

# Wout Bittremieux

University of Antwerp  
Middelheimlaan 1 – 2020 Antwerp – Belgium

✉ [wout.bittremieux@uantwerpen.be](mailto:wout.bittremieux@uantwerpen.be) • [bittremieux.be](https://www.bittremieux.be)  
@ [@wout@sigmoid.social](https://twitter.com/wout@sigmoid.social) • [bittremieux](https://www.github.com/bittremieux) • [0000-0002-3105-1359](https://orcid.org/0000-0002-3105-1359)

## Employment

- 2022–... **Assistant Professor** (Computer Science)  
University of Antwerp, Antwerp, Belgium
- 2019–22 **Postdoctoral Researcher** (Pharmacy and Pharmaceutical Sciences)  
University of California San Diego, La Jolla, CA, USA  
Advisor: Pieter C. Dorrestein, PhD
- 2017–19 **Postdoctoral Researcher** (Genome Sciences)  
University of Washington, Seattle, WA, USA  
Advisor: William Stafford Noble, PhD

## Education

- 2013–17 **PhD in Computer Science**  
University of Antwerp, Antwerp, Belgium  
Thesis: *Computational Solutions for Quality Control of Mass Spectrometry-based Proteomics*  
Advisors: Kris Laukens, PhD and Bart Goethals, PhD
- 2016 **Visiting Researcher**  
Stellenbosch University, Cape Town, South Africa
- 2010–12 **MSc in Computer Science**  
Hasselt University, Diepenbeek, Belgium  
Thesis: *Time Series Similarity Search*  
Advisors: Marc Gyssens, PhD
- 2007–10 **BSc in Computer Science**  
Hasselt University, Diepenbeek, Belgium  
Thesis: *Extending a Web Browser With Additional Navigation Options*  
Advisors: Jan Van den Bussche, PhD

## Awards and Honors

- 2022 **Early Career Researcher Manuscript Competition Award**  
Human Proteome Organization
- 2021 **Rising Stars in Proteomics and Metabolomics: 40 Under 40**  
*Journal of Proteome Research*
- 2020 **Postdoctoral Career Development Award**  
American Society for Mass Spectrometry
- 2019 **Travel Fellowship to the Human Proteome Organization – Proteomics Standards Initiative Spring Meeting 2019 (Cape Town, South Africa)**  
Research Foundation – Flanders

- 2017 **Travel Fellowship (nine months) to the University of Washington (Seattle, WA, USA),** Research Foundation – Flanders
- 2017 **Travel Fellowship to the Annual Conference of the American Society for Mass Spectrometry 2017 (Indianapolis, IN, USA),** Research Foundation – Flanders
- 2016 **Travel Fellowship (three months) to Stellenbosch University (Cape Town, South Africa),** Research Foundation – Flanders
- 2016 **Travel Fellowship to the Annual Conference of the American Society for Mass Spectrometry 2016 (San Antonio, TX, USA),** Research Foundation – Flanders
- 2015 **Best Oral Presentation Award,** Benelux Bioinformatics Conference 2015

## Key Publications

(\* indicates equal contributions)

- [23] **Wout Bittremieux**, Lev Levitsky, Matteo Pilz, Timo Sachsenberg, Florian Huber, Mingxun Wang, and Pieter C. Dorrestein. “Unified and Standardized Mass Spectrometry Data Processing in Python Using Spectrum\_utils.” In: *Journal of Proteome Research* (Jan. 23, 2023). DOI: [10.1021/acs.jproteome.2c00632](https://doi.org/10.1021/acs.jproteome.2c00632).
- [22] Issar Arab, William E. Fondrie, Kris Laukens, and **Wout Bittremieux**. “Semisupervised Machine Learning for Sensitive Open Modification Spectral Library Searching.” In: *Journal of Proteome Research* (Jan. 23, 2023). DOI: [10.1021/acs.jproteome.2c00616](https://doi.org/10.1021/acs.jproteome.2c00616).
- [21] **Wout Bittremieux**, Mingxun Wang, and Pieter C. Dorrestein. “The Critical Role That Spectral Libraries Play in Capturing the Metabolomics Community Knowledge.” In: *Metabolomics* 18.94 (Nov. 19, 2022). DOI: [10.1007/s11306-022-01947-y](https://doi.org/10.1007/s11306-022-01947-y).
- [20] Charlotte Adams, Kurt Boonen, Kris Laukens, and **Wout Bittremieux**. “Open Modification Searching of SARS-CoV-2–Human Protein Interaction Data Reveals Novel Viral Modification Sites.” In: *Molecular & Cellular Proteomics* (Oct. 2022), p. 100425. DOI: [10.1016/j.mcpro.2022.100425](https://doi.org/10.1016/j.mcpro.2022.100425).
- [19] Wout Bittremieux\*, Robin Schmid\*, Florian Huber, Justin J.J. van der Hooft, Mingxun Wang, and Pieter C. Dorrestein. “Comparison of Cosine, Modified Cosine, and Neutral Loss Based Spectral Alignment for Discovery of Structurally Related Molecules.” In: *Journal of The American Society for Mass Spectrometry* 33.9 (Aug. 12, 2022), pp. 1733–1744. DOI: [10.1021/jasms.2c00153](https://doi.org/10.1021/jasms.2c00153).
- [18] Julia M. Gauglitz\*, Kiana A. West\*, Wout Bittremieux\*, Candace L. Williams, Kelly C. Weldon, Morgan Panitchpakdi, Francesca Di Ottavio, Christine M. Aceves, Elizabeth Brown, Nicole C. Sikora, Alan K. Jarmusch, Cameron Martino, Anupriya Tripathi, Michael J. Meehan, Kathleen Dorrestein, Justin P. Shaffer, Roxana Coras, Fernando Vargas, Lindsay DeRight Goldasich, Tara Schwartz, MacKenzie Bryant, Gregory Humphrey, Abigail J. Johnson, Katharina Spengler, Pedro Belda-Ferre, Edgar Diaz, Daniel McDonald, Qiyun Zhu, Emmanuel O. Elijah, Mingxun Wang, Clarisse Marotz, Kate E. Sprecher, Daniela Vargas-Robles, Dana Withrow, Gail Ackermann, Lourdes Herrera, Barry J. Bradford, Lucas Maciel Mauriz Marques, Juliano Geraldo Amaral, Rodrigo Moreira Silva, Flavio Protasio Veras, Thiago Mattar Cunha, Rene Donizeti Ribeiro Oliveira, Paulo Louzada-Junior, Robert H. Mills, Paulina K. Piotrowski, Stephanie L. Servetas, Sandra M. Da Silva, Christina M. Jones, Nancy J. Lin, Katrice A. Lippa, Scott A. Jackson, Rima Kaddurah Daouk, Douglas Galasko, Parambir S. Dulai, Tatyana I. Kalashnikova, Curt Wittenberg, Robert Terkeltaub, Megan M. Doty, Jae H. Kim, Kyung E. Rhee, Julia Beauchamp-Walters, Kenneth P. Wright, Maria Gloria Dominguez-Bello, Mark Manary, Michelli F. Oliveira, Brigid S. Boland, Norberto Peporine Lopes, Monica Guma, Austin D. Swafford, Rachel J. Dutton, Rob Knight, and Pieter C. Dorrestein. “Enhancing Untargeted Metabolomics Using Metadata-Based Source Annotation.” In: *Nature Biotechnology* 40 (July 7, 2022), pp. 1774–1779. DOI: [10.1038/s41587-022-01368-1](https://doi.org/10.1038/s41587-022-01368-1).
- [17] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. “A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra.” In: *Nature Methods* 19 (May 30, 2022), pp. 675–678. DOI: [10.1038/s41592-022-01496-1](https://doi.org/10.1038/s41592-022-01496-1).

