

Requirement:

In section 3.2.8 Enzymatic phosphate assay, lines 4-8, you made some mistakes in numbers or units in the description of plate layout compared to the kit manual. Can you check it and present the correction?

Questions:

1. Concerning the section 4.2 Docking NS3 and NS5, you described the crosslinking experiment done by Dr. Zdeněk Franta and interacting residues of the proteins. Despite the discrepancy of the results, can you show these residues at the structural model, just for illustration, compared to the HADDOCK prediction result side by side?
2. In methodology section 3.2.2 and results 4.3 you described Q5 PCR mutagenesis and problem with GC-rich primers. Did you try to use Q5 High GC enhancer or some other troubleshooting option?

In the future, be careful mainly about page numbers, tables and figures layout and other typing mistakes.

Conclusion:

**In conclusion, I recommend the thesis for the defense and I suggest the grade
Excellent (1)**

In **České Budějovice** date **6.6.2022**

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signature