Markus Heinonen | PhD — AI research scientist

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Impact | **68 publications** | **2.8K citations** | **27 H-index** | **3.2M funding secured** | **18x PhD advisor**

Domains | Deep learning, GenAI, ODEs/SDEs/PDEs, diffusion, Bayesian statistics, bioinformatics, proteins

Skills | Python, PyTorch, JAX, numpy, wandb, rdkit, git, slurm, latex, C++, MATLAB, R, Java, SQL

Experience

Academy Research Fellow | Principal investigator — Aalto University, Finland 2020–2025
– Leader in project *Deep learning with differential equations* — budget 0.57M
– Co-lead an 12 university 5 pharma AI drug design EU consortium — total budget 3.92M
– Co-lead an AI drug design project — budget 0.96M
– Co-lead an autonomous learning consortium — budget 1.02M

Academy postdoctoral fellow | Principal investigator — Aalto University 2016–2019
– Leader in project *Next-generation statistical learning for synthetic enzyme engineering* — budget 0.37M

Postdoctoral researcher | prof. Harri Lähdesmäki lab — Aalto University 2015–2016
– Bayesian enzyme optimisation to modify substrate specificity; metabolic modelling

Postdoctoral researcher | prof. Florence d'Alché-Buc lab — TeleCom ParisTech, France 2013–2014
– Modelling temporal gene expression under irradiation damage

Research highlights

(1) Y Verma, M Heinonen, V Garg (ICLR 2024). ClimODE: Climate forecasting with physics-informed neural ODEs | Oral presentation (top 4% of 2260 papers)

We propose a physics-inspired weather predictor that is up to 100x smaller than major transformer competitors (eg. NVIDIA, Microsoft), while having 10-30% improved performance.

(2) T Trinh, M Heinonen, L Acerbi, S Kaski (ICML 2022). Tackling covariate shift with node-based Bayesian neural networks | Oral presentation (top 10% of 1233 papers)

We present 1000x more efficient Bayesian networks by treating hidden nodes as stochastic instead of weights, which allows turning pre-trained networks into Bayesian ones for improved calibration and performance.

(3) S Rissanen, M Heinonen, A Solin (ICLR 2023). Generative modelling with inverse heat dissipation

We introduce a novel diffusion model that reduces signal by blurring instead of adding noise. The blurry diffusion organises the data distribution in a detail hierarchy, offering smooth generation and fast training.

(4) Y Verma, M Heinonen, V Garg (ICML 2023). AbODE: Ab initio antibody design using conjoined ODEs

We show SOTA performance on conditional generation of antibodies given antigens using a principled and simple flow generation over the protein coordinates and residue labels.

(5) P Hegde, M Heinonen, H Lähdesmäki, S Kaski (AISTATS 2019). Deep learning with differential Gaussian process flows | Best paper award (top 1% of 360 papers)

We introduce diffusion classifiers (before diffusion models) where an SDE morphs the data to be maximally separable by a subsequent classifier. We show outsanding performance on Gaussian process benchmarks.

Education

PhD Computer Science | supervisor prof. Juho Rousu — University of Helsinki, Finland 2013
– Thesis *Computational methods for small molecules* with Distinction
MSc Computer Science — University of Helsinki 2008

Research funding

Deep learning with differential equations — Academy of Finland
Principal investigator for two researchers (12 FTE, 570K), acceptance ratio 11% — 2020–2025

Next-generation statistical learning for synthetic enzyme engineering — Academy of Finland
Principal investigator (3 FTE, 370K), acceptance ratio 15% — 2016–2018

Advanced machine learning for Innovative Drug Discovery (AIDD) — EU-H2020-MSCA-ITN-EID
2 researchers for 3 years (6 FTE, 259K) — 2021–2024
Co-Supervisor for 2 phd students

Human-steered next-generation machine learning for reviving drug design (HEALED) — Academy of Finland
4 researchers for 4 years (16 FTE, 960K) — 2021–2025
Co-supervisor for 1 phd student, 1 postdoc

Bridging the Reality Gap in Autonomous Learning (B-REAL) — Academy of Finland
3 researchers for 3 years (9 FTE, 1020K) — 2020–2022
Co-supervisor for 1 phd student, 1 postdoc

Artificial Intelligence for SynBio Powerhouse (AI4SynBio) — Sitra
Principal investigator (1 FTE) — 2018