- [16] Xiyang Luo\*, Wout Bittremieux\*, Johannes Griss, Eric W. Deutsch, Timo Sachsenberg, Lev I. Levitsky, Mark V. Ivanov, Julia A. Bubis, Ralf Gabriels, Henry Webel, Aniel Sanchez, Mingze Bai, Lukas Käll, and Yasset Perez-Riverol. "A Comprehensive Evaluation of Consensus Spectrum Generation Methods in Proteomics." In: *Journal of Proteome Research* 21.6 (May 13, 2022), pp. 1566–1574. DOI: [10.1021/acs.jproteome.2c00069](https://doi.org/10.1021/acs.jproteome.2c00069).
- [15] **Wout Bittremieux**, Rohit S Advani, Alan K Jarmusch, Shaden Aguirre, Aileen Lu, Pieter C Dorrestein, and Shirley M Tsunoda. "Physicochemical Properties Determining Drug Detection in Skin." In: *Clinical and Translational Science* 15.3 (Mar. 2022), pp. 761–770. DOI: [10.1111/cts.13198](https://doi.org/10.1111/cts.13198).
- [14] **Wout Bittremieux**, Kris Laukens, William Stafford Noble, and Pieter C Dorrestein. "Large-Scale Tandem Mass Spectrum Clustering Using Fast Nearest Neighbor Searching." In: *Rapid Communications in Mass Spectrometry* (June 25, 2021), e9153. DOI: [10.1002/rcm.9153](https://doi.org/10.1002/rcm.9153).
- [13] **Wout Bittremieux**, David Bouyssié, Viktoria Dorfer, Marie Locard-Paulet, Yasset Perez-Riverol, Veit Schwämmle, Julian Uszkoreit, and Tim Van Den Bossche. "The European Bioinformatics Community for Mass Spectrometry (EuBIC-MS): An Open Community for Bioinformatics Training and Research." In: *Rapid Communications in Mass Spectrometry* (Apr. 16, 2021), e9087. DOI: [10.1002/rcm.9087](https://doi.org/10.1002/rcm.9087).
- [12] **Wout Bittremieux**, Charlotte Adams, Kris Laukens, Pieter C Dorrestein, and Nuno Bandeira. "Open Science Resources for the Mass Spectrometry-Based Analysis of SARS-CoV-2." In: *Journal of Proteome Research* 20.3 (Feb. 19, 2021), pp. 1464–1475. DOI: [10.1021/acs.jproteome.0c00929](https://doi.org/10.1021/acs.jproteome.0c00929).
- [11] **Wout Bittremieux**. "spectrum\_utils: A Python Package for Mass Spectrometry Data Processing and Visualization." In: *Analytical Chemistry* 92.1 (Jan. 7, 2020), pp. 659–661. DOI: [10.1021/acs.analchem.9b04884](https://doi.org/10.1021/acs.analchem.9b04884).
- [10] Lindsay Pino, Andy Lin, and **Wout Bittremieux**. "2018 YPIC Challenge: A Case Study in Characterizing an Unknown Protein Sample." In: *Journal of Proteome Research* 18.11 (Sept. 26, 2019), pp. 3936–3943. DOI: [10.1021/acs.jproteome.9b00384](https://doi.org/10.1021/acs.jproteome.9b00384).
- [9] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "Extremely Fast and Accurate Open Modification Spectral Library Searching of High-Resolution Mass Spectra Using Feature Hashing and Graphics Processing Units." In: *Journal of Proteome Research* 18.10 (Aug. 26, 2019), pp. 3792–3799. DOI: [10.1021/acs.jproteome.9b00291](https://doi.org/10.1021/acs.jproteome.9b00291).
- [8] Sander Willems, David Bouyssié, Dieter Deforce, Viktoria Dorfer, Vladimir Gorshkov, Dominik Kopczynski, Kris Laukens, Marie Locard-Paulet, Veit Schwämmle, Julian Uszkoreit, Dirk Valkenburg, Marc Vaudel, and **Wout Bittremieux**. "Proceedings of the EuBIC Developer's Meeting 2018." In: *Journal of Proteomics* 187 (Sept. 15, 2018), pp. 25–27. DOI: [10.1016/j.jprot.2018.05.015](https://doi.org/10.1016/j.jprot.2018.05.015).
- [7] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Journal of Proteome Research* 17.10 (Oct. 5, 2018), pp. 3463–3474. DOI: [10.1021/acs.jproteome.8b00359](https://doi.org/10.1021/acs.jproteome.8b00359).
- [6] **Wout Bittremieux**, David L Tabb, Francis Impens, An Staes, Evy Timmerman, Lennart Martens, and Kris Laukens. "Quality Control in Mass Spectrometry-Based Proteomics." In: *Mass Spectrometry Reviews* 37.5 (Sept. 2018), pp. 697–711. DOI: [10.1002/mas.21544](https://doi.org/10.1002/mas.21544).
- [5] **Wout Bittremieux**, Mathias Walzer, Stefan Tenzer, Weimin Zhu, Reza M Salek, Martin Eisenacher, and David L Tabb. "The Human Proteome Organization–Proteomics Standards Initiative Quality Control Working Group: Making Quality Control More Accessible for Biological Mass Spectrometry." In: *Analytical Chemistry* 89.8 (Apr. 18, 2017), pp. 4474–4479. DOI: [10.1021/acs.analchem.6b04310](https://doi.org/10.1021/acs.analchem.6b04310).
- [4] **Wout Bittremieux**, Dirk Valkenburg, Lennart Martens, and Kris Laukens. "Computational Quality Control Tools for Mass Spectrometry Proteomics." In: *PROTEOMICS* 17.3-4 (Feb. 2017), p. 1600159. DOI: [10.1002/pmic.201600159](https://doi.org/10.1002/pmic.201600159).
- [3] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Dirk Valkenburg, and Kris Laukens. "Unsupervised Quality Assessment of Mass Spectrometry Proteomics Experiments by Multivariate Quality Control Metrics." In: *Journal of Proteome Research* 15.4 (Apr. 1, 2016), pp. 1300–1307. DOI: [10.1021/acs.jproteome.6b00028](https://doi.org/10.1021/acs.jproteome.6b00028).
- [2] **Wout Bittremieux**, Hanny Willems, Pieter Kelchtermans, Lennart Martens, Kris Laukens, and Dirk Valkenburg. "iMonDB: Mass Spectrometry Quality Control through Instrument Monitoring." In: *Journal of Proteome Research* 14.5 (May 1, 2015), pp. 2360–2366. DOI: [10.1021/acs.jproteome.5b00127](https://doi.org/10.1021/acs.jproteome.5b00127).

- [1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenburg, Lennart Martens, and Kris Laukens. “jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format.” In: *Journal of Proteome Research* 13.7 (July 3, 2014), pp. 3484–3487. DOI: [10.1021/pr401274z](https://doi.org/10.1021/pr401274z).

