

Research Internship: Activity report

Mass Spectrometry Data Cleaning for Improved Identification of Post Translational Modifications

Nathan Marckx

1st Master Biomedical Sciences

Promotor: Lennart Martens


Copromotor: Robbin Bouwmeester



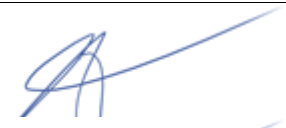



Mentor: Arthur Declercq





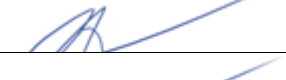

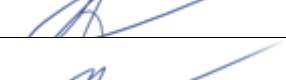



Academic year 2022-203








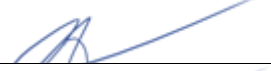
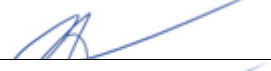



Activity report






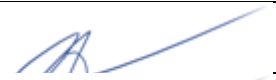






Title reseach internship	Student	Promotor	Co-promotor	Mentor
Mass Spectrometry Data Cleaning for Improved Identification of PTMs	Nathan Marckx	Lennart Martens	Robbin Bouwmeester	Arthur Declercq



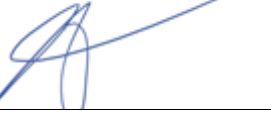




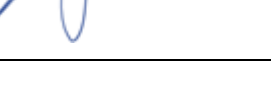
Date	Activity	Contact (name)	Signature
02/10/2022	<p>Literature study on articles provided with the topic</p> <ul style="list-style-type: none"> Degroeve, S., Gabriels, R., Velghe, K., Bouwmeester, R., Tichshenko, N., & Martens, L. (2021). ionbot: a novel, innovative and sensitive machine learning approach to LC-MS/MS peptide identification. bioRxiv. Declercq, A., Bouwmeester, R., Hirschler, A., Carapito, C., Degroeve, S., Martens, L., & Gabriels, R. (2022). MS2Rescore: Data-driven rescoring dramatically boosts immunopeptide identification rates. Molecular & Cellular Proteomics, 100266. Abdrakhimov, D. A., Bubis, J. A., Gorshkov, V., Kjeldsen, F., Gorshkov, M. V., & Ivanov, M. V. (2021). Biosaur: An open-source Python software for liquid chromatography–mass spectrometry peptide feature detection with ion mobility support. Rapid Communications in Mass Spectrometry, e9045. Kong, A. T., Leprevost, F. V., Avtonomov, D. M., Mellacheruvu, D., & Nesvizhskii, A. I. (2017). MSFragger: ultrafast and comprehensive peptide identification in mass spectrometry–based proteomics. Nature methods, 14(5), 513-520. <p>(3u)</p>	/	

08/10/2022	<p>Literature study & watching videos</p> <ul style="list-style-type: none"> • Deep Learning in Proteomics Bo Wen,* Wen-Feng Zeng, Yuxing Liao, Zhiao Shi, Sara R. Savage, Wen Jiang, and Bing Zhang* • https://www.youtube.com/watch?v=D5YQ3ZLESZM • https://www.youtube.com/watch?v=j2e2xiXVla4 • https://www.youtube.com/watch?v=tOGM2gOHKPc <p>(2u)</p>	/	
09/10/2022	<p>Literature study on PubMed & watching videos</p> <ul style="list-style-type: none"> • https://www.youtube.com/watch?v=2oPUylbPxLo • DeepLC can predict retention times for peptides that carry as-yet unseen modifications Robbin Bouwmeester 1,2, Ralf Gabriels 1,2, Niels Hulstaert1,2, Lennart Martens 1,2 ✉ and Sven Degroeve1,2 • Comprehensive and Empirical Evaluation of Machine Learning Algorithms for Small Molecule LC Retention Time Prediction. Robbin Bouwmeester,†,‡ Lennart Martens,* ,†,‡ and Sven Degroeve†,‡ • The Age of Data-Driven Proteomics: How Machine Learning Enables Novel Workflows. Robbin Bouwmeester, Ralf Gabriels, Tim Van Den Bossche, Lennart Martens,* and Sven Degroeve <p>(4u)</p>	/	
11/10/2022	<ul style="list-style-type: none"> • First meeting with promotor, co-promotor & mentor • Introduction to the topic <p>(2u)</p>	Lennart Martens Robbin Bouwmeester Arthur Declercq	
24/10/2022	<p>Lab Training @ Zwijnaarde Proteomics Extravaganza</p> <p>(8u)</p>	Robbin Bouwmeester Arthur Declercq	
12/11/2022	<p>Literature study</p> <p>(4u)</p>	/	
16/11/2022	<p>Lab training @ Zwijnaarde Peptide and Protein identification CompOmics Tutorials 1.1 (Database Generation) & 1.2 (Peak List Generation)</p> <p>(6u)</p>	Robbin Bouwmeester	

