

## Julien BOCCARD

🇨🇭 January 4<sup>th</sup> 1978, Geneva  
Swiss - Married (two children)

School of Pharmaceutical Sciences  
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### RESEARCH INTERESTS

- ★ Chemometrics
- ★ Multivariate analysis
- ★ Metabolomics
- ★ Data fusion
- ★ Bioinformatics
- ★ Machine learning

### ACADEMIC QUALIFICATIONS

- 2009 **PhD in Sciences (with distinction).** "Knowledge discovery in pharmaceutical sciences, from metabolomics to molecular modelling". University of Geneva
- 2004 **Master of Advanced Studies in Bioinformatics.** Swiss Institute of Bioinformatics, University of Geneva
- 2002 **Master of Science in Biology.** University Medical Centre, University of Geneva
- 2000 **Bachelor of Science in Biology.** University of Geneva

### PROFESSIONAL EXPERIENCE

- since 2022 **Lecturer.** School of Pharmaceutical Sciences, University of Geneva
- 2016-2021 **Senior Research Associate.** School of Pharmaceutical Sciences, University of Geneva
- 2013-2015 **Research and Teaching Fellow.** School of Pharmaceutical Sciences, University of Geneva
- 2012 **Post-doctoral Researcher.** "Advanced chemometric analysis and integration of multiple Omics data: assessment of dioxin toxicity in human". AgroParisTech, Paris (France)
- 2009-2011 **Post-doctoral Researcher.** Swiss Centre for Applied Human Toxicology (SCAHT), Geneva
- 2004-2009 **Research and Teaching Assistant.** School of Pharmaceutical Sciences, University of Geneva

### LANGUAGES

- French Native  
English Full professional proficiency  
German Limited professional proficiency

### PROFESSIONAL ACTIVITIES

#### ACADEMIC ORGANIZATIONS

- Board member of the Swiss Metabolomics Society (SMS) since 2017
- Board member of the French-speaking Metabolomics and Fluxomics network (RFMF) 2015-2023
- Board member of the Mass Spectrometry & Advances in the Clinical Lab (MSACL) conference European Scientific Committee 2018-2020
- Member of the Metabolomics Society, the Swiss Chemical Society (SCS), the French Statistical Society (SFdS), the Centre of Competence in Analytical Chemistry and Toxicology (ccCTA)

#### CONGRESS CO-ORGANISER

- Chimométrie XVI, University of Geneva 19-21.01.2015
- 10<sup>èmes</sup> Journées Scientifiques du RFMF, Montpellier 30.05-02.06.2016
- 34th International Symposium on Pharmaceutical and Biomedical Analysis, Geneva 09.09-12.09.2024
- Annual Meetings of the Swiss Metabolomics Society (since 2018)

## GRANTS

**Project funding.** (Co-applicant, 2017) "Steroidomics, an innovative metabolomic approach to extend the steroid profile monitoring in human". Swiss National Science Foundation. 31003A\_166658/1, 525'000 CHF.

**Fellowship for advanced researcher.** (Responsible applicant, 2012) "Advanced chemometric analysis and integration of multiple Omics data: assessment of dioxin toxicity in human". Swiss Foundation for Grants in Biology and Medicine. PASMP3\_140064/1, 50'360 CHF.

## BIBLIOMETRICS

### 5 PUBLICATION HIGHLIGHTS

- ★ **Assessing variable importance stability using resampling strategies to enhance model interpretability and reliability in metabolomics.** J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2026), 1397, 345258.
- ★ **Integration of multifactorial omics data from several sources using multiblock methods.** M. de Figueiredo, S. Rudaz, J. Boccard. *Chemometrics and Intelligent Laboratory Systems* (2025), 262, 105403.
- ★ **Gaining insights into metabolic networks using chemometrics and bioinformatics: chronic kidney disease as a clinical model.** J. Boccard, D. Schvartz, S. Codesido, M. Hanafi, Y. Gagnebin, B. Ponte, F. Jourdan, S. Rudaz. *Frontiers in Molecular Biosciences* (2021), 8, 682559.
- ★ **Network principal component analysis: a versatile tool for the investigation of multigroup and multiblock datasets.** S. Codesido, M. Hanafi, Y. Gagnebin, V. González-Ruiz, S. Rudaz, J. Boccard. *Bioinformatics* (2021), 37(9), 1297-1303.
- ★ **A consensus OPLS-DA strategy for multiblock Omics data fusion.** J. Boccard, D.N. Rutledge. *Analytica Chimica Acta* (2013), 769, 30-39.

Research articles: **119**  
Book chapters: **11**  
Protocols: **4**

Reviews & tutorials: **12**  
Short communications & perspectives: **4**

**h-index: 45**                      **i10-index: 104**  
**citations: >6'400** (Google Scholar, April 2026)

Oral communications: **29**

Posters (as first author): **17**

External invited lectures: **34** (Denmark, Greece, France, Belgium, Switzerland)

PhD/Master thesis jury or advisory committee: **38** (AgroParisTech, Paris-Saclay University, ONIRIS, Grenoble Alpes University, Clermont Auvergne University, University of Perpignan Via Domitia, Toulouse III - Paul Sabatier University, INRAE, University of Liège, University of Lausanne, University of Geneva)

PhD co-directions: **4** (University of Geneva, University Clermont Auvergne)

### EDITORIAL & PEER REVIEW ACTIVITIES

since 2022                      Associate editor of the Metabolomics section of *Frontiers in Molecular Biosciences*  
since 2021                      Editorial board member of *Metabolites*

Ad hoc reviewer for *Analytical Chemistry*, *Analytica Chimica Acta*, *Metabolomics*, *Bioinformatics*, *BMC Bioinformatics*, *PLOS Computational Biology*, *Chemometrics and Intelligent Laboratory Systems*, *Journal of Chemometrics*, *Journal of Chromatography A*, *Talanta*, *Analytical and Bioanalytical Chemistry*, *Journal of Pharmaceutical and Biomedical Analysis*, *Current Opinion in Toxicology*, *Forensic Science International*, *Metabolites*, *Molecules*, *Computer Methods and Programs in Biomedicine*, *Computational and Structural Biotechnology Journal*, *Phytochemistry*, *Chemosphere*, *Flavour and Fragrance Journal*, *Food Chemistry*, *Food Research International*, *LWT - Food Science and Technology*, *Journal of the Brazilian Chemical Society*, *Planta Medica*, *PeerJ*.

## TEACHING

### **SCHOOL OF PHARMACEUTICAL SCIENCES (UNIVERSITY OF GENEVA, SWITZERLAND)**

- Statistics & Pharmaceutical Methodology (Bachelor 2, since 2008, 28 h/y)
- Pharmaceutical Methodology (Bachelor 3, since 2010, 48 h/y)
- Practical work of Biomedical Analysis (Bachelor 3, since 2023, 88 h/y)
- Multivariate Analysis (Doctoral program, since 2011, 16 h/y)
- Design of Experiments (Doctoral program, since 2011, 16 h/y)
- Validation of analytical methods (Doctoral program, since 2018, 16 h/y)

### **FACULTY OF SCIENCES (UNIVERSITY OF GENEVA, SWITZERLAND)**

- Biostatistics (MAS in Toxicology, since 2013, 32 h/2y)
- Metabolomics (MAS in Drug Discovery and Clinical Development, since 2017, 2 h/y)
- Elements of Proteomics & Metabolomics (Master, since 2017, 6 h/y)

### **SWISS INSTITUTE OF BIOINFORMATICS**

- Multiomics Data Analysis and Integration (Training course, since 2023)

### **SCHOOL OF CRIMINAL SCIENCES (UNIVERSITY OF LAUSANNE, SWITZERLAND)**

- Design of Experiments (Master, since 2016, 2 h/y)

### **INTERUNIVERSITY DOCTORAL PROGRAM « STAROMICS » (UNIVERSITIES OF GENEVA, LAUSANNE, NEUCHÂTEL, FRIBOURG AND BERN, SWITZERLAND)**

- Multivariate Analysis in Metabolomics (Doctoral program, since 2017, 3 h/y)

### **INTERUNIVERSITY DOCTORAL PROGRAM IN ORGANISMAL BIOLOGY (UNIVERSITIES OF GENEVA, LAUSANNE, NEUCHÂTEL, FRIBOURG AND BERN, SWITZERLAND)**

- Metabolomics Data Analysis (Doctoral program, since 2014, 6 h/2y)

### **CENTRE OF COMPETENCES IN ANALYTICAL CHEMISTRY AND TOXICOLOGY (SWITZERLAND)**

- Statistics in Toxicology (Continuing education, since 2011, 8 h/y)
- Multivariate Analysis (Continuing education, since 2015, 8 h/y)

### **SIGMA PLUS/DYNACENTRIX (PARIS, FRANCE)**

- Multivariate Analysis of Omics Data (Training course, since 2011)

### **BIOSCIENCES & CO (LYON, FRANCE)**

- Analysis of MultiOmics Data (Training course, since 2023)

### **MASSIVE OPEN ONLINE COURSES**

- CheMoocs (Chemometrics, since 2015)
- UseMetabo (Metabolomics, since 2018)

### **BARCAMPS / TRAINING WORKSHOPS**

- ChemOmics (Chemometrics/Metabolomics, since 2019)