## Additional Peer-Reviewed Publications

- [29] Eric W. Deutsch, Juan Antonio Vizcaíno, Andrew R. Jones, Pierre-Alain Binz, Henry Lam, Joshua Klein, **Wout Bittremieux**, Yasset Perez-Riverol, David L. Tabb, Mathias Walzer, Sylvie Ricard-Blum, Henning Hermjakob, Steffen Neumann, Tytus D. Mak, Shin Kawano, Luis Mendoza, Tim Van Den Bossche, Ralf Gabriels, Nuno Bandeira, Jeremy Carver, Benjamin Pullman, Zhi Sun, Nils Hoffmann, Jim Shofstahl, Yunping Zhu, Luana Licata, Federica Quaglia, Silvio C. E. Tosatto, and Sandra E. Orchard. “Proteomics Standards Initiative at Twenty Years: Current Activities and Future Work.” In: *Journal of Proteome Research* (Jan. 10, 2023). DOI: [10.1021/acs.jproteome.2c00637](https://doi.org/10.1021/acs.jproteome.2c00637).
- [28] Justin P. Shaffer, Louis-Félix Nothias, Luke R. Thompson, Jon G. Sanders, Rodolfo A. Salido, Sneha P. Couvillion, Asker D. Brejnrod, Franck Lejzerowicz, Niina Haiminen, Shi Huang, Holly L. Lutz, Qiyun Zhu, Cameron Martino, James T. Morton, Smruthi Karthikeyan, Mélissa Nothias-Esposito, Kai Dührkop, Sebastian Böcker, Hyun Woo Kim, Alexander A. Aksenov, **Wout Bittremieux**, Jeremiah J. Minich, Clarisse Marotz, MacKenzie M. Bryant, Karenina Sanders, Tara Schwartz, Greg Humphrey, Yoshiki Vásquez-Baeza, Anupriya Tripathi, Laxmi Parida, Anna Paola Carrieri, Kristen L. Beck, Promi Das, Antonio González, Daniel McDonald, Joshua Ladau, Søren M. Karst, Mads Albertsen, Gail Ackermann, Jeff DeReus, Torsten Thomas, Daniel Petras, Ashley Shade, James Stegen, Se Jin Song, Thomas O. Metz, Austin D. Swafford, Pieter C. Dorrestein, Janet K. Jansson, Jack A. Gilbert, Rob Knight, the Earth Microbiome Project 500 (EMP500) Consortium, Lars T. Angenent, Alison M. Berry, Leonora S. Bittleston, Jennifer L. Bowen, Max Chavarría, Don A. Cowan, Dan Distel, Peter R. Girguis, Jaime Huerta-Cepas, Paul R. Jensen, Lingjing Jiang, Gary M. King, Anton Lavrinienko, Aurora MacRae-Crerar, Thulani P. Makhalanyane, Tapio Mappes, Ezequiel M. Marzinelli, Gregory Mayer, Katherine D. McMahon, Jessica L. Metcalf, Sou Miyake, Timothy A. Mousseau, Catalina Murillo-Cruz, David Myrold, Brian Palenik, Adrián A. Pinto-Tomás, Dorota L. Porazinska, Jean-Baptiste Ramond, Forest Rowher, Taniya RoyChowdhury, Stuart A. Sandin, Steven K. Schmidt, Henning Seedorf, Ashley Shade, J. Reuben Shipway, Jennifer E. Smith, James Stegen, Frank J. Stewart, Karen Tait, Torsten Thomas, Yael Tucker, Jana M. U’Ren, Phillip C. Watts, Nicole S. Webster, Jesse R. Zaneveld, and Shan Zhang. “Standardized Multi-Omics of Earth’s Microbiomes Reveals Microbial and Metabolite Diversity.” In: *Nature Microbiology* 7.12 (Nov. 28, 2022), pp. 2128–2150. DOI: [10.1038/s41564-022-01266-x](https://doi.org/10.1038/s41564-022-01266-x).
- [27] Bart Cuypers, Pieter Meysman, Ionas Erb, **Wout Bittremieux**, Dirk Valkenburg, Geert Baggerman, Inge Mertens, Shyam Sundar, Basudha Khanal, Cedric Notredame, Jean-Claude Dujardin, Malgorzata A. Domagalska, and Kris Laukens. “Four Layer Multi-Omics Reveals Molecular Responses to Aneuploidy in Leishmania.” In: *PLOS Pathogens* 18.9 (Sept. 23, 2022). Ed. by Christian R. Engwerda, e1010848. DOI: [10.1371/journal.ppat.1010848](https://doi.org/10.1371/journal.ppat.1010848).
- [26] Raphael Reher, Allegra T. Aron, Pavla Fajtová, Paolo Stincone, Berenike Wagner, Alicia I. Pérez-Lorente, Chenxi Liu, Ido Y. Ben Shalom, **Wout Bittremieux**, Mingxun Wang, Kyowon Jeong, Marie L. Matos-Hernandez, Kelsey L. Alexander, Eduardo J. Caro-Diaz, C. Benjamin Naman, J. H. William Scanlan, Phil M. M. Hochban, Wibke E. Diederich, Carlos Molina-Santiago, Diego Romero, Khaled A. Selim, Peter Sass, Heike Brötz-Oosterhelt, Chambers C. Hughes, Pieter C. Dorrestein, Anthony J. O’Donoghue, William H. Gerwick, and Daniel Petras. “Native Metabolomics Identifies the Rivulariapeptolide Family of Protease Inhibitors.” In: *Nature Communications* 13.1 (Aug. 8, 2022), p. 4619. DOI: [10.1038/s41467-022-32016-6](https://doi.org/10.1038/s41467-022-32016-6).
- [25] Melih Yilmaz, William E. Fondrie, **Wout Bittremieux**, Sewoong Oh, and William Stafford Noble. “De Novo Mass Spectrometry Peptide Sequencing with a Transformer Model.” In: *Proceedings of the 39th International Conference on Machine Learning - ICML ’22*. Vol. 162. Proceedings of Machine Learning Research. Baltimore, MD, USA: PMLR, July 17, 2022, pp. 25514–25522.
- [24] Richard D. LeDuc, Eric W. Deutsch, Pierre-Alain Binz, Ryan T. Fellers, Anthony J. Cesnik, Joshua A. Klein, Tim Van Den Bossche, Ralf Gabriels, Arshika Yalavarthi, Yasset Perez-Riverol, Jeremy Carver, **Wout Bittremieux**, Shin Kawano, Benjamin Pullman, Nuno Bandeira, Neil L. Kelleher, Paul M. Thomas, and Juan Antonio Vizcaíno. “Proteomics Standards Initiative’s ProForma 2.0: Unifying