Academic supervision

Postdocs
Maryam Sabzevari 2018–19 (PI), Charles Gadd 2019–2021 (advisor), Anton Mallasto 2020–2022 (advisor)

PhD students (co-supervision)
Rafal Karczewski 2023–, Nawja Laabid 2023–, Yogesh Verma 2022–, Yasmine Nahal 2022–, Severi Rissanen 2021–, Arslan Masood 2021–, Trunh Tring 2021–, Anirudh Jain 2020–

PhD degrees (co-supervision)
Valerii Iakovlev (2025), Emmi Jokinen (2024), Pashupati Hegde (2023), Zheyang Shen (2022), Cagatay Yildiz (2022), Mohammad Moein (2022), Sami Remes (2019), Huibin Shen (2017), Hongyu Su (2015)

Master degrees (co-supervision)
Pashupati Hegde (2018), Zheyang Shen (2018), Kenneth Blomqvist (2018), Parisa Mapar (2018), Anni Antikainen (2017), Emmi Jokinen (2016)

Doctoral evaluation committees

David Frich Hansen — DTU, Denmark, 2023
Towards real time Raman molecular imaging of living organisms

Tuomo Hartonen — University of Helsinki, Finland, 2022
Novel computational methods for studying the role and interactions of transcription factors in gene regulation

Joseph Sakaya — University of Helsinki, Finland, 2020
From Approximations to Decisions

Teaching

Gaussian processes (co-lecturer) — Aalto University, Finland, 2019, 2021–23
Machine learning in Bioinformatics (guest lecturer) — Aalto 2017
Special course in Bioinformatics II (guest lecturer) — Aalto 2015–17
Kernel Methods (guest lecturer) — Aalto 2016

Machine Learning: Basic Principles (co-lecturer) Aalto 2016–17
From data to knowledge (coordinator) Aalto 2015
Computational methods for Systems biology (co-lecturer) University of Helsinki 2012

Honors

Notable paper award **(top 1%)**, *Deep learning with differential GP flows*, AISTATS 2019

Best presentation award, MLSB 2014

Oral presentations: ICML 2022, ICLR 2024, AISTATS 2025

Highlight presentations: NeurIPS 2024, ICLR 2024

Top reviewer: ICML 2020, NeurIPS 2022, AISTATS 2022–23, TMLR

Academic service

Organiser

ELLIS Robust ML workshop Helsinki, Finland 2024
ELLIS Robust ML workshop Espoo, Finland 2023
Dagstuhl Seminar: *Differential Equations and Continuous-Time Deep Learning* Wadern, Germany 2022
Workshop on Deep structures Espoo, Finland 2019
Workshop on Machine learning in Systems biology Strasbourg, France 2014
Workshop on Mass Spectrometry Informatics in Systems biology Helsinki, Finland 2010
Machine Learning Coffee Seminar, Finnish Center of AI 2019–2024

Associate editor

Pattern Recognition 2023–
Transaction in Machine Learning Research 2024–

Senior program committee

AAAI, IJCAI

Program committee

NeurIPS, ICML, AISTATS, ICLR, ECML, ISMB

Reviewer

Neural networks, Bioinformatics, BMC Bioinformatics, Molecular Biosystems, J Am soc for Mass Spectrometry, PLOS ONE, Mass Spectrometry Reviews, IEEE Signal Processing Letters, JMLR, TMLR, Machine Learning, IEEE Transactions on Pattern Analysis and Machine Intelligence, Engineering Applications of Artificial Intelligence, Nature Communications Medicine

Funding committees

Medical Research Council UK 2017, 2019
National Science Centre Poland 2019, 2021

Board member: Finnish society for bioinformatics 2010–2013

Invited talks

Bayesian repulsive ensembles with a Jacobian twist KAUST, Saudi Arabia, 2024

Learning continuous-time dynamics under uncertainty Doshi-Velez lab, Harvard, 2024