- 119. Integrated workflow for univariate and multivariate evaluation of batch correction reliability.** E. Salanon, B. Comte, D. Centeno, S. Durand, E. Pujos-Guillot, J. Boccard. Accepted in *Metabolomics* (in press).
- 118. Characterization of residual kidney function in chronic hemodialysis patients using plasma metabolomics.** D. Jaques, J. Boccard, O. Strassel, M.-A. Monat, G. Visconti, V. Jotterand, N. Marangon, P. Saudan, S. De Seigneux, S. Rudaz, B. Ponte. *Scientific Reports* (2026), 16, 11701.
- 117. Heterologous internal calibration for Multiplexed Internal Quantification in Targeted LC-MS/MS Bioanalysis.** O. Strassel, M. Feinberg, G. Visconti, J. Boccard, S. Rudaz. *Journal of Pharmaceutical and Biomedical Analysis* (2026), 277, 117487.
- 116. Lipidomic profiling of extracellular vesicles from breast and metastatic triple-negative breast cancer cell lines for identification of potential biomarkers.** O.B. Majchrzak, C. Lopes Silva, S. Tankov, J. Boccard, S. Rudaz, O. Jordan, P.R. Walker, I. Meister, G. Borchard. *European Journal of Pharmaceutical Sciences* (2026), 221, 107514.
- 115. Assessing variable importance stability using resampling strategies to enhance model interpretability and reliability in metabolomics.** J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2026), 1397, 345258.
- 114. Cannabis consumption is associated with altered steroid metabolism in young men.** M. Galmiche, I. Meister, F. Zufferey, M. F. Rossier, R. Rahban, A. Senn, S. Nef, J. Boccard, S. Rudaz. *Communications Medicine* (2026), 6, 224.
- 113. A comprehensive metabolomics approach for enhanced detection of growth promoting practices in livestock.** C. Cloteau, M. Letertre, J. Boccard, M. Pezzolato, E. Bozzeta, B. Le Bizec, G. Dervilly. *Food Additives and Contaminants: Part A* (2026), 43(3), 421-434.
- 112. A cooperative learning framework for the integration of metabolomic data from multiple cohorts and common phenotype identification.** E. Salanon, E. Jules, B. Comte, J. Boccard, E. Pujos-Guillot. *Computational and Structural Biotechnology Journal* (2026), 31, 346-354.
- 111. Neurotoxicity of Propylene Glycol Butyl Ether: Multiomic Evidence from Human BrainSpheres.** D. Lopez-Rodriguez, D. Pamies, J. Boccard, I. Meister, M. Galmiche, T. Sajic, E. Maret, N. Héritier, M. Frangiamone, A. Thomas, N.B. Hopf h, S. Rudaz, M.-G. Zurich. *Environment International* (2025), 205, 109852.
- 110. Improving metabolomics data comparability without long term quality controls using a post-acquisition correction strategy.** E. Salanon, B. Comte; D. Centeno, S. Durand, J. Boccard, E. Pujos-Guillot. *Analytica Chimica Acta* (2025), 1380, 344753.
- 109. PCK1-mediated cataplerosis is required to maintain mitochondrial fitness and to avoid kidney disease progression.** D. Dalga, A. Rinaldi, X. Fu, L. C. Chanvillard, A. Huber, A Faivre, D. Jaques, L. Berchtold, J. Boccard, G. Arnoux, A. Lyon, J. M. Rutkowski, Q. Gex, D. Paolucci, M. Kreuzfeld, N. Hulo, T. Cagarell, L. Lutz, A. Longchamp, S. Moll, B. Ponte, S. Burgess, P. E. Cippà, T. Verissimo, S. de Seigneux. *Kidney International* (2025), 108(5), 827-847.
- 108. Integration of multifactorial omics data from several sources using multiblock methods.** M. de Figueiredo, S. Rudaz, J. Boccard. *Chemometrics and Intelligent Laboratory Systems* (2025), 262, 105403.
- 107. Identification of lipid species signature in FOLFOXIRI-resistant colorectal cancer cells.** G. M. Ramzy, I. Meister, S. Rudaz, J. Boccard, P. Nowak-Sliwinska. *International Journal of Molecular Sciences* (2025), 26(3), 1169.
- 106. Hyperpolarized <sup>13</sup>C NMR metabolomics of urine samples at natural abundance applied to chronic kidney disease.** V. Ribay, B. Charrier, M. Croyal, B. Cariou, S. Hadjadj, J. Boccard, C. Cannet, J.-N. Dumez, M. P. M. Letertre, P. Giraudeau. *Journal of the American Chemical Society* (2025), 147(1), 644-650.
- 105. Early detection of bacterial pneumonia by characteristic induced odor signatures.** K. Arnold, A. Gómez-Mejja, M. de Figueiredo, J. Boccard, K. Dev Singh, S. Rudaz, P. Sinues, A. S. Zinkernagel. *BMC Infectious Diseases* (2024), 24, 1467.

- 104. Kernel-based bootstrap synthetic data to estimate measurement uncertainty in analytical sciences.** M. Feinberg, S. Clémenton, S. Rudaz, J. Boccard. *Journal of Chemometrics* (2024), 38(12), e3628.
- 103. An advanced metabolomic approach untangles oviposition preference of grape skin among cultivars by *Drosophila suzukii*.** R. Marcellin-Gros, S. Hévin, C. Chevalley, J. Boccard, V. Hofstetter, K. Gindro, J.-L. Wolfender, P. Kehrl. *Frontiers in Plant Science* (2024), 15, 1435943.
- 102. Assessment of the potential risk of oteseconazole and two other tetrazole antifungals to inhibit adrenal steroidogenesis and peripheral metabolism of corticosteroids.** M.-C. Jäger, V. González-Ruiz, F. L. Joos, D. V. Winter, J. Boccard, T. Degenhardt, S. Brand, S. Rudaz, G. R. Thompson, A. Odermatt. *Frontiers in Pharmacology* (2024), 15, 1394846.
- 101. An alternative for the robust assessment of the repeatability and reproducibility of analytical measurements using bivariate dispersion.** E. Salanon, B. Comte, D. Centeno, S. Durand, E. Pujos-Guillot, J. Boccard. *Chemometrics and Intelligent Laboratory Systems* (2024), 250, 105148.
- 100. Comprehensive plasma steroidomics in patients at the different stages of prostate cancer disease.** S. Girel, P. A. Markin, E. Tobolkin, J. Boccard, N. E. Moskaleva, S. Rudaz, S. A. Appolonova. *Scientific Reports* (2024), 14, 1557.
- 99. Mixture effects of pharmaceuticals carbamazepine, diclofenac and venlafaxine on *Mytilus galloprovincialis* mussel probed by metabolomics and proteogenomics combined approach.** T. Dumas, E. Gomez, J. Boccard, G. Ramirez, J. Armengaud, A. Escande, O. Matthieu, H. Fenet, F. Courant. *Science of the Total Environment* (2024), 907, 168015.
- 98. Multitargeted internal calibration for the quantification of chronic kidney disease related endogenous metabolites using liquid chromatography–mass spectrometry.** G. Visconti, M. de Figueiredo, O. Strassel, J. Boccard, N. Vuilleumier, D. Jaques, B. Ponte, S. Rudaz, S. *Analytical Chemistry* (2023), 95(36), 13546-13554.
- 97. Straightforward quantification of endogenous steroids with liquid chromatography–tandem mass spectrometry: a retrospective study comparing calibration approaches.** G. Visconti, M. de Figueiredo, O. Salamin, J. Boccard, N. Vuilleumier, R. Nicoli, T. Kuuranne, S. Rudaz. *Journal of Chromatography B* (2023), 1226, 123778.
- 96. A new multimodal paradigm for biomarkers longitudinal monitoring: a clinical application to women steroid profiles in urine and blood.** M. de Figueiredo, J. Saugy, M. Saugy, R. Faiss, O. Salamin, R. Nicoli, T. Kuuranne, S. Rudaz, F. Botrè, J. Boccard. *Analytica Chimica Acta* (2023), 1267, 341389.
- 95. Low-polarity untargeted metabolomic profiling as a tool to gain insight into seminal fluid.** E. Olesti, J. Boccard, R. Rahban, S. Girel, N. E. Moskaleva, F. Zufferey, M. F. Rossier, S. Nef, S. Rudaz, V. González-Ruiz. *Metabolomics* (2023), 19, 53.
- 94. A unified strategy to rebalance multifactorial designs with unequal group sizes: application to analysis of variance multiblock orthogonal partial least squares.** M. de Figueiredo, S. Rudaz, J. Boccard. *Analytica Chimica Acta* (2023), 1263, 341284.
- 93. Extended steroid profiling in H295R cells provides deeper insight into chemical-induced disturbances of steroidogenesis: exemplified by prochloraz and anabolic steroids.** M.-C. Jäger, M. Patt, V. González-Ruiz, J. Boccard, T. Wey, D.V. Winter, S. Rudaz, A. Odermatt. *Molecular and Cellular Endocrinology* (2023), 579, 111929.
- 92. Digoxin induces human astrocyte reaction in vitro.** D. Pamies, T. Vujic, D. Schvartz, J. Boccard, C. Repond, C. Nunes, S. Rudaz, J.-C. Sanchez, V. González-Ruiz, M.-G. Zurich. *Molecular Neurobiology* (2023), 60(1), 84-97.
- 91. Efficiently handling high-dimensional data from multifactorial designs with unequal group sizes using Rebalanced ASCA (RASCA).** M. de Figueiredo, S. Giannoukos, S. Rudaz, R. Zenobi, J. Boccard. *Journal of Chemometrics* (2023), 37(7), e3401.
- 90. An integrated metabolomics and proteogenomics approach reveals molecular alterations following carbamazepine exposure in the male mussel *Mytilus galloprovincialis*.** T. Dumas, F. Courant, C. Almunia, J. Boccard, D. Rosain, G. Duporté, J. Armengaud, H. Fenet, E. Gomez. *Chemosphere* (2022), 286, 131793.