- the Encoding of Proteoforms and Peptidoforms.” In: *Journal of Proteome Research* 21.4 (Mar. 15, 2022), pp. 1189–1195. DOI: [10.1021/acs.jproteome.1c00771](https://doi.org/10.1021/acs.jproteome.1c00771).
- [23] William E Fondrie, **Wout Bittremieux**, and William Stafford Noble. “ppx: Programmatic Access to Proteomics Data Repositories.” In: *Journal of Proteome Research* 20.9 (Aug. 3, 2021), pp. 4621–4624. DOI: [10.1021/acs.jproteome.1c00454](https://doi.org/10.1021/acs.jproteome.1c00454).
- [22] Eric W Deutsch, Yasset Perez-Riverol, Jeremy Carver, Shin Kawano, Luis Mendoza, Tim Van Den Bossche, Ralf Gabriels, Pierre-Alain Binz, Benjamin Pullman, Zhi Sun, Jim Shofstahl, **Wout Bittremieux**, Tytus Mak, Joshua Klein, Yunping Zhu, Henry Lam, Juan Antonio Vizcaino, and Nuno Bandeira. “Universal Spectrum Identifier for Mass Spectra.” In: *Nature Methods* 18 (June 28, 2021), pp. 768–770. DOI: [10.1038/s41592-021-01184-6](https://doi.org/10.1038/s41592-021-01184-6).
- [21] Youzhong Liu, Thomas De Vijlder, **Wout Bittremieux**, Kris Laukens, and Wouter Heyndrickx. “Current and Future Deep Learning Algorithms for MS/MS-based Small Molecule Structure Elucidation.” In: *Rapid Communications in Mass Spectrometry* (May 6, 2021), e9120. DOI: [10.1002/rcm.9120](https://doi.org/10.1002/rcm.9120).
- [20] Samantha L Wilson, Gregory P Way, **Wout Bittremieux**, Jean-Paul Armache, Melissa A Haendel, and Michael M Hoffman. “Sharing Biological Data: Why, When, and How.” In: *FEBS Letters* 595.7 (Apr. 11, 2021), pp. 847–863. DOI: [10.1002/1873-3468.14067](https://doi.org/10.1002/1873-3468.14067).
- [19] Pieter Moris, Joey De Pauw, Anna Postovskaya, Sofie Gielis, Nicolas De Neuter, **Wout Bittremieux**, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. “Current Challenges for Unseen-Epitope TCR Interaction Prediction and a New Perspective Derived from Image Classification.” In: *Briefings in Bioinformatics* (Dec. 21, 2020), bbaa318. DOI: [10.1093/bib/bbaa318](https://doi.org/10.1093/bib/bbaa318).
- [18] Christopher Ashwood, **Wout Bittremieux**, Eric W Deutsch, Nadezhda T Doncheva, Viktoria Dorfer, Ralf Gabriels, Vladimir Gorshkov, Surya Gupta, Andrew R Jones, Lukas Käll, Dominik Kopczynski, Lydie Lane, Ludwig Lautenbacher, Marc Legeay, Marie Locard-Paulet, Bart Mesuere, Yasset Perez-Riverol, Eugen Netz, Julianus Pfeuffer, Timo Sachsenberg, Renee Salz, Patroklos Samaras, Henning Schiebenhoefer, Tobias Schmidt, Veit Schwämmle, Alessio Soggiu, Julian Uszkoreit, Tim Van Den Bossche, Bart Van Puyvelde, Joeri Van Strien, Pieter Verschaffelt, Henry Webel, and Sander Willems. “Proceedings of the EuBIC-MS 2020 Developers’ Meeting.” In: *EuPA Open Proteomics* 24 (Nov. 24, 2020), pp. 1–6. DOI: [10.1016/j.euprot.2020.11.001](https://doi.org/10.1016/j.euprot.2020.11.001).
- [17] Alexander A Aksenov, Ivan Laponogov, Zheng Zhang, Sophie L F Doran, Ilaria Belluomo, Dennis Veselkov, **Wout Bittremieux**, Louis Felix Nothias, Mélissa Nothias-Esposito, Katherine N Maloney, Biswapriya B Misra, Alexey V Melnik, Aleksandr Smirnov, Xiuxia Du, Kenneth L Jones, Kathleen Dorrestein, Morgan Panitchpakdi, Madeleine Ernst, Justin J J van der Hooft, Mabel Gonzalez, Chiara Carazzone, Adolfo Amézquita, Chris Callewaert, James T Morton, Robert A Quinn, Amina Bouslimani, Andrea Albarracín Orío, Daniel Petras, Andrea M Smania, Sneha P Couvillion, Meagan C Burnet, Carrie D Nicora, Erika Zink, Thomas O Metz, Viatcheslav Artaev, Elizabeth Humston-Fulmer, Rachel Gregor, Michael M Meijler, Itzhak Mizrahi, Stav Eyal, Brooke Anderson, Rachel Dutton, Raphaël Lugan, Pauline Le Boulch, Yann Guitton, Stephanie Prevost, Audrey Poirier, Gaud Dervilly, Bruno Le Bizec, Aaron Fait, Noga Sikron Persi, Chao Song, Kelem Gashu, Roxana Coras, Monica Guma, Julia Manasson, Jose U Scher, Dinesh Kumar Barupal, Saleh Alseekh, Alisdair R Fernie, Reza Mirnezami, Vasilis Vasilidou, Robin Schmid, Roman S Borisov, Larisa N Kulikova, Rob Knight, Mingxun Wang, George B Hanna, Pieter C Dorrestein, and Kirill Veselkov. “Auto-Deconvolution and Molecular Networking of Gas Chromatography–Mass Spectrometry Data.” In: *Nature Biotechnology* 39 (Nov. 9, 2020), pp. 169–173. DOI: [10.1038/s41587-020-0700-3](https://doi.org/10.1038/s41587-020-0700-3).
- [16] Sofie Gielis, Pieter Moris, **Wout Bittremieux**, Nicolas De Neuter, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. “Identification of Epitope-Specific T Cells in T-cell Receptor Repertoires.” In: *Bioinformatics for Cancer Immunotherapy*. Ed. by Sebastian Boegel. Vol. 2120. New York, NY: Springer US, Mar. 3, 2020, pp. 183–195. DOI: [10.1007/978-1-0716-0327-7\\_13](https://doi.org/10.1007/978-1-0716-0327-7_13).
- [15] Youzhong Liu, Aida Mrzic, Pieter Meysman, Thomas De Vijlder, Edwin P Romijn, Dirk Valkenburg, **Wout Bittremieux**, and Kris Laukens. “MESSAR: Automated Recommendation of Metabolite Substructures from Tandem Mass Spectra.” In: *PLOS ONE* 15.1 (Jan. 16, 2020), e0226770. DOI: [10.1371/journal.pone.0226770](https://doi.org/10.1371/journal.pone.0226770).
- [14] Sofie Gielis, Pieter Moris, **Wout Bittremieux**, Nicolas De Neuter, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. “Detection of Enriched T Cell Epitope Specificity in Full T Cell Receptor Sequence Repertoires.” In: *Frontiers in Immunology* 10 (Nov. 29, 2019), p. 2820. DOI: [10.3389/fimmu.2019.02820](https://doi.org/10.3389/fimmu.2019.02820).