Can neural ODEs forecast global weather? Tubingen, Germany, 2024

Can neural ODEs forecast global weather?	Linköping, Sweden, 2024
Efficient Bayesian neural networks with node parameterisation	EURECOM, France, 2023
Efficient Bayesian neural networks with node parameterisation	DTU, Denmark, 2023
Generative models for molecules	Shonan, Japan, 2023
New perspectives to generation and decision-making	Dagstuhl, Germany, 2022
Tackling covariate shift with node-based Bayesian neural networks	ICLM, USA, 2022
Continuous-time models under uncertainty	ICSB, Germany, 2022
From differential learning to diffusion models	CMS, London, 2022
Learning continuous-time dynamics	GenU, Denmark, 2021
Learning continuous-time dynamics	Telecom Paristech, France, 2021
Spectral kernels	GP summer school, 2021
Deploying deep learning-based models in projects and real-world cases	AstraZeneca, Sweden, 2021
Infinitely deep models with differential Gaussian process flows	U Manchester, Imperial, Prowler.AI, UK, 2019
Deep learning with differential Gaussian process flows	AISTATS, Japan, 2019
Towards deep learning with differential equations	Bosch AI, Germany, 2019
Towards automated molecular design: Bayesian deep learning perspectives	AstraZeneca, Sweden, 2019
Output-sparse latent Gaussian processes	CMS, Italy, 2018
Approximating Rosetta with machine learning	RosettaCon, USA, 2017

Publications (peer-reviewed)

68 publications, **27** H-index, **2800** citations scholar.google.com/citations?user=hFtfHZoAAAAJ

[1] Anirudh Jain, Markus Heinonen, Heikki Käsnänen, Julius Sipilä, and Samuel Kaski. Multi-target property prediction and optimization using latent spaces of generative model. *Machine Learning: Science and Technology*, 2025.

[2] Severi Rissanen, RuiKang OuYang, Jiajun He, Wenlin Chen, Markus Heinonen, Arno Solin, and José Miguel Hernández-Lobato. Progressive tempering sampling with diffusion. In *ICML*, 2025.

[3] Rafal Karczewski, Markus Heinonen, and Vikas Garg. Devil is in the details: Density guidance for detail-aware generation with flow models. In *ICML*, 2025.

[4] Sofie Lundgren, Jani Huuhtanen, ..., and Satu Mustjoki. Single-cell analysis of aplastic anemia reveals a convergence of NK and NK-like CD8+ T cells with a disease-associated TCR signature. *Science Translational Medicine*, 18, 2025.

[5] Quentin Bouniot, Ievgen Redko, Anton Mallasto, Charlotte Laclau, Karol Arndt, Oliver Struckmeier, Markus Heinonen, Ville Kyrki, and Samuel Kaski. From alexnet to transformers: Measuring the non-linearity of deep neural networks with affine optimal transport. In *CVPR*, 2025.

[6] Rafal Karczewski, Markus Heinonen, and Vikas Garg. Diffusion models as cartoonists! The curious case of high density regions. In *ICLR*, 2025.

[7] Severi Rissanen, Markus Heinonen, and Arno Solin. Free hunch: Denoiser covariance estimation for diffusion models without extra costs. In *ICLR*, 2025.

[8] Najwa Laabid, Severi Rissanen, Markus Heinonen, Arno Solin, and Vikas Garg. Alignment is key for applying diffusion models to retrosynthesis. In *ICLR*, 2025.

[9] Alexandru Dumitrescu, Dani Korpela, Markus Heinonen, Yogesh Verma, Valerii Iakovlev, Vikas Garg, and Harri Lähdesmäki. Field-based molecule generation. In *ICLR*, 2025.

[10] Rafal Karczewski, Samuel Kaski, Markus Heinonen, and Vikas Garg. What ails generative structure-based drug design: Too little or too much expressivity? In *AISTATS*, 2025. Oral presentation (top 2%).

[11] Markus Heinonen, Ba-Hien Tran, Michael Kampffmeyer, and Maurizio Filippone. Robust classification by coupling data mollification with label smoothing. In *AISTATS*, 2025.

[12] Ossi Arasalo, Arttu Lehtonen, Mari Kielosto, Markus Heinonen, and Juho Pokki. Probabilistic analysis of spatial viscoelastic cues in 3d cell culture using magnetic microrheometry. *Biophysical Journal*, 2024.

[13] Yasmine Nahal, Janosch Menke, Julien Martinelli, Markus Heinonen, Mikhail Kabeshov, Jon Paul Janet, Eva Nittinger, Ola Engkvist, and Samuel Kaski. Human-in-the-loop active learning for goal-oriented molecule generation. *J Chemoinformatics*, 2024.

[14] Trung Trinh, Markus Heinonen, Luigi Acerbi, and Samuel Kaski. Improving robustness to corruptions with multiplicative weight perturbations. In *NeurIPS*, 2024. Highlight presentation (8% of accepted).