- 89. Longitudinal evaluation of multiple biomarkers for the detection of testosterone gel administration in women with normal menstrual cycle.** O. Salamin, R. Nicoli, T. Langer, J. Boccard, C. Schweizer Grundisch, C. Xu, S. Rudaz, N. Pitteloud, M. Saugy, T. Kuuranne. *Drug Testing and Analysis* (2022), 14(5), 833-850.
- 88. Steroid profiling by UHPLC-MS/MS in dried blood spots collected from healthy women with and without testosterone gel administration.** O. Salamin, R. Nicoli, C. Xu, J. Boccard, S. Rudaz, M. Saugy, N. Pitteloud, T. Kuuranne. *Journal of Pharmaceutical and Biomedical Analysis* (2021), 204, 114280.
- 87. Gaining insights into metabolic networks using chemometrics and bioinformatics: chronic kidney disease as a clinical model.** J. Boccard, D. Schwartz, S. Codesido, M. Hanafi, Y. Gagnebin, B. Ponte, F. Jourdan, S. Rudaz. *Frontiers in Molecular Biosciences* (2021), 8, 682559.
- 86. Neuroinflammatory response to TNF $\alpha$  and IL1 $\beta$  cytokines is accompanied by an increase of glycolysis in human astrocytes in vitro.** D. Pamies, C. Sartori, D. Schwartz, V. González-Ruiz, L. Pellerin, C. Nunes, D. Tavel, V. Maillard, J. Boccard, S. Rudaz, J.-C. Sanchez, M.-G. Zurich. *International Journal of Molecular Sciences* (2021), 22(8), 4065.
- 85. Wipe sampling procedure optimization for the determination of 23 antineoplastic drugs used in hospital pharmacy.** N. Guichard, J. Boccard, S. Rudaz, P. Bonnabry, S. Fleury-Souverain. *European Journal of Hospital Pharmacy* (2021), 28(2), 94-99.
- 84. Metatypes of Pseudomonas aeruginosa correlate with antibiotic resistance, virulence and clinical outcome in cystic fibrosis chronic infections.** O. Moyne, F. Castelli, D.J. Bicout, J. Boccard, B. Camara, B. Cournoyer, E. Faudry, S. Terrier, D. Hannani, S. Huot-Marchand, C. Leger, M. Maurin, T. Dung Ngo, C. Plazy, R.A. Quinn, I. Attree, F. Fenaille, B. Toussaint, A. Le Gouëllec. *Metabolites* (2021), 11(2), 63.
- 83. Network principal component analysis: a versatile tool for the investigation of multigroup and multiblock datasets.** S. Codesido, M. Hanafi, Y. Gagnebin, V. González-Ruiz, S. Rudaz, J. Boccard. *Bioinformatics* (2021), 37(9), 1297-1303.
- 82. Evaluation of different tandem MS/MS acquisition modes to support metabolite annotation in human plasma using ultra high-performance liquid chromatography high-resolution mass spectrometry for untargeted metabolomics.** J. Pezzatti, V. González-Ruiz, J. Boccard, D. Guillaume, S. Rudaz. *Metabolites* (2020), 10(11), 464.
- 81. Exploring blood alterations in chronic kidney disease and haemodialysis using metabolomics.** Y. Gagnebin, D.A. Jaques, S. Rudaz, S. de Seigneux, J. Boccard, B. Ponte. *Scientific Reports* (2020), 10, 19502.
- 80. Inhibition of enteric methanogenesis in dairy cows induces changes in plasma metabolome highlighting metabolic shifts and potential markers of emission.** B. Yanibada, U. Hohenester, M. Pétéra, C. Canlet, S. Durand, F. Jourdan, J. Boccard, C. Martin, M. Eugène, D. Morgavi, H. Boudra. *Scientific Reports* (2020), 10, 15591.
- 79. Insights on the structural and metabolic resistance of potato (Solanum tuberosum) cultivars to tuber black dot (Colletotrichum coccodes).** J. Massana-Codina, S. Schnee, P.-M. Allard, A. Rutz, J. Boccard, E. Michellod, M. Cléroux, S. Schürch, K. Gindro, J.-L. Wolfender. *Frontiers in Plant Science* (2020), 11, 1287.
- 78. Multifactorial analysis of environmental metabolomic data in ecotoxicology: wild marine mussel exposed to WWTP effluent as a case study.** T. Dumas, J. Boccard, E. Gomez, H. Fenet, F. Courant. *Metabolites* (2020), 10(7), 269.
- 77. Development and validation of an UHPLC-MS/MS method for extended serum steroid profiling in female populations.** O. Salamin, F. Ponzetto, J. Boccard, S. Rudaz, M. Saugy, T. Kuuranne, R. Nicoli. *Bioanalysis* (2020), 12(11), 753-768.
- 76. Comprehensive examination of the mouse lung metabolome following Mycobacterium tuberculosis infection using a multiplatform mass spectrometry approach.** M. Fernández-García, F. Rey-Stolle, J. Boccard, V. Reddy, A. García, B. Cumming, A. Steyn, S. Rudaz, C. Barbas. *Journal of Proteome Research* (2020), 19(5), 2053-2070.
- 75. Cultivar, site or harvest date: the Gordian knot of Wine Terroir.** L. M. Schmidtke, G. Antalick, K. Šuklje, J. W. Blackman, J. Boccard, A. Deloire. *Metabolomics* (2020), 16, 52.

- 74. Applicability of supercritical fluid chromatography – mass spectrometry to metabolomics. II- Assessment of a comprehensive library of metabolites and evaluation of biological matrices.** G. L. Losacco, O. Ismail, J. Pezzatti, V. González-Ruiz, J. Boccard, S. Rudaz, J.-L. Veuthey, D. Guillaume. *Journal of Chromatography A* (2020), 1620, 461021.
- 73. Metabolomics approach reveals disruption of metabolic pathways in the marine bivalve *Mytilus galloprovincialis* exposed to a WWTP effluent extract.** T. Dumas, B. Bonnefille, E. Gomez, J. Boccard, N. Ariza Castro, H. Fenet, F. Courant. *Science of the Total Environment* (2020), 712, 136551.
- 72. Profiling of anabolic androgenic steroids and selective androgen receptor modulators for interference with adrenal steroidogenesis.** M. Patt, K. R. Beck, T. Di Marco, M.-C. Jäger, V. González-Ruiz, J. Boccard, S. Rudaz, C. van Koppen, M. Grill, A. Odermatt. *Biochemical Pharmacology* (2020), 172, 113781.
- 71. Supercritical Fluid Chromatography - Mass Spectrometry in routine anti-doping analyses: estimation of retention time variability under reproducible conditions.** G. L. Losacco, E. Marconetto, R. Nicoli, T. Kuuranne, J. Boccard, S. Rudaz, J.-L. Veuthey, D. Guillaume. *Journal of Chromatography A* (2020), 1616, 460780.
- 70. Steroid profile analysis by LC-HR-MS in human seminal fluid.** E. Olesti, A. Garcia, R. Rahban, M. Rossier, J. Boccard, S. Nef, V. González-Ruiz, S. Rudaz. *Journal of Chromatography B* (2020), 1136, 121929.
- 69. Combining the advantages of multilevel and orthogonal partial least squares data analysis for longitudinal metabolomics: application to kidney transplantation.** Y. Gagnebin, J. Pezzatti, P. Lescuyer, J. Boccard, B. Ponte, S. Rudaz. *Analytica Chimica Acta* (2020), 109, 26-38.
- 68. Choosing an optimal sample preparation in *Caulobacter crescentus* for untargeted metabolomics approaches.** J. Pezzatti, M. Bergé, J. Boccard, S. Codesido, Y. Gagnebin, P. H. Viollier, V. González-Ruiz, S. Rudaz. *Metabolites* (2019), 9(10), 193.
- 67. Processing of NMR and MS metabolomics data using chemometrics methods: a global tool for fungi biotransformation reactions monitoring.** C. Palaric, S. Pilard, J.-X. Fontaine, J. Boccard, D. Mathiron, S. Rigaud, D. Cailleu, F. Mesnard, Y. Gut, T. Renaud, A. Petit, J.-Y. Beaumal, R. Molinié. *Metabolomics* (2019), 15, 107.
- 66. Protein pathway analysis to study development-dependent effects of acute and repeated Trimethyltin (TMT) treatments in 3D rat brain cell cultures.** D. Schwartz, V. González-Ruiz, N. Walter, P. Antinori, F. Jeanneret, D. Tonoli, J. Boccard, M.-G. Zurich, S. Rudaz, F. Tschudi-Monnet, J. Sandström, J.-C. Sanchez. *Toxicology in Vitro* (2019), 60, 281-292.
- 65. Steroidomics for highlighting novel serum biomarkers of testosterone doping.** F. Ponzetto, J. Boccard, R. Nicoli, T. Kuuranne, M. Saugy, S. Rudaz. *Bioanalysis* (2019), 11(12), 1171-1187.
- 64. DynaStI: A dynamic retention time database for steroidomics.** S. Codesido, G. M. Randazzo, F. Lehmann, V. González-Ruiz, A. García, I. Xenarios, R. Liechti, A. Bridge, J. Boccard, S. Rudaz. *Metabolites* (2019), 9(5), 85.
- 63. An integrative multi-omics workflow to address multifactorial toxicology experiments.** V. González-Ruiz, D. Schwartz, J. Sandström, J. Pezzatti, F. Jeanneret, D. Tonoli, J. Boccard, F. Monnet-Tschudi, J.-C. Sanchez, S. Rudaz. *Metabolites* (2019), 9(4), 79.
- 62. In vitro models to study insulin and glucocorticoids modulation of Trimethyltin (TMT)-induced neuroinflammation and neurodegeneration, and in vivo validation in db/db mice.** J. Sandström, D. Kratschmar, A. Broyer, O. Poirot, P. Marbet, B. Chantong, F. Zufferey, T. Dos Santos, J. Boccard, R. Christ, A. Odermatt, F. Monnet-Tschudi. *Archives of Toxicology* (2019), 93(6), 1649-1664.
- 61. Toward a better understanding of chronic kidney disease with complementary chromatographic methods hyphenated with mass spectrometry for improved polar metabolome coverage.** Y. Gagnebin, J. Pezzatti, P. Lescuyer, J. Boccard, B. Ponte, S. Rudaz. *Journal of Chromatography B* (2019), 1116, 9-18.
- 60. Chemical composition and anti-inflammatory activity of the decoction from leaves of a cultivated specimen of *Myracrodruon urundeuva*.** N. C. Aquino, E. F. Queiroz, L. Marcourt, L. B. N. Freitas, E. V. O. Araújo, L. K. A. M. Leal, A. M. E. Bezerra, J. Boccard, J.-L. Wolfender, E. R. Silveira. *Journal of the Brazilian Chemical Society* (2019), 30(8), 1616-1623.