- [13] Pieter Meysman, Yvan Saeys, Ehsan Sabaghian, **Wout Bittremieux**, Yves van de Peer, Bart Goethals, and Kris Laukens. "Mining the Enriched Subgraphs for Specific Vertices in a Biological Graph." In: *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 16.5 (Sept. 2019), pp. 1496–1507. DOI: [10.1109/TCBB.2016.2576440](https://doi.org/10.1109/TCBB.2016.2576440).
- [12] Charlie Beirnaert, Laura Peeters, Pieter Meysman, **Wout Bittremieux**, Kenn Foubert, Deborah Custers, Anastasia Van der Auwera, Matthias Cuykx, Luc Pieters, Adrian Covaci, and Kris Laukens. "Using Expert Driven Machine Learning to Enhance Dynamic Metabolomics Data Analysis." In: *Metabolites* 9.3 (Mar. 20, 2019), p. 54. DOI: [10.3390/metabo9030054](https://doi.org/10.3390/metabo9030054).
- [11] Dominik Kopczynski, **Wout Bittremieux**, David Bouyssié, Viktoria Dorfer, Marie Locard-Paulet, Bart Van Puyvelde, Veit Schwämmle, Alessio Soggiu, Sander Willems, and Julian Uszkoreit. "Proceedings of the EuBIC Winter School 2019." In: *EuPA Open Proteomics* 22–23 (Mar. 2019), pp. 4–7. DOI: [10.1016/j.euprot.2019.07.002](https://doi.org/10.1016/j.euprot.2019.07.002).
- [10] Aida Mrzic, Pieter Meysman, **Wout Bittremieux**, Pieter Moris, Boris Cule, Bart Goethals, and Kris Laukens. "Grasping Frequent Subgraph Mining for Bioinformatics Applications." In: *BioData Mining* 11.20 (Sept. 3, 2018). DOI: [10.1186/s13040-018-0181-9](https://doi.org/10.1186/s13040-018-0181-9).
- [9] Nicolas De Neuter, **Wout Bittremieux**, Charlie Beirnaert, Bart Cuypers, Aida Mrzic, Pieter Moris, Arvid Suls, Viggo Van Tendeloo, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. "On the Feasibility of Mining CD8+ T-cell Receptor Patterns Underlying Immunogenic Peptide Recognition." In: *Immunogenetics* 70.3 (Mar. 2018), pp. 159–168. DOI: [10.1007/s00251-017-1023-5](https://doi.org/10.1007/s00251-017-1023-5).
- [8] Eric W Deutsch, Sandra Orchard, Pierre-Alain Binz, **Wout Bittremieux**, Martin Eisenacher, Henning Hermjakob, Shin Kawano, Henry Lam, Gerhard Mayer, Gerben Menschaert, Yasset Perez-Riverol, Reza M Salek, David L Tabb, Stefan Tenzer, Juan Antonio Vizcaino, Mathias Walzer, and Andrew R Jones. "Proteomics Standards Initiative: Fifteen Years of Progress and Future Work." In: *Journal of Proteome Research* 16.12 (Dec. 1, 2017), pp. 4288–4298. DOI: [10.1021/acs.jproteome.7b00370](https://doi.org/10.1021/acs.jproteome.7b00370).
- [7] Juan Antonio Vizcaino, Mathias Walzer, Rafael C Jiménez, **Wout Bittremieux**, David Bouyssié, Christine Carapito, Fernando Corrales, Myriam Ferro, Albert JR Heck, Peter Horvatovich, Martin Hubalek, Lydie Lane, Kris Laukens, Fredrik Levander, Frederique Lisacek, Petr Novak, Magnus Palmblad, Damiano Piovesan, Alfred Pühler, Veit Schwämmle, Dirk Valkenborg, Merlijn van Rijswijk, Jiri Vondrasek, Martin Eisenacher, Lennart Martens, and Oliver Kohlbacher. "A Community Proposal to Integrate Proteomics Activities in ELIXIR [Version 1; Referees: 2 Approved]." In: *F1000Research* 6 (June 13, 2017), p. 875. DOI: [10.12688/f1000research.11751.1](https://doi.org/10.12688/f1000research.11751.1).
- [6] Evelyne Maes, Pieter Kelchtermans, **Wout Bittremieux**, Kurt De Grave, Sven Degroeve, Jef Hooyberghs, Inge Mertens, Geert Baggerman, Jan Ramon, Kris Laukens, Lennart Martens, and Dirk Valkenborg. "Designing Biomedical Proteomics Experiments: State-of-the-Art and Future Perspectives." In: *Expert Review of Proteomics* 13.5 (Apr. 25, 2016), pp. 495–511. DOI: [10.1586/14789450.2016.1172967](https://doi.org/10.1586/14789450.2016.1172967).
- [5] Pieter Meysman, Yvan Saeys, Ehsan Sabaghian, **Wout Bittremieux**, Yves Van de Peer, Bart Goethals, and Kris Laukens. "Discovery of Significantly Enriched Subgraphs Associated with Selected Vertices in a Single Graph." In: *Proceedings of the 14th International Workshop on Data Mining in Bioinformatics - BIODKDD '15*. Sydney, Australia, Aug. 10, 2015, p. 8.
- [4] Stefan Naulaerts, Pieter Meysman, **Wout Bittremieux**, Trung Nghia Vu, Wim Vanden Berghe, Bart Goethals, and Kris Laukens. "A Primer to Frequent Itemset Mining for Bioinformatics." In: *Briefings in Bioinformatics* 16.2 (Mar. 2015), pp. 216–231. DOI: [10.1093/bib/bbt074](https://doi.org/10.1093/bib/bbt074).
- [3] Trung Nghia Vu, **Wout Bittremieux**, Dirk Valkenborg, Bart Goethals, Filip Lemièrre, and Kris Laukens. "Efficient Reduction of Candidate Matches in Peptide Spectrum Library Searching Using the Top k Most Intense Peaks." In: *Journal of Proteome Research* 13.9 (Sept. 5, 2014), pp. 4175–4183. DOI: [10.1021/pr401269z](https://doi.org/10.1021/pr401269z).
- [2] Mathias Walzer, Lucia Espona Pernas, Sara Nasso, **Wout Bittremieux**, Sven Nahnsen, Pieter Kelchtermans, Peter Pichler, Henk W P van den Toorn, An Staes, Jonathan Vandenbussche, Michael Mazanek, Thomas Taus, Richard A Scheltema, Christian D Kelstrup, Laurent Gatto, Bas van Breukelen, Stephan Aiche, Dirk Valkenborg, Kris Laukens, Kathryn S Lilley, Jesper Velgaard Olsen, Albert J R Heck, Karl Mechtler, Ruedi Aebersold, Kris Gevaert, Juan Antonio Vizcaino, Henning Hermjakob, Oliver Kohlbacher, and Lennart Martens. "qcML: An Exchange Format for Quality Control Metrics from Mass Spectrometry Experiments." In: *Molecular & Cellular Proteomics* 13.8 (Aug. 1, 2014), pp. 1905–1913. DOI: [10.1074/mcp.M113.035907](https://doi.org/10.1074/mcp.M113.035907).

- [1] Pieter Kelchtermans, **Wout Bittremieux**, Kurt De Grave, Sven Degroeve, Jan Ramon, Kris Laukens, Dirk Valkenburg, Harald Barsnes, and Lennart Martens. "Machine Learning Applications in Proteomics Research: How the Past Can Boost the Future." In: *PROTEOMICS* 14.4-5 (Mar. 2014), pp. 353–366. DOI: [10.1002/pmic.201300289](https://doi.org/10.1002/pmic.201300289).

