

Opponent's Report

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Title: Comparison of fast single-molecule experiments and simulation of translocation through the SecY translocon

A computational framework based on Monte carlo simulation was developed in the bachelor's thesis to estimate a mechanism of protein translocation through SecYEG translocon.

The structure and properties of SecYEG followed by description of translocation mechanism models are explained in the Introduction. In the Methods the student describes used algorithms and physical model integrated into the simulation. A scheme and achieved results are presented in the next chapter followed by discussion and conclusion. There are 65 references closely related to the aim of the bachelor's thesis. Supplementary figures are also enclosed.

The work is well-structured and easy to follow. However, there are a lot of orthographic mistakes, sometimes the sentence is not finished, a verb is missing (*e. g.* page 2–3, 14), the same sentence or word are repeated (*e. g.* “between within” on page 12, description of Figure 13). It would be better to repeat citation again to be more clear where equations or statements are coming from (*e. g.* Allen et al., page 11, equations on pages 14–15). In the work, there is a good explanation of symbols used in equations but in the chapters 2.3 and 2.4 the symbol description is missing. There are sections 3.1–3.4 but chapter 3 is missing. A lot of figures are incorrectly referred (Figure 2, Figures 6–9) and Figure 4 is not referred in the text at all. Description of Figure 9 and supplementary figures are not sufficient. There is no paragraph division in the text. The chapter Discussion should be extended.

The simulation of protein translocation using SecYEG complex would have a great impact for dispatching of biochemistry experiments. I suppose that selection of physical models and code writing were hard and time consuming work. The potential of created package has been shown in the work and it is very promising for future application. In advance the package offers modularity. Unfortunately, the bachelor's thesis contains a lot of formal mistakes. The problem is also in a very brief description of results. Even a few more sentences would make it easier to understand the biological impact of presented observations.

Nevertheless, I would recommend the bachelor's thesis for defense with evaluation mark of B.

Some question to think about and answer:

1. Which approximation was done to omit density function in equation (7)?
2. Why is the axes length in the Figure 5 on page 19 different?
3. Can you describe the Figure 9 in bigger details?
4. Residue Cross Correlation in the Figure 12 is very interesting method but only briefly discussed in work. Please, provide more information including the possibility to see the time scale.
5. Do you plan to provide public access to the package?

In České Budějovice, 17th May, 2018


Filip Dyčka