- 59. A scoring approach for multi-platform acquisition in metabolomics.** J. Pezzatti, V. González-Ruiz, S. Codesido, Y. Gagnebin, A. Joshi, D. Guillarme, J. Schappler, D. Picard, J. Boccard, S. Rudaz. *Journal of Chromatography A* (2019), 1592, 47-54.
- 58. Removal of batch effects using stratified subsampling of metabolomic data for *in vitro* endocrine disruptors screening.** J. Boccard, D. Tonoli, P. Strajhar, F. Jeanneret, A. Odermatt, S. Rudaz. *Talanta* (2019), 195, 77-86.
- 57. Steroid profiles in both blood serum and seminal plasma are not correlated and do not reflect sperm quality: study on the male reproductive health of fifty young Swiss men.** F. Zufferey, R. Rahban, A. Garcia, Y. Gagnebin, J. Boccard, D. Tonoli, F. Jeanneret, E. Stettler, A. Senn, S. Nef, S. Rudaz, M. Rossier. *Clinical Biochemistry* (2018), 62, 39-46.
- 56. Dynamics of metabolite induction in fungal co-cultures by metabolomics at both volatile and non-volatile levels.** A. Azzollini, L. Boggia, J. Boccard, B. Sgorbini, N. Lecoultre, P.-M. Allard, P. Rubiolo, S. Rudaz, K. Gindro, C. Bicchì, J.-L. Wolfender. *Frontiers in Microbiology* (2018), 9, 72.
- 55. Unravelling the effects of multiple experimental factors in metabolomics, analysis of human neural cells with Hydrophilic Interaction Liquid Chromatography hyphenated to High Resolution Mass Spectrometry.** V. González-Ruiz, J. Pezzatti, A. Roux, L. Stoppini, J. Boccard, S. Rudaz. *Journal of Chromatography A* (2017), 1527, 53-60.
- 54. Enhanced metabolite annotation via dynamic retention time prediction: steroidogenesis alterations as a case study.** G. M. Randazzo, D. Tonoli, P. Strajhar, I. Xenarios, A. Odermatt, J. Boccard, S. Rudaz. *Journal of Chromatography B* (2017), 1071, 11-18.
- 53. Optimized selection of liquid chromatography conditions for wide range analysis of natural compounds.** A. Périat, D. Guillarme, J.-L. Veuthey, J. Boccard, S. Moco, D. Barron, A. Grand-Guillaume Perrenoud. *Journal of Chromatography A* (2017), 1504, 91-104.
- 52. High resolution mass spectrometry as an alternative detection method to tandem mass spectrometry for the analysis of endogenous steroids in serum.** F. Ponzetto, J. Boccard, N. Baume, T. Kuuranne, S. Rudaz, M. Saugy, R. Nicoli. *Journal of Chromatography B* (2017), 1052, 34-42.
- 51. Steroid profiling in H295R cells to identify chemicals potentially disrupting the production of adrenal steroids.** P. Strajhar, D. Tonoli, F. Jeanneret, R. M. Imhof, V. Malagnino, M. Patt, D. V. Kratschmar, J. Boccard, S. Rudaz, A. Odermatt. *Toxicology* (2017), 381, 51-63.
- 50. Metabolomic analysis of urine samples by UHPLC-QTOF-MS: impact of normalization strategies.** Y. Gagnebin, D. Tonoli, P. Lescuyer, B. Ponte, S. de Seigneux, P.-Y. Martin, J. Schappler, J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2017), 955, 27-35.
- 49. Targeted metabolomics shows plasticity in the evolution of signaling lipids and uncovers old and new endocannabinoids in the plant kingdom.** M. S. Gachet, A. Schubert, S. Calarco, J. Boccard, J. Gertsch. *Scientific Reports* (2017), 7, 41177.
- 48. Indirect Quantitative Structure-Retention Relationship for Steroid Identification: A chemometric challenge at "Chimiométrie 2016".** G. M. Randazzo, E. Vigneau, P. Courcoux, C. Harrouet, Y. Lijour, P. Dardenne, J. Boccard, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2017), 160, 52-58.
- 47. Structured plant metabolomics for the simultaneous exploration of multiple factors.** N. Vasilev, J. Boccard, G. Lang, U. Grömping, R. Fischer, S. Goepfert, S. Rudaz, S. Schillberg. *Scientific Reports* (2016), 6, 37390.
- 46. A Standardized LCxLC-ELSD Fractionation Procedure for the Identification of Minor Bioactives via the Enzymatic Screening of Natural Extracts.** P. Coulerie, Y. Ratinaud, S. Moco, L. Merminod, M. Naranjo Pinta, J. Boccard, L. Bultot, M. Deak, K. Sakamoto, E. Queiroz, J.-L. Wolfender, D. Barron. *Journal of Natural Products* (2016), 79(11), 2856-2864.
- 45. High throughput identification of monoclonal antibodies after compounding by UV spectroscopy coupled to chemometrics analysis.** E. Jaccoulet, J. Boccard, M. Taverna, A. Santos Azevedos, S. Rudaz, C. Smadja. *Analytical and Bioanalytical Chemistry* (2016), 408, 5915-5924.

- 44. Ultra-high Performance Supercritical Fluid Chromatography coupled with quadrupole-time-of-flight mass spectrometry as a performing tool for bioactive analysis.** A. Grand-Guillaume Perrenoud, D. Guillaume, J. Boccard, J.-L. Veuthey, D. Barron, S. Moco. *Journal of Chromatography A* (2016), 1450, 101–111.
- 43. Exploring Omics data from designed experiments using Analysis of Variance Multiblock Orthogonal Partial Least Squares.** J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2016), 920, 18-28.
- 42. Prediction of retention time in reversed-phase liquid chromatography as a tool for steroid identification.** G. M. Randazzo, D. Tonoli, S. Hambye, D. Guillaume, F. Jeanneret, A. Nurisso, L. Goracci, J. Boccard, S. Rudaz. *Analytica Chimica Acta* (2016), 916, 8-16.
- 41. Statistical correlations between HPLC activity-based profiling results and NMR/MS microfractions data to deconvolute bioactive compounds in mixture.** S. Bertrand, A. Azzollini, A. Nievergelt, J. Boccard, S. Rudaz, M. Cuendet, J.-L. Wolfender. *Molecules* (2016), 21 (3), 259.
- 40. Longitudinal monitoring of endogenous steroids in human serum by UHPLC-MS/MS as a tool to detect testosterone abuse in sport.** F. Ponzetto, F. Mehl, J. Boccard, N. Baume, S. Rudaz, M. Saugy, R. Nicoli. *Analytical and Bioanalytical Chemistry* (2016), 408(3), 705-719.
- 39. Systematic evaluation of matrix effects in hydrophilic interaction chromatography versus reversed phase liquid chromatography coupled to mass spectrometry.** A. Périat, I. Kohler, A. Thomas, R. Nicoli, J. Boccard, J.-L. Veuthey, J. Schappler, D. Guillaume. *Journal of Chromatography A* (2016), 1439, 42–53.
- 38. Evaluation and identification of dioxin exposure biomarkers in human urine by high-resolution metabolomics, multivariate analysis and in vitro synthesis.** F. Jeanneret, D. Tonoli, D. Hochstrasser, J.-H. Saurat, O. Sorg, J. Boccard, S. Rudaz. *Toxicology Letters* (2016), 240(1), 22–31.
- 37. Rumen microbial communities influence metabolic phenotypes in lambs.** D. Morgavi, E. Rathahao-Paris, M. Popova, J. Boccard, K. Fog Nielsen, H. Boudra. *Frontiers in Microbiology* (2015), 6, 1060.
- 36. Steroidomic footprinting based on ultra-high performance liquid chromatography coupled with qualitative and quantitative high-resolution mass spectrometry for the evaluation of endocrine disrupting chemicals in H295R cells.** D. Tonoli, C. Fürstenberger, J. Boccard, D. Hochstrasser, F. Jeanneret, A. Odermatt, S. Rudaz. *Chemical Research in Toxicology* (2015), 28(5), 955–966.
- 35. Assessing susceptibility to epilepsy in three rat strains using brain metabolic profiling based on HRMAS NMR spectroscopy and chemometrics.** F. Fauvelle, J. Boccard, F. Cavarec, A. Depaulis, C. Deransart. *Journal of Proteome Research* (2015), 14(5), 2177–2189.
- 34. Integrating metabolomic data from multiple analytical platforms for a comprehensive characterisation of lemon essential oils.** F. Mehl, G. Marti, P. Merle, E. Delort, L. Baroux, H. Sommer, J.-L. Wolfender, S. Rudaz, J. Boccard. *Flavour and Fragrance Journal* (2015), 30, 131–138.
- 33. Multi-way PLS regression: Monotony convergence of tri-linear PLS2 and optimality of parameters.** M. Hanafi, S. Ouertani, G. Mazerolles, J. Boccard, S. Rudaz. *Computational Statistics and Data Analysis* (2015), 83, 129–139.
- 32. Retention time prediction for dereplication of natural products (C<sub>x</sub>H<sub>y</sub>O<sub>z</sub>) in LC-MS metabolite profiling.** P.J. Eugster, J. Boccard, B. Debrus, L. Bréant, J.-L. Wolfender, S. Martel, P.-A. Carrupt. *Phytochemistry* (2014), 108, 196-207.
- 31. Untargeted profiling of urinary steroid metabolites after testosterone ingestion: opening new perspectives for anti-doping testing.** J. Boccard, F. Badoud, N. Jan, R. Nicoli, C. Schweizer, F. Pralong, J.-L. Veuthey, N. Baume, S. Rudaz, M. Saugy. *Bioanalysis* (2014), 6(19), 2523-2536.
- 30. Quantitative monitoring of tamoxifen in human plasma extended to forty metabolites using LC-HR-MS: New investigation capabilities for clinical pharmacology.** E. Dahmane, J. Boccard, C. Csajka, S. Rudaz, L. Décosterd, E. Genin, B. Duret, M. Bromirski, K. Zaman, B. Testa, B. Rochat. *Analytical and Bioanalytical Chemistry* (2014), 406(11), 2627-2640.