17/11/2022	Lab Training @Zwijnaarde Peptide and Protein identification CompOmics Tutorials 1.3 (Peptide to Spectrum Matching) & 1.4 (Browsing Identification Results) (5u)	Robbin Bouwmeester	
18/11/2022	Lab Training @Zwijnaarde Peptide and Protein identification CompOmics Tutorials 1.5 (Peptide and Protein Validation), 1.6 (PTM Analysis) & 1.7 (De Novo Peptide Identification) (5u)	Robbin Bouwmeester	
23/11/2022	Literature study (2u)	/	
24/11/2022	Lab Training Kaggle online course "Pandas" (4u)	Robbin Bouwmeester	
29/11/2022	Literature study (3u)	/	
08/12/2022	Lab Training GitHub (2u)	Robbin Bouwmeester	
14/12/2022	Literature Study (4u)	/	
15/12/2022	Lab Training GitHub (2u)	Robbin Bouwmeester	
14/02/2023	Lab Training Python Programming (Dodona) (4u)	Robbin Bouwmeester	
24/02/2023	Lab Training Statistical Analysis in Proteomics – Chapter 1 (3u)	Robbin Bouwmeester	

02/03/2023	Lab Training Statistical Analysis in Proteomics – Chapter 3 (4u)	Robbin Bouwmeester	
07/03/2023	<ul style="list-style-type: none"> Meeting with co-promotor and mentor concerning section “Rationale & positioning with regard to the state-of-the-art” & “Scientific research objectives” @Zwijnaarde Writing proposal & literature study (4u)	Robbin Bouwmeester Arthur Declercq	
11/03/2023	Proposal Writing (2u)	/	
22/03/2023	Lab Training Sage (3u)	Robbin Bouwmeester	
24/03/2023	Lab Training Python Programming (Dodona) (5u)	Robbin Bouwmeester	
03/04/2023	Proposal Writing (1u)	/	
06/04/2023	Proposal Writing (8u)	/	
07/04/2023	Proposal Writing (6u)	/	
08/03/2023	Proposal Writing (3u)	/	
10/04/2023	Proposal Writing (4u)	/	
12/04/2023	Proposal Writing (3u)	/	
14/04/2023	Proposal Writing (3u)	/	

15/04/2023	Proposal Writing (6u)	/	
18/04/2023	Lab Training Kaggle online course "Intro to Machine Learning" (5u)	Robbin Bouwmeester	
19/04/2023	Lab Training Kaggle online course "Intro to Machine Learning" (6u)	Robbin Bouwmeester	
26/04/2023	Feedback on section "Rationale & positioning with regard to the state-of-the-art" & "Scientific research objectives" (2u)	Arthur Declercq	
27/04/2023	<ul style="list-style-type: none"> Meeting with co-promotor and mentor concerning section "Research methodology & work plan" @Zwijnaarde Writing proposal & literature study (4u)	Robbin Bouwmeester Arthur Declercq	
02/05/2023	Proposal Writing (8u)	/	
03/05/2023	Proposal Writing (6u)	/	
03/05/2023	Feedback on section "Rationale & positioning with regard to the state-of-the-art" (1u)	Arthur Declercq	
05/05/2023	Proposal Writing (3u)	/	
05/05/2023	Feedback on section "Rationale & positioning with regard to the state-of-the-art" (1u)	Arthur Declercq	
06/05/2023	Proposal Writing (7u)	/	
07/05/2023	Proposal Writing (5u)	/	

08/05/2023	Lab Training Kaggle online course "Data Cleaning" + Python programming (Dodona) (6u)	Robbin Bouwmeester	
09/05/2023	Lab Training Kaggle online course "Data Visualization" (5u)	Robbin Bouwmeester	
10/05/2023	Feedback on section "Rationale & positioning with regard to the state-of-the-art" & "Research methodology & work plan" (2u)	Robbin Bouwmeester	
11/05/2023	Proposal Writing (1u)	/	
12/05/2023	Proposal Writing (2u)	/	
13/05/2023	Proposal Writing (4u)	/	
15/05/2023	Meeting with co-promotor and mentor concerning finalization of the proposal @Zwijnaarde (1u)	Robbin Bouwmeester Arthur Declercq	
16/05/2023	Proposal Writing (3u)	/	
18/05/2023	Final feedback + submission RI & activity report (1u)	Lennart Martens Robbin Bouwmeester Arthur Declercq	