## Other Manuscripts

- [5] Melih Yilmaz, William E. Fondrie, **Wout Bittremieux**, Rowan Nelson, Varun Ananth, Sewoong Oh, and William Stafford Noble. *Sequence-to-Sequence Translation from Mass Spectra to Peptides with a Transformer Model*. Jan. 3, 2023. DOI: [10.1101/2023.01.03.522621](https://doi.org/10.1101/2023.01.03.522621).
- [4] Alan K. Jarmusch, Allegra T. Aron, Daniel Petras, Vanessa V. Phelan, **Wout Bittremieux**, Deepa D. Acharya, Mohammed M. A. Ahmed, Anelize Bauermeister, Matthew J. Bertin, Paul D. Boudreau, Ricardo M. Borges, Benjamin P. Bowen, Christopher J. Brown, Fernanda O. Chagas, Kenneth D. Cleverger, Mario S. P. Correia, William J. Crandall, Max Crüsemann, Tito Damiani, Oliver Fiehn, Neha Garg, William H Gerwick, Jeffrey R. Gilbert, Daniel Globisch, Paulo Wender P. Gomes, Steffen Heuckeroth, C. Andrew James, Scott A. Jarmusch, Sarvar A. Kakhkhorov, Kyo Bin Kang, Roland D Kersten, Hyunwoo Kim, Riley D. Kirk, Oliver Kohlbacher, Eftychia E. Kontou, Ken Liu, Itzel Lizama-Chamu, Gordon T. Luu, Tal Luzzatto Knaan, Michael T. Marty, Andrew C. McAvoy, Laura-Isobel McCall, Osama G. Mohamed, Omri Nahor, Timo H.J. Niedermeyer, Trent R. Northen, Kirsten E. Overdahl, Tomáš Pluskal, Johannes Rainer, Raphael Reher, Elys Rodriguez, Timo T. Sachsenberg, Laura M. Sanchez, Robin Schmid, Cole Stevens, Zhenyu Tian, Ashootosh Tripathi, Hiroshi Tsugawa, Kozo Nishida, Yuki Matsuzawa, Justin J.J. van der Hooft, Andrea Vicini, Axel Walter, Tilmann Weber, Quanbo Xiong, Tao Xu, Haoqi Nina Zhao, Pieter C. Dorrestein, and Mingxun Wang. "A Universal Language for Finding Mass Spectrometry Data Patterns." In: *bioRxiv* (Aug. 7, 2022). DOI: [10.1101/2022.08.06.503000](https://doi.org/10.1101/2022.08.06.503000).
- [3] Ceder Dens, **Wout Bittremieux**, Fabio Affaticati, Kris Laukens, and Pieter Meysman. "Interpretable Deep Learning to Uncover the Molecular Binding Patterns Determining TCR–Epitope Interactions." In: *bioRxiv* (May 2, 2022). DOI: [10.1101/2022.05.02.490264](https://doi.org/10.1101/2022.05.02.490264).
- [2] **Wout Bittremieux**, Nicole E. Avalon, Sydney P. Thomas, Sarvar A. Kakhkhorov, Alexander A. Aksenov, Paulo Wender Portal Gomes, Christine M. Aceves, Andres Mauricio Caraballo Rodriguez, Julia M. Gauglitz, William H. Gerwick, Alan K. Jarmusch, Rima F. Kaddurah-Daouk, Kyo Bin Kang, Hyun Woo Kim, Todor Kondic, Helena Mannocho-Russo, Michael J. Meehan, Alexey Melnik, Louis-Felix Nothias, Claire O'Donovan, Morgan Panitchpakdi, Daniel Petras, Robin Schmid, Emma L. Schymanski, Justin J. J. van der Hooft, Kelly C. Weldon, Heejung Yang, Jasmine Zemlin, Mingxun Wang, and Pieter C. Dorrestein. "Open Access Repository-Scale Propagated Nearest Neighbor Suspect Spectral Library for Untargeted Metabolomics." In: *bioRxiv* (May 15, 2022). DOI: [10.1101/2022.05.15.490691](https://doi.org/10.1101/2022.05.15.490691).
- [1] **Wout Bittremieux**, Christopher Chen, Pieter C Dorrestein, Emma L Schymanski, Tobias Schulze, Steffen Neumann, Rene Meier, Simon Rogers, and Mingxun Wang. "Universal MS/MS Visualization and Retrieval with the Metabolomics Spectrum Resolver Web Service." In: *bioRxiv* (Sept. 26, 2020). DOI: [10.1101/2020.05.09.086066](https://doi.org/10.1101/2020.05.09.086066).

## Invited/Keynote Presentations

- [6] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *HUPO Annual Conference Cancun, Mexico* (Dec. 7, 2022).
- [5] **Wout Bittremieux**. "Introduction to Machine Learning." In: *Imaging Mass Spectrometry Workshop, ASMS Annual Conference Minneapolis, MN, USA* (June 7, 2022).
- [4] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *Best of US HUPO 2022* (May 3, 2022). DOI: [10.5281/ZENODO.6515099](https://doi.org/10.5281/ZENODO.6515099).

- [3] **Wout Bittremieux**, Nicole Avalon, Sydney P. Thomas, Mingxun Wang, and Pieter C. Dorrestein. "Leveraging Public Untargeted Metabolomics Data to Propagate Structurally Related Molecule Annotations to Millions of MS/MS Spectra." In: *Applied Bioinformatics in Life Sciences* Leuven, Belgium (Mar. 11, 2022). DOI: [10.5281/ZENODO.6346949](https://doi.org/10.5281/ZENODO.6346949).
- [2] **Wout Bittremieux**. "Shedding Light on Complex Mass Spectrometry Proteomics Processes through Advanced Data Mining." In: *Faculty of Science Research Day* Antwerp, Belgium (Jan. 13, 2017). DOI: [10.5281/zenodo.242392](https://doi.org/10.5281/zenodo.242392).
- [1] **Wout Bittremieux** and Dirk Valkenburg. "iMonDB: Mass Spectrometry Instrument Monitoring for Quality Control." In: *Methods and Tools for Intra- and Inter-experiment LC MS Performance Tracking Workshop, ASMS Annual Conference* St. Louis, MO, USA (June 1, 2015).

## Oral Presentations

- [12] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *US HUPO 2022* Charleston, SC, USA (Mar. 1, 2022). DOI: [10.5281/ZENODO.6320843](https://doi.org/10.5281/ZENODO.6320843).
- [11] **Wout Bittremieux**, Julia Gauglitz, Alexander Aksenov, Alan K Jarmusch, Louis-Felix Nothias, Daniel Petras, Mingxun Wang, and Pieter C Dorrestein. "Repository-Scale Propagated Spectral Library of Suspects." In: *SoCal Science @Home Lollapalooza* (Dec. 1, 2020). DOI: [10.5281/zenodo.4300710](https://doi.org/10.5281/zenodo.4300710).
- [10] **Wout Bittremieux**, Damon H May, Jeffrey Bilmes, and William Stafford Noble. "Deep Neural Network Embedding for Efficient Repository-Scale Analysis of Hundreds of Millions of Mass Spectra." In: *ASMS 2020 Reboot* (June 8, 2020). DOI: [10.5281/zenodo.3831052](https://doi.org/10.5281/zenodo.3831052).
- [9] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "Identifying Millions of Protein Modifications Using GPU-powered Approximate Nearest Neighbor Searching." In: *GPU Technology Conference* (Mar. 26, 2020). DOI: [10.5281/zenodo.3831055](https://doi.org/10.5281/zenodo.3831055).
- [8] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Cascadia Proteomics Symposium* Seattle, WA, USA (July 23, 2018). DOI: [10.5281/zenodo.1319035](https://doi.org/10.5281/zenodo.1319035).
- [7] **Wout Bittremieux**. "Git: How Version Control Can Power Your Research." In: *Biomina Lunch Talks* Antwerp, Belgium (June 24, 2016). DOI: [10.5281/zenodo.56352](https://doi.org/10.5281/zenodo.56352).
- [6] **Wout Bittremieux**, Dirk Valkenburg, and Kris Laukens. "Optimized Open Modification Spectral Library Searching Using Approximate Nearest Neighbor Techniques." In: *ASMS Annual Conference* San Antonio, TX, USA (June 9, 2016). DOI: [10.5281/zenodo.55999](https://doi.org/10.5281/zenodo.55999).
- [5] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Bart Goethals, Dirk Valkenburg, and Kris Laukens. "Approaches for Mass Spectrometry Quality Control." In: *Biomina Research Day* Antwerp, Belgium (Dec. 9, 2015). DOI: [10.5281/zenodo.56004](https://doi.org/10.5281/zenodo.56004).
- [4] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Bart Goethals, Dirk Valkenburg, and Kris Laukens. "Analysis of Mass Spectrometry Quality Control Metrics." In: *Benelux Bioinformatics Conference* Antwerp, Belgium (Dec. 7, 2015). DOI: [10.5281/zenodo.56001](https://doi.org/10.5281/zenodo.56001).
- [3] **Wout Bittremieux** and Kris Laukens. "Precursor-Free and Fast Spectral Library Search Using Approximate Nearest Neighbor Techniques." In: *Benelux Bioinformatics Conference Student Council Symposium* Antwerp, Belgium (Dec. 6, 2015). DOI: [10.5281/zenodo.56002](https://doi.org/10.5281/zenodo.56002).
- [2] **Wout Bittremieux**, Emmanuel Müller, Dirk Valkenburg, Lennart Martens, Bart Goethals, and Kris Laukens. "Pattern Mining of Mass Spectrometry Quality Control Data." In: *Benelux Bioinformatics Conference* Luxembourg, Luxembourg (Dec. 9, 2014). DOI: [10.5281/zenodo.56000](https://doi.org/10.5281/zenodo.56000).
- [1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenburg, Lennart Martens, and Kris Laukens. "Collecting and Mining Mass Spectrometry Quality Control Data." In: *Biomina Research Day* Antwerp, Belgium (Feb. 20, 2014). DOI: [10.5281/zenodo.56003](https://doi.org/10.5281/zenodo.56003).