- 29. Multi-way PLS for discrimination: Compact form equivalent to the tri-linear PLS2 procedure and its monotony convergence.** S. Ouertani, M. Hanafi, G. Mazerolles, J. Boccard, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2014), 133, 25-32.
- 28. Iterative weighting of multiblock data in the Orthogonal Partial Least Squares framework.** J. Boccard, D.N. Rutledge. *Analytica Chimica Acta* (2014), 813, 25–34.
- 27. Human urinary biomarkers of dioxin exposure: analysis by metabolomics and biologically-driven data dimensionality reduction.** F. Jeanneret, J. Boccard, F. Badoud, O. Sorg, D. Pelcova, S. Vlckova, D.N. Rutledge, C. F. Samer, D. Hochstrasser, J.-H. Saurat, S. Rudaz. *Toxicology Letters* (2014), 230, 234-243.
- 26. Comprehensive profiling and marker identification in non-volatile citrus oil residues by mass spectrometry and nuclear magnetic resonance.** G. Marti, J. Boccard, F. Mehl, B. Debrus, L. Marcourt, P. Merle, E. Delort, L. Baroux, H. Sommer, S. Rudaz, J.-L. Wolfender. *Food Chemistry* (2014), 150, 235-245.
- 25. Differentiation of lemon essential oil based on volatile and non-volatile fractions with various analytical techniques: a metabolomic approach.** F. Mehl, G. Marti, J. Boccard, B. Debrus, P. Merle, E. Delort, L. Baroux, V. Raymo, M.I. Velazco, H. Sommer, J.-L. Wolfender, S. Rudaz. *Food Chemistry* (2014), 143, 325-335.
- 24. Systematic comparison of sensitivity between HILIC-MS and RPLC-MS using columns packed with sub-2 µm particles.** A. Périat, J. Boccard, J.-L. Veuthey, S. Rudaz, D. Guillaume. *Journal of Chromatography A* (2013), 1312, 49-57.
- 23. Différentiation d'huile essentielle de citron basée sur l'analyse des fractions volatile et non-volatile par plusieurs techniques analytiques : une approche métabolomique.** F. Mehl, G. Marti, J. Boccard, B. Debrus, P. Merle, E. Delort, L. Baroux, V. Raymo, M. I. Velazco, H. Sommer, J.-L. Wolfender, S. Rudaz. *Spectra Analyse* (2013), 294, 48-58.
- 22. Profiling of steroid metabolites after transdermal and oral administration of testosterone by ultra-high pressure liquid chromatography coupled to quadrupole time-of-flight mass spectrometry.** F. Badoud, J. Boccard, C. Schweizer, F. Pralong, M. Saugy, N. Baume. *Journal of Steroid Biochemistry and Molecular Biology* (2013), 138, 222-235.
- 21. A consensus OPLS-DA strategy for multiblock Omics data fusion.** J. Boccard, D.N. Rutledge. *Analytica Chimica Acta* (2013), 769, 30-39.
- 20. Metabolomics reveals herbivore-induced metabolites of resistance and susceptibility in maize leaves and roots.** G. Marti, M. Erb, J. Boccard, G. Glauser, G.D. Doyen, N. Villard, C.A.M. Robert, T.C.J. Turlings, S. Rudaz, J.-L. Wolfender. *Plant, Cell and Environment* (2013), 36(3), 621-639.
- 19. Analysis of basic compounds by supercritical fluid chromatography: Attempts to improve peak shape and maintain mass spectrometry compatibility.** A. Grand-Guillaume Perrenoud, J. Boccard, J.-L. Veuthey, D. Guillaume. *Journal of Chromatography A* (2012), 1262, 205-213.
- 18. Analyse métabolomique dans l'urine par UHPLC-QTOF-MS<sup>E</sup>: profilage des stéroïdes appliqué au dépistage anti-dopage.** J. Boccard, F. Badoud, E. Grata, S.S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Spectra Analyse* (2012), 41 (284), 48-54.
- 17. Method development for pharmaceuticals: Some solutions for tuning selectivity in reversed phase and hydrophilic interaction liquid chromatography.** J. Ruta, Josephine; J. Boccard, D. Cabooter, S. Rudaz, G. Desmet, J.-L. Veuthey, D. Guillaume. *Journal of Pharmaceutical and Biomedical Analysis* (2012), 63, 95-105.
- 16. A steroidomic approach for biomarkers discovery in doping control.** J. Boccard, F. Badoud, E. Grata, S.S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Forensic Science International*. (2011), 213(1-3), 85-94.
- 15. Quantification of glucuronidated and sulfated steroids in human urine by ultra-high pressure liquid chromatography quadrupole time-of-flight mass spectrometry.** F. Badoud, E. Grata, J. Boccard, D. Guillaume, J.-L. Veuthey, S. Rudaz, M. Saugy. *Analytical and Bioanalytical Chemistry* (2011), 400(2), 503-516.

- 14. Analysis of experimental design with multivariate response: A contribution using multiblock techniques.** G. Mazerolles, J. Boccard, M. Hanafi, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2011), 106(1), 65-72.
- 13. Phenotypic and molecular characterization of proliferating and differentiated GnRH-expressing GnV-3 cells.** V. Mansuy, S. Geller, J.-P. Rey, C. Campagne, J. Boccard, P. Poulain, V. Prevot, F. Pralong. *Molecular and Cellular Endocrinology* (2011), 332(1-2), 97-105.
- 12. Standard machine learning algorithms applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in *Arabidopsis thaliana*.** J. Boccard, A. Kalousis, M. Hilario, P. Lantéri, M. Hanafi, G. Mazerolles, J.-L. Wolfender, P.-A. Carrupt, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2010), 104(1), 20-27.
- 11. IEF pattern classification-derived criteria for the identification of epoetin- $\delta$  in urine.** S. Lamon, J. Boccard, P.-E. Sottas, N. Glatz, G. Wuerzner, N. Robinson, M. Saugy. *Electrophoresis* (2010), 31(12), 1918-1924.
- 10. Mass spectrometry-based metabolomics oriented by correlation analysis for wound-induced molecule discovery: identification of a novel jasmonate glucoside.** G. Glauser, J. Boccard, S. Rudaz, J.-L. Wolfender. *Phytochemical Analysis* (2010), 21(1), 95-101.
- 9. Breast cancer resistance protein (BCRP/ABCG2): New inhibitors and QSAR studies by a 3D linear solvation energy approach.** E. Nicolle, J. Boccard, D. Guilet, M.-G. Dijoux-Franca, F. Zelefac, S. Macalou, J. Grosseclin, J. Schmidt, P.-A. Carrupt, A. Di Pietro, A. Boumendjel. *European Journal of Pharmaceutical Sciences* (2009), 38(1), 39-46.
- 8. Metabolite profiling of plant extracts by ultra-high-pressure liquid chromatography at elevated temperature coupled to time-of-flight mass spectrometry.** E. Grata, D. Guillaume, G. Glauser, J. Boccard, P.-A. Carrupt, J.-L. Veuthey, S. Rudaz, J.-L. Wolfender. *Journal of Chromatography A* (2009), 1216(30), 5660-5668.
- 7. A 3D linear solvation energy model to quantify the affinity of flavonoid derivatives toward P-glycoprotein.** J. Boccard, F. Bajot, A. Di Pietro, S. Rudaz, A. Boumendjel, E. Nicolle, P.-A. Carrupt. *European Journal of Pharmaceutical Sciences* (2009), 36(2-3), 254-264.
- 6. UPLC-TOF-MS for plant metabolomics: A sequential approach for wound marker analysis in *Arabidopsis thaliana*.** E. Grata, J. Boccard, D. Guillaume, G. Glauser, P.-A. Carrupt, E.E. Farmer, J.-L. Wolfender, S. Rudaz. *Journal of Chromatography B* (2008), 871(2), 261-270.
- 5. Antimitotic and antiproliferative activities of chalcones: forward structure-activity relationship.** A. Boumendjel, J. Boccard, P.-A. Carrupt, E. Nicolle, M. Blanc, A. Geze, L. Choisnard, D. Wouessidjewe, E.-L. Matera, C. Dumontet. *Journal of Medicinal Chemistry* (2008), 51(7), 2307-2310.
- 4. Optimized liquid chromatography-mass spectrometry approach for the isolation of minor stress biomarkers in plant extracts and their identification by capillary nuclear magnetic resonance.** G. Glauser, D. Guillaume, E. Grata, J. Boccard, A. Thiocone, P.-A. Carrupt, J.-L. Veuthey, S. Rudaz, J.-L. Wolfender. *Journal of Chromatography A* (2008), 1180(1-2), 90-98.
- 3. Development of a two-step screening ESI-TOF-MS method for rapid determination of significant stress-induced metabolome modifications in plant leaf extracts: the wound response in *Arabidopsis thaliana* as a case study.** E. Grata, J. Boccard, G. Glauser, P.-A. Carrupt, E.E. Farmer, J.-L. Wolfender, S. Rudaz. *Journal of Separation Science* (2007), 30(14), 2268-2278.
- 2. Multivariate data analysis of rapid LC-TOF/MS experiments from *Arabidopsis thaliana* stressed by wounding.** J. Boccard, E. Grata, A. Thiocone, J.-Y. Gauthier, P. Lanteri, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Chemometrics and Intelligent Laboratory Systems* (2007), 86(2), 189-197.
- 1. CD40-CD40 ligand disruption does not prevent hyperoxia-induced injury.** C. Barazzone Argiroffo, Y.R. Donati, J. Boccard, A.F. Rochat, C. Vesin, C.-D. Kan, P.-F. Piguet. *American Journal of Pathology* (2002), 160(1), 67-71.

