Research Trip Summary Report

Task 2. Foreign mobility of WUST doctoral students

I. Data of the doctoral student

1.Full name: **Daniel Wiczew**

2.Year of studies: **2**

3. Educational discipline: **Biomedical engineering**

II. Foreign research trip (research visit)

1. Research institute in which the foreign research was implemented: **Pompeu Fabra / Parc de Recerca Biomèdica de Barcelona in Barcelona**

2. Name and surname of the host person (mentor): **Gianni de Fabritiis**

3. Dates of the research trip: **01.10.2021 – 31.12.2021**

4. Title and date of a seminar delivered during the research trip: **"Applying curiosity-driven reinforcement learning to molecular dynamics simulations", 03.10.2021**; Furthermore, there were weekly meetings with presentations on the regular basis.

5. Description of work carried out during the research trip:

During the research trip, fallowing was carried out:

- Weekly meeting with the host's research group;
- Research and discussion with the group on the Reinforcement Learning based algorithm that was proposed in the Individual Research Plan (further called IPB) from 2019;
- Learning constructing synthetic mathematical molecular environments to benchmark machine learning algorithms applied to molecular dynamics;
- Evaluating performance of available deep-learning-based dimensionality reduction model (Reversible Vampnet) based on the host's molecular dynamics data;

6. Description of the main results obtained:

During the research trip, the reinforcement learning algorithm from point 2.1.1 of IPB (Point: "Investigating reinforcement learning as enhancing sampling of a high-dimensional space of molecular simulation") was assessed based on the

synthetically constructed molecular environments. This helped to decide further the steps with regard to the step from the research plan (IPB).

7. Future collaborations (if applicable):

May be considered in the future

8. Title and date of a seminar presenting the results of the trip delivered at Wroclaw University of Science and Technology after returning from the research trip: Constructing synthetic mathematical molecular models to evaluate machine learning based algorithms, 24.01.2022.

III. Doctoral student's signature

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(Date)
(doctoral student's signature)

IV. Confirmation and information from the host

1. Confirmation of compliance of the information contained in the report: I CONFIRM / DO NOT CONFIRM. (*In justified cases, the confirmation of the host may be sent by e-mail to the Dean's Office of the Doctoral School email: interdocschool@pwr.edu.pl)*

2. Additional information and comments from host (mentor)

Daniel was present at Parc de Recerca Biomèdica de Barcelona between 01.10.2021 – 31.12.2021. Furthermore, he actively attended weekly group meetings and presented his part of the research.

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(Date)
(signature(s) of Host)