## Poster Presentations

- [15] Charlotte Adams, Issar Arab, William E. Fondrie, Kurt Boonen, Kris Laukens, and **Wout Bittremieux**. "Semi-Supervised Rescoring For Open Modification Searching Reveals Protein Modifications During SARS-CoV-2 Infection." In: *HUPO Annual Conference* Cancun, Mexico (Dec. 6, 2022).



- [14] **Wout Bittremieux**, Robin Schmid, Florian Huber, Justin J.J. van der Hooft, Mingxun Wang, and Pieter C. Dorrestein. "Comparison of Spectrum Similarity Measures for Discovery of Structurally Related Molecules." In: *ASMS Annual Conference* Minneapolis, MN, USA (June 8, 2022). DOI: [10.5281/ZENODO.6609002](https://doi.org/10.5281/ZENODO.6609002).
- [13] **Wout Bittremieux**, Nicole Avalon, Sydney P. Thomas, Mingxun Wang, and Pieter C. Dorrestein. "Leveraging Public Untargeted Metabolomics Data to Propagate Annotations to Millions of MS/MS Spectra." In: *US HUPO 2022* Charleston, SC, USA (Mar. 1, 2022). DOI: [10.5281/ZENODO.6303580](https://doi.org/10.5281/ZENODO.6303580).
- [12] **Wout Bittremieux**, Sydney P Thomas, Mingxun Wang, and Pieter C Dorrestein. "Repository Scale Propagated Spectral Library of Suspects for Untargeted Metabolomics." In: *ASMS Annual Conference* Philadelphia, PA, USA (Nov. 2, 2021). DOI: [10.5281/ZENODO.5609253](https://doi.org/10.5281/ZENODO.5609253).
- [11] **Wout Bittremieux**, Damon H May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *Machine Learning in Computational Biology* Vancouver, BC, Canada (Dec. 14, 2019). DOI: [10.5281/zenodo.3576516](https://doi.org/10.5281/zenodo.3576516).
- [10] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "ANN-SoLo: Extremely Fast and Accurate Open Modification Spectral Library Searching." In: *ASMS Annual Conference* Atlanta, GA, USA (June 3, 2019). DOI: [10.5281/zenodo.3242687](https://doi.org/10.5281/zenodo.3242687).
- [9] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Department of Genome Sciences Retreat* Leavenworth, WA, USA (Sept. 17, 2018). DOI: [10.5281/zenodo.1418397](https://doi.org/10.5281/zenodo.1418397).
- [8] **Wout Bittremieux**, Dirk Valkenburg, and Kris Laukens. "Towards the Smart Lab: A Comprehensive Approach to Mass Spectrometry Quality Control." In: *ASMS Annual Conference* Indianapolis, IN, USA (June 8, 2017). DOI: [10.5281/zenodo.584052](https://doi.org/10.5281/zenodo.584052).
- [7] **Wout Bittremieux** and Kris Laukens. "Mass Spectrometry Proteomics: Ready for the Deep Learning (r)Evolution?" In: *ASMS Annual Conference* Indianapolis, IN, USA (June 8, 2017). DOI: [10.5281/zenodo.584067](https://doi.org/10.5281/zenodo.584067).
- [6] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Dirk Valkenburg, and Kris Laukens. "Automatic Quality Assessment of Mass Spectrometry Experiments by Multivariate Quality Control Metrics." In: *ASMS Annual Conference* San Antonio, TX, USA (June 9, 2016). DOI: [10.5281/zenodo.55998](https://doi.org/10.5281/zenodo.55998).
- [5] **Wout Bittremieux**, Hanny Willems, Lennart Martens, Dirk Valkenburg, and Kris Laukens. "Mass Spectrometry Quality Control: Instrument Monitoring and Pattern Mining Insights." In: *ASMS Annual Conference* St. Louis, MO, USA (June 2, 2015). DOI: [10.5281/zenodo.55992](https://doi.org/10.5281/zenodo.55992).
- [4] **Wout Bittremieux**, Hanny Willems, Lennart Martens, Bart Goethals, Dirk Valkenburg, and Kris Laukens. "A Comprehensive Approach to Mass Spectrometry Quality Control." In: *Two-day Symposium of the Belgian Proteomics Association* Brussels, Belgium (Dec. 18, 2014). DOI: [10.5281/zenodo.55990](https://doi.org/10.5281/zenodo.55990).
- [3] **Wout Bittremieux**, Dirk Valkenburg, Aida Mrzic, Hanny Willems, Bart Goethals, and Kris Laukens. "Pattern Mining of Mass Spectrometry Quality Control Data." In: *European Conference on Computational Biology* Strasbourg, France (Sept. 7, 2014). DOI: [10.5281/zenodo.55989](https://doi.org/10.5281/zenodo.55989).
- [2] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenburg, Lennart Martens, Bart Goethals, and Kris Laukens. "Mining Mass Spectrometry Quality Control Data." In: *ASMS Annual Conference* Baltimore, MD, USA (June 16, 2014). DOI: [10.5281/zenodo.55988](https://doi.org/10.5281/zenodo.55988).
- [1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenburg, Lennart Martens, and Kris Laukens. "jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format." In: *Benelux Bioinformatics Conference* Brussels, Belgium (Dec. 9, 2013). DOI: [10.5281/zenodo.55986](https://doi.org/10.5281/zenodo.55986).

## Scientific Software Contributions

**ANN-SoLo:** A spectral library search engine for fast and accurate open modification searching.

Homepage: <https://github.com/bittremieux/ANN-SoLo>

Role: creator and maintainer

**falcon:** A tool for efficient clustering of millions of mass spectra.  
 Homepage: <https://github.com/bittremieux/falcon>  
 Role: creator and maintainer

**GLEAMS:** A deep neural network to convert mass spectrometry data to vector embeddings.  
 Homepage: <https://github.com/bittremieux/GLEAMS>  
 Role: creator and maintainer

**iMonDB:** A Java tool to automatically extract, store, manage, and visualize mass spectrometer instrument parameters from raw data files.  
 Homepage: <https://github.com/bittremieux/iMonDB>  
 Role: creator and maintainer

**jqcML:** A Java API for the standard qcML file format for mass spectrometry quality control data.  
 Homepage: <https://github.com/bittremieux/jqcML>  
 Role: creator and maintainer

**Metabolomics USI:** A web tool for FAIR mass spectrometry data.  
 Homepage: <https://metabolomics-usi.ucsd.edu/>  
 Role: creator and maintainer