## PEER-REVIEWED SCIENTIFIC REVIEWS & TUTORIALS

- 12. From fundamentals in calibration to modern methodologies: A tutorial for small molecules quantification in liquid chromatography–mass spectrometry bioanalysis.** G. Visconti, J. Boccard, M. Feinberg, S. Rudaz. *Analytica Chimica Acta* (2023), 1240, 340711.
- 11. Challenges in ESI-MS based untargeted metabolomics.** E. Tobolkina, V. González-Ruiz, I. Meister, M. de Figueiredo, D. Guillaume, J. Boccard, S. Rudaz. *Chimia* (2022), 76(1-2), 90-100.
- 10. Approaches in metabolomics for regulatory toxicology applications.** E. Olesti, V. González-Ruiz, M.F. Wilks, J. Boccard, S. Rudaz. *Analyst* (2021), 146, 1820-1834.
- 9. From a single steroid to the steroidome: trends and analytical challenges.** E. Olesti, J. Boccard, G. Visconti, V. González-Ruiz, S. Rudaz. *Journal of Steroid Biochemistry and Molecular Biology* (2021), 206:105797.
- 8. Implementation of liquid chromatography-high resolution mass spectrometry methods for untargeted metabolomic analyses of biological samples: a tutorial.** J. Pezzatti, J. Boccard, S. Codesido, Y. Gagnebin, A. Joshi, D. Picard, V. González-Ruiz, S. Rudaz. *Analytica Chimica Acta* (2020), 1105, 28-44.
- 7. Metabolomics in chronic kidney disease: Strategies for extended metabolome coverage.** Y. Gagnebin, J. Boccard, B. Ponte, S. Rudaz. *Journal of Pharmaceutical and Biomedical Analysis* (2018), 161, 313-325.
- 6. Evaluation of steroidomics by liquid chromatography hyphenated to mass spectrometry as a powerful analytical strategy for measuring human steroid perturbations.** F. Jeanneret, D. Tonoli, M. Rossier, M. Saugy, J. Boccard, S. Rudaz. *Journal of Chromatography A* (2016), 1430, 97–112.
- 5. Harnessing the complexity of metabolomic data with chemometrics.** J. Boccard, S. Rudaz. *Journal of Chemometrics* (2014), 28(1), 1-9.
- 4. New Insights in Pharmaceutical Analysis.** D. Guillaume, J. Schappler, J. Boccard, J.-L. Veuthey, S. Rudaz. *Chimia* (2012), 66, 330-334.
- 3. Analytical aspects in doping control: Challenges and perspectives.** F. Badoud, D. Guillaume, J. Boccard, E. Grata, M. Saugy, S. Rudaz, J.-L. Veuthey. *Forensic Science International*. (2011), 213(1-3), 49-61.
- 2. Knowledge discovery in metabolomics: an overview of MS data handling.** J. Boccard, J.-L. Veuthey, S. Rudaz. *Journal of Separation Science* (2010), 33(3), 290-304.
- 1. MS-based plant metabolomic approaches for biomarker discovery.** J.-L. Wolfender, G. Glauser, J. Boccard, S. Rudaz. *Natural Product Communications* (2009), 4(10), 1417-1430.

## SHORT COMMUNICATIONS & PERSPECTIVES

- 4. Why do we need to go beyond overall biological variability assessment in metabolomics?** J. Boccard, S. Rudaz. *Frontiers in Analytical Science* (2023), 3, 1112390.
- 3. Longitudinal Monitoring of Endogenous Blood Steroids as a Tool to Detect Testosterone Abuse in Sport.** F. Ponzetto, J. Boccard, N. Baume, S. Rudaz, M. Saugy, R. Nicoli, *Chimia* (2016), 70(3), 208.
- 2. Plant Metabolomics – Strategies for Biomarker Detection, Isolation and Identification.** E. Grata, J. Boccard, G. Glauser, D. Guillaume, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz, *Chimia* (2008), 62(7/8), 685.
- 1. Synergy at the 'Ecole de Pharmacie Geneve-Lausanne': Methodology developments for the treatment of complex metabolomic datasets with data mining.** A. Thiocone, E. Grata, J. Boccard, P.-A. Carrupt, S. Rudaz, J.-L. Wolfender. *Chimia* (2005), 59(6), 362-365.

## PROTOCOLS

- 4. Extended steroid profiling in human serum and plasma with simultaneous quantitative determination using one-point internal calibration.** M. Galmiche, O. Strassel, M.-A. Monat, I. Meister, J. Boccard, S. Rudaz. *Journal of Separation Science* (2025), 48(4), e70147.
- 3. Identification of a predictive metabolic signature of response to immune checkpoint inhibitors in non-small cell lung cancer: METABO-ICI clinical study protocol.** S. Sannicolo, M. Giay Levra, A. Le Gouellec, C. Aspod, J. Boccard, L. Chaperot, B. Toussaint, D. Moro-Sibilot, D. Hannani, A.-C. Toffart. *Respiratory Medicine and Research* (2021), 80, 100845.
- 2. UHPLC-HRMS analysis for steroid profiling in serum (steroidomics) in *Metabolic Profiling: Methods and Protocols*,** F. Ponzetto, J. Boccard, R. Nicoli, T. Kuuranne, M. Saugy, S. Rudaz. Springer (2018).
- 1. Extracting knowledge from MS clinical metabolomic data: Processing and analysis strategies in *Clinical Metabolomics: Methods and Protocols*,** J. Boccard, S. Rudaz. Springer (2018).

## BOOK CHAPTERS

- 11. Extracting knowledge from MS clinical metabolomic data: Processing and analysis strategies in *Clinical Metabolomics: Methods and Protocols (Second Edition)*,** I. Meister, J. Boccard, S. Rudaz. Springer (2025).
- 10. Workflow for knowledge discovery from metabolomic data using chemometrics in *A Practical Guide to Metabolomics Applications in Health and Disease: From Samples to Insights into Metabolism*,** M. de Figueiredo, S. Rudaz, J. Boccard. Springer (2024).
- 9. Data analysis strategies in CE-MS for metabolomics in *Capillary Electrophoresis-Mass Spectrometry for Proteomics and Metabolomics: Principles and Applications*,** N. Drouin, J. Boccard, S. Rudaz, V. González-Ruiz. Wiley-VCH (2022).
- 8. Evaluation of prototype CE-MS interfaces in *Capillary Electrophoresis-Mass Spectrometry*,** S. Ferré, J. Boccard, S. Rudaz, V. González-Ruiz. Springer (2022).
- 7. Analysis of metabolomic data – A chemometrics perspective in *Comprehensive Chemometrics (Second Edition)*,** J. Boccard, S. Rudaz. Elsevier (2020).
- 6. Mass spectrometry metabolomic data handling for biomarker discovery in *Proteomic and Metabolomic Approaches to Biomarker Discovery (Second Edition)*,** J. Boccard, V. González-Ruiz, S. Codesido, S. Rudaz. Academic Press (2020).
- 5. Integration of metabolomic data from multiple analytical platforms: toward extensive coverage of the metabolome in *Data Analysis for Omic Sciences: Methods and Applications*,** J. Boccard, S. Rudaz. Elsevier (2018).
- 4. Methods for Doping Detection in *Sports Endocrinology*,** F. Ponzetto, S. Giraud, N. Leuenberger, J. Boccard, R. Nicoli, N. Baume, S. Rudaz, M. Saugy. Karger (2016).
- 3. From raw signals to identified metabolites: recent tools for enhancing LC-MS untargeted metabolomic data processing in *Metabolomic Data Processing and Analysis*,** D. Tonoli, F. Jeanneret, J. Boccard, S. Rudaz. Future Science (2015).
- 2. Mass spectrometry metabolomic data handling for biomarker discovery in *Proteomic and Metabolomic Approaches to Biomarker Discovery*,** J. Boccard, S. Rudaz. Academic Press (2013).
- 1. Metabolomics: Application in plant sciences in *Metabolomics In Practice: Successful Strategies to Generate and Analyze Metabolic Data*,** G. Glauser, J. Boccard, J.-L. Wolfender, S. Rudaz. Wiley-VCH (2013).

