

fakulta v Českých Budějovicích
Faculty University of South Bohemia
of Science in České Budějovice

## SUPERVISOR'S STATEMENT ON BACHELOR THESIS

Name of the student: Marc Ninou Codina **Biological Chemistry** Study program:

Department/Institute:

**Institute of Chemistry** 

Thesis title:

Theoretical study of bacteriochlorophyll aggregates using methods of

quantum chemistry and molecular mechanics

Supervisor:

Mgr. David Řeha, Ph.D.

**Supervisor's affiliation:** University of South Bohemia, Institute of Chemistry

	Point scale <sup>1</sup>	Points
(1) FORMAL REQUIREMENTS		
Formal and graphical quality of the thesis	0-3	3
Ability to work with literature	0-3	3
Language and stylistics	0-3	2
Formal requirements – points in total		8
(2) PRACTICAL REQUIREMENTS		
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 results and their discussion with the literature	0-3	3
Experimental difficulty of the thesis, independence in experimental work	0-3	3
Contribution of the thesis to the knowledge in the field and the possibility to publish the results (after eventual supplementary experiments)	0-3	3
Practical requirements – points in total		15
POINTS IN TOTAL (MAX/AWARDED)	24	23

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

## Comments of the supervisor on the student and the thesis:

Marc has started his work on this project in autumn 2017. The main aim of the project is to study the self-aggregation of bacteriochlorophyll molecules into the curved aggregates found in chlorosomes. Marc's task was to attempt to identify the origin of curvature formation in those aggregates from a local energy perspective, using QM and QM/MM calculations.

Marc was very enthusiastic and hardworking student, who was able to learn very difficult subjects — Quantum Mechanics and Methods of QM and QM/MM calculations in chemistry and their application on biomolecules. He has also independently studied the literature and familiarized himself with work about chlorosomes and current state of our project. He has used every free time he had during very challenging coursework to come to the lab and work on his part of the project. Mars is also very social person who can nicely interact with other people, which makes him a perfect team member. Marc's results proved to be important for our overall project. Although he has not found the origin of curvature formation in bacteriochlorophyll aggregates, but he can exclude the local energy as the contributing factor. This has allowed us to focus on the other underlying causes of the curvature formation (global energy, entropy).

## Conclusion:

In conclusion, I highly

r e c o m m e n d

the thesis for the defense.

In České Budějovice date 28.1.2020

signature