[15] Trung Trinh, Markus Heinonen, Luigi Acerbi, and Samuel Kaski. Input gradient diversity for neural network ensembles. In *ICLR*, 2024. Highlight presentation (15% of accepted).

[16] Yogesh Verma, Markus Heinonen, and Vikas Garg. ClimODE: Climate forecasting with physics-informed neural ODEs. In *ICLR*, 2024. Oral presentation (4% of accepted).

[17] Valerii Iakovlev, Markus Heinonen, and Harri Lähdesmäki. Learning space-time continuous latent neural PDEs from partially observed states. In *NeurIPS*, 2023.

[18] Giulio Franzese, Giulio Corallo, Simone Rossi, Markus Heinonen, Maurizio Filippone, and Pietro Michiardi. Continuous-time functional diffusion processes. In *NeurIPS*, 2023.

[19] Mohammad Moein, Markus Heinonen, Natalie Mesens, Ronnie Chamanza, Chidozie Amuzie, Yvonne Will, Hugo Ceulemans, Samuel Kaski, and Dorota Herman. Chemistry-based modelling on phenotype-based drug-induced liver injury annotation: from public to proprietary data. *Chemical Research in Toxicology*, 2023.

[20] Oliver Struckmeier, Ievgen Redko, Anton Mallasto, Karol Arndt, Markus Heinonen, and Ville Kyrki. Learning representations that are closed-form Monge mapping optimal with application to domain adaptation. *TMLR*, 2023.

[21] Aarne Talman, Hande Celikkanat, Sami Virpioja, Markus Heinonen, and Jörg Tiedemann. Uncertainty-aware natural language inference with stochastic weight averaging. In *NoDaLiDa*, 2023.

[22] Yogesh Verma, Markus Heinonen, and Vikas Garg. AbODE: Ab initio antibody design using conjoined ODEs. In *ICML*, 2023.

[23] Magnus Ross and Markus Heinonen. Learning energy conserving dynamics efficiently with Hamiltonian Gaussian processes. *TMLR*, 2023.

[24] Vishnu Raj, Tianyu Cui, Markus Heinonen, and Pekka Marttinen. Incorporating functional summary information in Bayesian neural networks using a Dirichlet process likelihood approach. In *AISTATS*, 2023.

[25] Valerii Iakovlev, Cagatay Yildiz, Markus Heinonen, and Harri Lähdesmäki. Latent neural ODEs with sparse Bayesian multiple shooting. In *ICLR*, 2023.

[26] Severi Rissanen, Markus Heinonen, and Arno Solin. Generative modelling with inverse heat dissipation. In *ICLR*, 2023.

[27] Iiris Sundin, Alexey Voronov, Haoping Xiao, Kostas Papadopoulos, Esben Bjerrum, Markus Heinonen, Atanas Patronov, Samuel Kaski, and Ola Engkvist. Human-in-the-loop assisted de novo molecular design. *Journal of chemoinformatics*, 4, 2022.

[28] Emmi Jokinen, Alexandru Dumitrescu, Jani Huuhtanen, Vladimir Gligorijevic, Satu Mustjoki, Richard Bonneau, Markus Heinonen, and Harri Lähdesmäki. TCRconv: predicting recognition between T cell receptors and epitopes using contextualized motifs. *Bioinformatics*, 2022.

[29] Yogesh Verma, Samuel Kaski, Markus Heinonen, and Vikas Garg. Modular flows: Differential molecular generation. In *NeurIPS*, 2022.

[30] Trung Trinh, Markus Heinonen, Luigi Acerbi, and Samuel Kaski. Tackling covariate shift with node-based Bayesian neural networks. In *ICML*, 2022. Oral presentation (10% of accepted).

[31] Pashupati Hegde, Cagatay Yildiz, Harri Lähdesmäki, Samuel Kaski, and Markus Heinonen. Variational multiple shooting for Bayesian ODEs with Gaussian processes. In *UAI*, 2022.

[32] Alexander Aushev, Henri Pesonen, Markus Heinonen, Jukka Corander, and Samuel Kaski. Likelihood-free inference with deep Gaussian processes. *Computational Statistics & Data Analysis*, 174:1–19, 2022.

[33] Anni Antikainen, Markus Heinonen, and Harri Lähdesmäki. Modeling binding specificities of transcription factor pairs with random forests. *BMC Bioinformatics*, 23, 2022.