## ORAL COMMUNICATIONS

- 29. Improving model interpretability in metabolomics by assessing variable importance stability.** *Chimiométrie XXV*, February 2026, Nancy (France).
- 28. Improving model interpretability in metabolomics by assessing variable importance stability via resampling.** *17<sup>èmes</sup> Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, June 2025, Paris (France).
- 27. Multiomics data analysis and integration.** *34<sup>th</sup> International Symposium on Pharmaceutical and Biomedical Analysis*, September 2024, Geneva (Switzerland).
- 26. New insights in bioanalytical and metabolomic readout for toxicology.** *SCAHT Retreat*, August 2023, Bern (Switzerland).
- 25. From data structures to relevant metabolic patterns.** *8<sup>th</sup> Swiss Metabolomics Society Annual Meeting*, September 2022, Lausanne (Switzerland)
- 24. Advanced analysis of metabolomics data: Data Structures as a key to knowledge discovery.** *Metabolomics2021*, June 2021, online.
- 23. Facing the data deluge: a practical survival guide.** *33<sup>rd</sup> Seminar in Pharmaceutical Sciences*, September 2019, Zermatt (Switzerland).
- 22. Facing the data deluge: a practical guide to biomarker discovery.** *CITB seminar series*, June 2019, Geneva (Switzerland).
- 21. Stratified subsampling for effective removal of batch effects in metabolomics: application to endocrine disruptors screening.** *Chimiométrie XX*, February 2019, Montpellier (France).
- 20. Steroidomic profiling in an adrenal cell model,** *6<sup>th</sup> SCAHT Science Advisory Board Meeting*, August 2018, Olten (Switzerland).
- 19. Exploring human urinary biomarkers of dioxin exposure using metabolomics and biologically-driven data dimensionality reduction.** *3<sup>rd</sup> Meeting of the Swiss Metabolomics Society*, November 2017, Bern (Switzerland).
- 18. Toward a better understanding of neuroinflammation using proteomic and metabolomic data integration.** *SCAHT Retreat*, August 2017, Neuchâtel (Switzerland).
- 17. Multiblock data integration and its application to plant metabolomics.** *French Flax Research Network*, May 2017, Amiens (France).
- 16. Metabolomic profiles alterations induced by neuroinflammatory conditions,** *5<sup>th</sup> SCAHT Science Advisory Board Meeting*, July 2016, Bern (Switzerland).
- 15. Exploring metabolomic data from designed experiments using ANOVA-Multiblock Orthogonal Partial Least Squares.** *12<sup>th</sup> Annual Conference of the Metabolomics Society*, June 2016, Dublin (Ireland).
- 14. ANOVA-Multiblock Orthogonal Partial Least Squares (AMOPLS) for exploring metabolomic data from designed experiments.** *Chimiométrie XVII*, January 2016, Namur (Belgium).
- 13. Analysis of metabolomic data from designed experiments using ANOVA Multiblock Orthogonal Partial Least Squares.** *9<sup>èmes</sup> Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, June 2015, Lille (France).
- 12. A consensus OPLS-DA strategy for multiblock data fusion: Application to plant metabolomics.** *8<sup>èmes</sup> Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, May 2014, Lyon (France).
- 11. Extension du profilage urinaire des stéroïdes par une approche stéroïdomique pour le dépistage antidopage.** *7<sup>èmes</sup> Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, June 2013, Amiens (France).

10. **Pondération itérative de tableaux multiples dans le cadre de la modélisation OPLS multiblocs.** *Chimie XIV*, December 2012, Lille (France).
9. **A multiblock OPLS-DA strategy for Omics data fusion.** *DIM Analytics Inaugural Symposium*. June 2012. Saclay (France).
8. **A steroidomic strategy for profile monitoring in doping control analysis.** *Annual Meeting of the Swiss Group for Mass Spectrometry*, October 2011, Beatenberg (Switzerland).
7. **A metabolomic approach to extend the steroid profile monitoring for doping control analysis.** *36<sup>th</sup> International Symposium on High-Performance Liquid Phase Separations and Related Techniques*, June 2011, Budapest (Hungary).
6. **Machine learning applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in *Arabidopsis thaliana*.** *Chimie XI*, December 2009, Paris (France).
5. **Analyses métabolomiques en phytochimie.** with J.-L. Wolfender, *Journées Scientifiques du ccCTA*, September 2008, Les Diablerets (Suisse).
4. **Data mining of UPLC-TOF/MS metabolic fingerprints for the detection of wound biomarkers in *Arabidopsis thaliana*.** *PhD Day*, June 2008, Archamps (France).
3. **Analyse solvatochromique 3D des forces d'interactions moléculaires dirigeant la liaison de dérivés de flavonoïdes à la glycoprotéine P.** *Chimie IX*, November 2007, Lyon (France).
2. **Analyse multivariée de données obtenues par gradient rapide LCTOF-MS dans le cadre d'une étude métabolomique chez *A. thaliana*.** *Chimie VII*, December 2005, Lille (France).
1. **Statistical comparison of LC-MS ion maps in metabolomic studies.** *Fall Meeting of the Swiss Chemical Society*, October 2004, Zürich (Suisse).

## EXTERNAL INVITED LECTURES

34. **Harnessing Experimental Design for Improved Knowledge Discovery in Metabolomics.** *Workflow4Experimenters workshop*, Rouen University, April 2026, Rouen (France).
33. **Kernel-based bootstrap synthetic data to estimate measurement uncertainty in analytical sciences.** *METAS Colloquium*, December 2025, Wabern (Switzerland).
32. **Making Sense of Metabolomics and Lipidomics - Linking Data Structures to Chemometric Strategies.** *11<sup>th</sup> Swiss Metabolomics Society Annual Meeting*, October 2025, Bern (Switzerland).
31. **Harnessing Data Structures for Improved Knowledge Discovery in Analytical Chemistry: Applications in Metabolomics.** *Journées Scientifiques Nantes Université*, May 2025, Nantes (France).
30. **Chemometrics for multiomics data analysis & integration.** *Staromics Retreat 2024*, October 2024, Leysin (Switzerland).
29. **Integration of metabolomic data from multiple sources: Challenges and strategies in chemometrics.** *RFMF webinar series*, July 2023, online.
28. **Intégration de données métabolomiques multi-sources: Enjeux et apports de la chimie.** *15<sup>ème</sup> Congrès Francophone sur les Sciences Séparatives*, March 2023, Paris (France).
27. **Integration of omics data from multiple sources.** *LEM symposium*, March 2023, Lyon (France).
26. **Aspects méthodologiques pour l'acquisition et le traitement de données métabolomiques.** *Workshop. Chimie XXII*, June 2022, Brest (France).
25. **Data structures as a key to knowledge discovery in metabolomics.** *Metabolomics Society Early Member Network webinars*, December 2021, online.

- 24. Des données à l'information biologique : aspects statistiques et bioinformatiques en métabolomique.** Short course. *14<sup>ème</sup> Congrès Francophone sur les Sciences Séparatives*, October 2021, Paris (France).
- 23. De l'acquisition aux données : aspects analytiques et méthodologiques en métabolomique.** Short course. *14<sup>ème</sup> Congrès Francophone sur les Sciences Séparatives*, October 2021, Paris (France).
- 22. Débuter dans l'analyse multivariée pour traiter ses données expérimentales.** *ccCTA seminar series*, June 2021, online.
- 21. Approches méthodologiques en métabolomique: de l'acquisition à l'analyse de données.** Workshop. *eChimométrie*, January 2021, online.
- 20. Aspects méthodologiques pour l'acquisition et le traitement de données métabolomiques.** Workshop. *Chimométrie XXI*, January 2020, Liège (Belgium).
- 19. Advanced approaches for the analysis of metabolomics data: From experimental design to knowledge discovery.** *RFMF-Metabomeeting*, January 2020, Toulouse (France).
- 18. On the trail of biomarkers: Principles and chemometric approaches for the analysis of metabolomic data.** *LABERCA seminar series*, July 2019, Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA), ONIRIS, Nantes (France).
- 17. Data integration in metabolomics: food for thought in bioinformatics and chemometrics.** *Data Integration Workshop, 12<sup>èmes</sup> Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, May 2019, Clermont-Ferrand (France).
- 16. Current challenges in metabolomics: From experimental design to knowledge discovery,** *MetaToul seminars*, May 2019, Toulouse (France).
- 15. Chemometrics and bioinformatics for metabolomics,** *Bioinformatic Network Workshop*, April 2019, Geneva (Switzerland).
- 14. L'Analyse multivariée des données expérimentales.** Tutorial. *13<sup>ème</sup> Congrès Francophone sur les Sciences Séparatives*, March 2019, Paris (France).
- 13. Multivariate analysis of metabolomic data.** *Metabolomics for life and health scientists*, December 2018, Lausanne (Switzerland).
- 12. Data structures and advanced chemometric tools in metabolomics.** *Workflow4Experimenters workshop, Pasteur Institute*, October 2018, Paris (France).
- 11. Data structures and chemometric strategies in metabolomics.** *BIOPI seminars, University of Picardy Jules Verne*, June 2018, Amiens (France).
- 10. Chemometric approaches for meta<sup>2</sup>bolomics.** *Meta-metabolomics Workshop, 11<sup>èmes</sup> Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, May 2018, Liège (Belgium).
- 9. A multiblock approach for the integration of multiple data sources in metabolomics.** *Club Lyonnais de Chromatographie, Forum Labo*, March 2018, Lyon (France).
- 8. Multivariate analysis of metabolomic data.** *Metabolomics: from data to publication*, June 2017, Lausanne (Switzerland).
- 7. Sur la piste des biomarqueurs : Traitement des données métabolomiques obtenues par chromatographie liquide couplée à la spectrométrie de masse.** *Société des Experts Chimistes de France*, June 2017, Solaize (France).
- 6. Advanced chemometric methods for MS-based metabolomics.** *Métabolomique: Outils et méthodologie*, April 2016, Clermont-Ferrand (France).
- 5. Chemometric approaches for the fusion of multiple data sources in metabolomics.** *Applied Statistics Workshop*, October 2015, Louvain-la-Neuve (Belgium).

**4. Harnessing the complexity of MS metabolomic data: From raw signals to biomarkers.** *4<sup>th</sup> Danish Symposium on Metabolomics*, November 2013, Copenhagen (Denmark).

**3. Réduction de la dimensionnalité dans le cadre de l'analyse de données LC-MS.** *Club Lyonnais de Chromatographie*, May 2012, Lyon (France).

**2. Analysis and integration of multiple data sources in metabolomics.** *Plant Metabolomics Workshop*, April 2011, Athens (Greece).