**spectrum\_utils:** A Python package for efficient MS/MS spectrum processing and visualization.  
 Homepage: [https://github.com/bittremieux/spectrum\\_utils](https://github.com/bittremieux/spectrum_utils)  
 Role: creator and maintainer

**Casanovo:** *De novo* mass spectrometry peptide sequencing with a transformer deep neural network.  
 Homepage: <https://github.com/Noble-Lab/casanovo>  
 Role: contributor

**Depthcharge:** A deep learning toolkit for building state-of-the-art models in mass spectrometry.  
 Homepage: <https://github.com/wfondrie/depthcharge>  
 Role: contributor

**GNPS:** A web-based mass spectrometry ecosystem for untargeted metabolomics.  
 Homepage: <https://gnps.ucsd.edu/>  
 Role: contributor

**ppx:** A Python package for programmatic access to proteomics data repositories.  
 Homepage: <https://github.com/wfondrie/ppx>  
 Role: contributor

**TCRex:** A web tool for predicting TCR-epitope binding for human T cell receptors.  
 Homepage: <https://tcrex.biodatamining.be/>  
 Role: contributor

## Student Supervision

2022-...	<b>Issar Arab</b> , PhD student PhD thesis: <i>Open Modification Search Methods for Tandem Mass Spectrometry</i> Computer Science; University of Antwerp, Antwerp, Belgium
2020-...	<b>Ceder Dens</b> , PhD student PhD thesis: <i>Interaction Modeling With Deep Learning for Data-Scarce Domains: An Application on Immune Receptors</i> Computer Science; University of Antwerp, Antwerp, Belgium
2020-...	<b>Charlotte Adams</b> , PhD student PhD thesis: <i>Unraveling the Role of Protein Post-Translational Modifications During Viral Infection by Large-Scale Reprocessing of Open Mass Spectrometry-Based Interactome</i> Computer Science; University of Antwerp, Antwerp, Belgium
2021	<b>Lies Van Olmen</b> , MSc student MSc thesis: <i>Identification of Post-Translational Modifications in Epitopes</i> Biotechnology; University of Antwerp, Antwerp, Belgium

- 2020 **Jens Settelmeier**, MSc student  
MSc thesis: *Deep Neural Embedding of Chimeric Tandem Mass Spectra*  
Machine Learning; Royal Institute of Technology, Stockholm, Sweden
- 2019 **Charlotte Adams**, MSc student  
MSc thesis: *Deep Reprocessing of Mass Spectrometry-Based Human and Virus-Host Protein Interaction Data Using Open Modification Searching*  
Biotechnology; University of Antwerp, Antwerp, Belgium
- 2019 **Charlotte Adams**, MSc student  
Internship: *Investigating the Advantages of Open Modification Searching to Identify Modified Proteins*  
Biotechnology; University of Antwerp, Antwerp, Belgium
- 2019 **Stephen Blaskowski**, PhD student  
Internship: *Using Machine Learning to Speed Up Calibration of Tandem Mass Spectrometry Database Search*  
Molecular Engineering; University of Washington, Seattle, WA, USA
- 2017 **Joeri Reynolds**, MSc student  
MSc thesis: *Protein Identification Using Deep Neural Networks*  
Computer Science; University of Antwerp, Antwerp, Belgium
- 2017 **Keerthana Sanala Prakash**, MSc student  
Internship: *Temporal Mining of Mass Spectrometry Quality Control Data*  
Computer Science; University of Antwerp, Antwerp, Belgium
- 2016 **Phui San Cheong**, MSc student  
Internship: *Implement Frequent Itemset-based Clustering in pyGCluster*  
Computer Science; University of Antwerp, Antwerp, Belgium
- 2016 **Robin Verachtert**, BSc student  
Internship: *Automatic Discovery of Artefacts in Mass Spectrometry Data*  
Computer Science; University of Antwerp, Antwerp, Belgium

## Teaching

### Training

- 2022 The Carpentries Instructor Training

### Experience

- 2022 Fundamentals of Machine Learning for Mass Spectrometry Data Analysis: Instructor, American Society for Mass Spectrometry – Annual Conference Short Course
- 2021 System-Wide Mass Spectrometry: Guest Lecturer, University of California San Diego – Cellular & Molecular Medicine
- 2017 Introduction to Computational Biology: Teaching Assistant, University of Antwerp – Bachelor of Computer Science
- 2016 Project Work: Teaching Assistant, University of Antwerp – Bachelor of Mathematics
- 2014–15 Data Mining: Teaching Assistant, University of Antwerp – Master of Biochemistry and Biotechnology
- 2015 Data Mining: Guest Lecturer, University of Antwerp – Master of Computer Science

## Funding Acquired

2022–23	Project: <i>Cross Repository Metabolomics Data and Workflow Integration</i> Co-investigator	Funding: \$302,764
2019–23	Project: <i>Transferable Deep Learning for Sequence Based Prediction of Molecular Interactions</i> Co-PI	Funding: €205,000
2017–20	Project: <i>Intelligent Quality Control for Mass Spectrometry-based Proteomics</i> Postdoctoral Fellowship	Funding: €265,300
2018–19	Project: <i>Prediction of Mass Spectrometry Spectral Libraries</i> Postdoctoral Fellowship	Funding: \$45,000

## Professional Activities

### Referee

**Journals** Analytical Chemistry, Artificial Intelligence in Medicine, Bioinformatics, BMC Bioinformatics, Genome Biology, IEEE/ACM Transactions on Computational Biology and Bioinformatics, Journal of Computational Biology, Journal of Open Source Software, Journal of Proteome Research, Mass Spectrometry Reviews, Metabolites, Nature Communications, PLOS Computational Biology, PLOS ONE, PROTEOMICS, Scientific Reports

**Conferences** Intelligent Systems for Molecular Biology (ISMB), Machine Learning in Computational Biology (MLCB), NIPS Workshop on Machine Learning in Computational Biology, Research in Computational Molecular Biology (RECOMB), Workshop on Data Mining in Bioinformatics (BIOKDD)

### Editor

Guest editor for PLOS Computational Biology and PROTEOMICS.

## Scientific Meetings Organized

2022	Intelligent Systems for Molecular Biology (Madison, WI, USA) – Computational Mass Spectrometry Track: Chair
2022	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Oeiras, Portugal): Organizing Committee Member
2022	US HUPO Annual Conference (Charleston, SC, USA) – Computational Proteomics: From Machine Learning to Human Insight Track: Chair
2021	American Society for Mass Spectrometry Annual Conference (Philadelphia, PA, USA) – Quality Control Workshop: Chair
2021	Intelligent Systems for Molecular Biology / European Conference on Computational Biology (online) – Computational Mass Spectrometry Track: Chair
2020	Intelligent Systems for Molecular Biology Conference (online) – Computational Mass Spectrometry Track: Co-chair
2020	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Nyborg, Denmark): Organizing Committee Member
2019	Machine Learning in Computational Biology (Vancouver, BC, Canada): Program Committee Member
2019	European Bioinformatics Community for Mass Spectrometry Winter School (Zakopane, Poland): Organizing Committee Member
2018	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Ghent, Belgium): Main Organizer
2015	Benelux Bioinformatics Community (Antwerp, Belgium): Organizing Committee Member

2014 Belgian Proteomics Association Symposium (Brussels, Belgium): Local Organizing Committee Member

## Professional Affiliations

2021-... Human Proteome Organization: Member

2017-... European Bioinformatics Community for Mass Spectrometry: Member

2016-... Human Proteome Organization – Proteomics Standards Initiative: Co-chair of the Quality Control Working Group

2014-... International Society for Computational Biology: Member

2013-... American Society for Mass Spectrometry: Member