[34] Jarkko Toivonen, Yrjö Koski, Esa Turkulainen, Femmeke Prinsze, Pietro della Briotta Parolo, Markus Heinonen, and Mikko Arvas. Prediction and impact of personalized donation intervals. *Vox Sanguinis*, 117, 2021.

[35] Anton Mallasto, Markus Heinonen, and Samuel Kaski. Bayesian inference for optimal transport with stochastic cost. In *ACML*, 2021.

[36] Zheyang Shen, Markus Heinonen, and Samuel Kaski. De-randomizing MCMC dynamics with the diffusion Stein operator. In *NeurIPS*, 2021.

[37] Cagatay Yildiz, Markus Heinonen, and Harri Lähdesmäki. Continuous-time model-based reinforcement learning. In *ICML*, 2021.

[38] Emmi Jokinen, Jani Huuhtanen, Satu Mustjoki, Markus Heinonen, and Harri Lähdesmäki. Predicting recognition between T cell receptors and epitopes with TCRGP. *PLoS computational biology*, 17, 2021.

[39] Valerii Iakovlev, Markus Heinonen, and Harri Lähdesmäki. Learning continuous-time PDEs from sparse data with graph neural networks. In *ICLR*, 2021.

[40] Simone Rossi, Markus Heinonen, Edwin Bonilla, Zheyang Shen, and Maurizio Filippone. Sparse Gaussian processes revisited: Bayesian approaches to inducing-variable approximations. In *AISTATS*, 2021.

[41] Sanni Voutilainen, Markus Heinonen, Martina Andberg, Emmi Jokinen, Hannu Maaheimo, Johan Pääkkönen, Nina Hakulinen, Juha Rouvinen, Harri Lähdesmäki, Samuel Kaski, Juho Rousu, Merja Penttilä, and Anu Koivula. Substrate specificity of 2-deoxy-d-ribose 5-phosphate aldolase (DERA) assessed by different protein engineering and machine learning methods. *Applied Microbiology and Biotechnology*, 104, 2020.

[42] Zheyang Shen, Markus Heinonen, and Samuel Kaski. Learning spectrograms with convolutional spectral kernels. In *AISTATS*, 2020.

[43] Kenneth Blomqvist, Samuel Kaski, and Markus Heinonen. Deep convolutional Gaussian processes. *ECML/PKDD*, 2019.

[44] Cagatay Yildiz, Markus Heinonen, and Harri Lähdesmäki. ODE^{2}VAE: Deep generative second order ODEs with Bayesian neural networks. In *NeurIPS*, 2019.

[45] Markus Heinonen, Maria Osmala, Henrik Mannerström, Sandra Castillo, Mikko Arvas, Harri Lähdesmäki, Samuel Kaski, and Juho Rousu. Bayesian metabolic flux analysis reveals the intracellular flux couplings. *Bioinformatics*, 35:i548–i557, 2019.

[46] Pashupati Hegde, Markus Heinonen, Harri Lähdesmäki, and Samuel Kaski. Deep learning with differential Gaussian process flows. In *AISTATS*, 2019. Notable paper award (1% of accepted).

[47] Zheyang Shen, Markus Heinonen, and Samuel Kaski. Harmonizable mixture kernels with variational Fourier features. In *AISTATS*, 2019.

[48] Cagatay Yildiz, Markus Heinonen, Henrik Mannerström, Jukka Intosalmi, and Harri Lähdesmäki. Learning stochastic differential equations with Gaussian processes without gradient matching. In *IEEE Workshop on Machine Learning for Signal Processing (MLSP)*, 2018.

[49] Markus Heinonen, Cagatay Yildiz, Henrik Mannerström, Jukka Intosalmi, and Harri Lähdesmäki. Learning unknown ODE models with Gaussian processes. In *ICML*, 2018.

[50] Pashupati Hegde, Markus Heinonen, and Samuel Kaski. Variational zero-inflated Gaussian processes with sparse kernels. In *UAI*, 2018.

[51] Markus Heinonen, Fabian Milliat, Mohamed Benadjaoud, Agnes Francois, Valerie Buard, Georges Tarlet, Florence d'Alche Buc, and Olivier Guipaud. Temporal clustering analysis of endothelial cell gene expression following exposure to a conventional radiotherapy dose fraction using Gaussian process clustering. *PLOS ONE*, 2018.

[52] Anna Cichonska, Tapio Pahikkala, Sandor Szedmak, Helil Julkunen, Antti Airola, Markus Heinonen, Tapio Aittokallio, and Juho Rousu. Learning with multiple pairwise kernels for drug bioactivity prediction. *Bioinformatics*, 34:i509–i518, 2018.

[53] Emmi Jokinen, Markus Heinonen, and Harri Lähdesmäki. mGPfusion: Predicting protein stability changes upon single and multiple mutations with Gaussian processes and data fusion. *Bioinformatics*, 34:i274–i283, 2018.

[54] Kyle Barlow, Shane Conchuir, Samuel Thompson, Pooja Suresh, James Lucas, Markus Heinonen, and Tanja Kortemme. Flex ddG: Rosetta ensemble-based estimation of changes in protein-protein binding affinity upon mutation. *Journal of Physical Chemistry B*, 122:5389–5399, 2018.

[55] Sami Remes, Markus Heinonen, and Samuel Kaski. A mutually-dependent Hadamard kernel for modelling latent variable couplings. In *ACML*, 2017.

[56] Sami Remes, Markus Heinonen, and Samuel Kaski. Non-stationary spectral kernels. In *NIPS*, 2017.

[57] Romain Brault, Markus Heinonen, and Florence d'Alche Buc. Random Fourier features for operator-valued kernels. In *ACML*, volume 63 of *PMLR*, pages 110–125, 2016.

[58] Markus Heinonen, Henrik Mannerström, Juho Rousu, Samuel Kaski, and Harri Lähdesmäki. Non-stationary Gaussian process regression with Hamiltonian Monte Carlo. In *AISTATS*, volume 51 of *PMLR*, pages 732–740, 2016.

[59] Tiina Pakula, Heli Nygren, Dorothee Barth, Markus Heinonen, Sandra Castillo, Merja Penttilä, and Mikko Arvas. Genome wide analysis of protein production load in Trichoderma reesei. *Biotechnology for Biofuels*, 9, 2016.

[60] Markus Heinonen, Olivier Guipaud, Fabien Milliat, Valerie Buard, Beatrice Micheau, Georges Tarlet, Marc Benderitter, Farida Zehraoui, and Florence d'Alche Buc. Detecting time periods of differential gene expression using Gaussian processes: An application to endothelial cells exposed to radiotherapy dose fraction. *Bioinformatics*, 31:728–735, 2015.

[61] Huibin Shen, Nicola Zamboni, Markus Heinonen, and Juho Rousu. Metabolite identification trough machine learning – Tackling CASMI challenge using FingerID. *Metabolites*, 3:484–505, 2013.

[62] Markus Heinonen, Huibin Shen, Nicola Zamboni, and Juho Rousu. Metabolite identification and fingerprint prediction via machine learning. *Bioinformatics*, 28:2333–41, 2012. Oral presentation at ISMB/ECCB.

[63] Markus Heinonen, Niko Välimäki, Velil Mäkinen, and Juho Rousu. Efficient path kernels for reaction function prediction. In *Proceedings of the International Conference on Bioinformatics Models, Methods and Algorithms*, pages 202–207, 2012.

[64] Markus Heinonen, Sampsa Lappalainen, Taneli Mielikäinen, and Juho Rousu. Computing atom mappings for biochemical reactions without subgraph isomorphism. *Journal of Computational Biology*, 18:43–58, 2011.

[65] Hongyu Su, Markus Heinonen, and Juho Rousu. Multilabel classification of drug-like molecules via max-margin conditional random fields. In *Proceedings of the Fifth European Workshop on Probabilistic Graphical Model*, pages 265–272. HIIT, 2010.

[66] Hongyu Su, Markus Heinonen, and Juho Rousu. Structured output prediction of anti-cancer drug activity. In *Proceedings of the 5th IAPR international conference on Pattern recognition in bioinformatics*, PRIB'10, pages 38–49. Springer-Verlag, 2010.

[67] Markus Heinonen, Ari Rantanen, Taneli Mielikäinen, Juha Kokkonen, Jari Kiuru, Raimo Ketola, and Juho Rousu. Fid: a software for *ab initio* structural identification of product ions from tandem mass spectrometric data. *Rapid Communications in Mass Spectrometry*, 22:3043–3052, 2008.

[68] Markus Heinonen, Ari Rantanen, Taneli Mielikäinen, Esa Pitkänen, Juha Kokkonen, and Juho Rousu. *Ab Initio* prediction of molecular fragments from tandem mass spectrometry data. In *German Conference on Bioinformatics*, volume P-83 of *LNI*, pages 40–53. GI, 2006.