**1. Knowledge discovery in high volume LC-MS metabolomic data.** *Séminaire Intégration des Données*, March 2010, Avignon (France).

## POSTER COMMUNICATIONS

**17. Longitudinal steroidomics of human serum by UHPLC-HRMS for testosterone abuse detection.** J. Boccard, F. Ponzetto, R. Nicoli, N. Baume, T. Kuuranne, M. Saugy, S. Rudaz. *Chimie X*, January 2018, Paris (France).

**16. Profilage stéroïdique des perturbateurs endocriniens : décomposition des sources de variabilité à l'aide de la chimométrie.** J. Boccard, D. Tonoli, P. Strajhar, F. Jeanneret, A. Odermatt, S. Rudaz. *12<sup>ème</sup> Congrès de l'Association Francophone des Sciences Séparatives*, March 2017, Paris (France).

**15. Multifactorial steroidomic footprinting for in vitro endocrine disruptor evaluation.** J. Boccard, D. Tonoli, P. Strajhar, F. Jeanneret, A. Odermatt, S. Rudaz. *Chimie XVIII*, January 2017, Paris (France).

**14. Simultaneous analysis of the spatial and temporal response to wounding in *Arabidopsis thaliana* using multifactorial metabolomics and chemometrics.** J. Boccard, S. Rudaz. *10<sup>èmes</sup> Journées Scientifiques du Réseau Français de Métabolisme et Fluxomique*, June 2016, Montpellier (France).

**13. Analyse métabolomique pour la recherche de biomarqueurs urinaires d'exposition à la dioxine chez l'Homme.** J. Boccard, F. Jeanneret, D. Tonoli, F. Badoud, O. Sorg, J.-H. Saurat, D. Hochstrasser, S. Rudaz. *Chimie XV*, September 2013, Brest (France).

**12. Discovery of biomarkers of dioxin intoxication in human urine: analysis by metabolomics and biologically-driven strategy.** J. Boccard, F. Jeanneret, O. Sorg, J.-H. Saurat, S. Vlckova, D. Pelclova, D.N. Rutledge, D. Hochstrasser, S. Rudaz. *Eurotox*, September 2013, Interlaken (Switzerland).

**11. Metabolomics applied to dioxin intoxication: biologically-driven strategy for the discovery of biomarkers in human urine.** J. Boccard, F. Jeanneret, O. Sorg, J.-H. Saurat, D. Pelclova, D.N. Rutledge, D. Hochstrasser, S. Rudaz. *Systems Toxicology*. April-May 2013, Ascona (Switzerland).

**10. Iterative weighting of multiblock data in the OPLS framework.** J. Boccard, D.N. Rutledge. *AfroData*, November 2012, Stellenbosch (South Africa).

**9. From targeted to extended steroid profile for doping analysis.** J. Boccard, F. Badoud, E. Grata, S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Chimie XII*, December 2010, Paris (France).

**8. Machine learning applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound markers in *Arabidopsis thaliana*.** J. Boccard, S. Rudaz, A. Kalousis, M. Hilario, P.-A. Carrupt, J.-L. Veuthey, J.-L. Wolfender. *Fall Meeting of the Swiss Chemical Society*, September 2009, EPFL, Lausanne (Suisse).

**7. Multiway 3D solvatochromic analysis of molecular interaction forces between flavonoid derivatives and P glycoprotein.** J. Boccard, F. Bajot, E. Nicolle, A. Boumendjel, S. Rudaz, P.-A. Carrupt. *Fall Meeting of the Swiss Chemical Society*, September 2007, EPFL, Lausanne (Suisse).

**6. Multiway PLS calibration based on 3D solvatochromic descriptors with artificial membrane PAMPA-skin experimental data.** J. Boccard, G. Ottaviani, S. Martel, S. Rudaz, P.-A. Carrupt. *GGMM*, May 2007, Autrans (France).

**5. Analyse multivariée par OSC-ACP/CAH de données métabolomiques obtenues par HPLC-TOF/MS chez *A. thaliana*.** J. Boccard, E. Grata, G. Glauser, P.-A. Carrupt, J.-Y. Gauthier, P. Lantéri, J.-L. Wolfender, S. Rudaz. *Chimie VIII*, November 2006, Paris (France).

**4. Chemometric analysis of LC-TOF/MS metabolomic data from wounded *Arabidopsis thaliana* specimens.** J. Boccard, E. Grata, G. Glauser, P.-A. Carrupt, J.-Y. Gauthier, P. Lantéri, J.-L. Wolfender, S. Rudaz. *Rencontre des Sciences Pharmaceutiques de l'Arc Alpin*, November 2006, Archamps (France).

**3. Stress biomarkers discovery in *Arabidopsis thaliana* after wounding based on rapid LC-TOF/MS experiments.** J. Boccard, E. Grata, G. Glauser, P.-A. Carrupt, J.-Y. Gauthier, P. Lantéri, J.-L. Wolfender, S. Rudaz. *Fall Meeting of the Swiss Chemical Society*, October 2006, Zurich (Suisse).

**2. Multivariate analysis of metabolomic data from *Arabidopsis thaliana* stressed by wounding with rapid LC/TOF-MS and gradient LC/quadrupole-MS analysis.** J. Boccard, E. Grata, C. Didon, A. Thiocone, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Fall Meeting of the Swiss Chemical Society*, October 2005, Lausanne (Suisse).

**1. Visualisation et comparaison de données obtenues par LC-APCI-MS dans le cadre d'une étude métabolomique chez *A. thaliana*.** J. Boccard, E. Grata, A. Thiocone, M. Muller, P.-A. Carrupt, J.-L. Wolfender, S. Rudaz. *Chimie VI*, November 2004, Paris (France).

## AWARDS AND DISTINCTIONS

**23. Rolin-Portais thesis award 2026. Integrative analysis of multiple study data for the identification of common metabolic syndrome phenotypes.** E. Salanon. Co-direction with Dre E. Pujos-Guillot. 18<sup>èmes</sup> *Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, May 2026, Lille (France).

**22. Best poster award, 1<sup>st</sup> prize. Multiblock Analysis of Metabolomics Data: Application to Mindfulness Meditation and Healthcare Student Well-Being.** C. Da Silva, M. Galmiche, O. Strassel, S. Girel, I. Meister, C. Piguët, F. Jermann, J. Boccard, S. Rudaz. *Chimie XXV*, February 2026, Nancy (France).

**21. Best poster award, 3<sup>rd</sup> prize. Mindfulness in Healthcare Students: exploring the Biological Basis of Well-Being through Chemometric and Metabolomic Analyses.** C. Da Silva, M. Galmiche, O. Strassel, S. Girel, T. Binz, C. Berchtold, C. Vögel, B. Meuleman, I. Meister, C. Piguët, F. Jermann, J. Boccard, S. Rudaz. 11<sup>th</sup> *Swiss Metabolomics Society Annual Meeting*, October 2025, Bern (Switzerland).

**20. Best poster award, 1<sup>st</sup> prize. Metabolomic insights into mindfulness: exploring the impact of non-judgmental self-awareness meditation on healthcare student well-being.** C. Da Silva, M. Galmiche, O. Strassel, S. Girel, M. Fiault, B. Meuleman, I. Meister, C. Piguët, F. Jermann, J. Boccard, S. Rudaz. 17<sup>èmes</sup> *Journées Scientifiques du Réseau Francophone de Métabolomique et Fluxomique*, June 2025, Paris (France).

**19. Best oral presentation for junior researcher, 1<sup>st</sup> prize. Investigating lipid raft composition of extracellular vesicles secreted by triple-negative breast cancer and non-cancerous breast cells to develop an optimal cancer-targeting EV-mimetic formulation.** O. Majchrzak, C. Lopes Silva, I. Meister, S. Tankov, J. Boccard, O. Jordan, P. Walker, S. Rudaz, G. Borchard. *International Society for Extracellular Vesicles Annual Meeting*, April 2025, Vienna (Austria).

**18. Best poster award, 1<sup>st</sup> prize. Metabolomic and lipidomic approaches in mindfulness-based intervention for health-care students.** I. Meister, S. Girel, I. Furlani, C. Holman, F. Jermann, J. Boccard, C. Piguët, S. Rudaz. *Swiss Metabolomics Society Annual Meeting*, September 2023, Zurich (Switzerland).

**17. Best poster award, 1<sup>st</sup> prize. Fast in-sample multiplexed quantification of endogenous metabolites associated with chronic kidney disease using liquid chromatography-mass spectrometry.** G. Visconti, M. de Figueiredo, O. Strassel, N. Vuilleumier, J. Boccard, D. Jaques, B. Ponte, S. Rudaz. *RDPA23*, September 2023, Novara (Italy).

**16. Editor's Choice article in *Metabolites*. Metabotypes of *Pseudomonas aeruginosa* Correlate with Antibiotic Resistance, Virulence and Clinical Outcome in Cystic Fibrosis Chronic Infections.** May 2023.

15. Best flash presentation, 1<sup>st</sup> prize. **Biosource-guided network annotation and visualization for untargeted metabolomics.** S. Codesido, V. González-Ruiz, E. Olesti, J. Boccard, S. Rudaz. *RFMF-Metabomeeting*, January 2020, Toulouse (France).
14. Best poster award, 2<sup>nd</sup> prize. **Metabolomics in chronic kidney disease: toward a better understanding of disease progression and hemodialysis.** Y. Gagnebin, J. Pezzatti, P. Lescuyer, S. De Seigneux, J. Boccard, S. Rudaz, B. Ponte, 32<sup>nd</sup> *International Symposium on Chromatography*, September 2018, Cannes (France).
13. Best poster award, 3<sup>rd</sup> prize. **Metabolomic analysis of urine samples by UHPLC-QTOF-MS: impact of normalization strategies.** Y. Gagnebin, D. Tonoli, P. Lescuyer, B. Ponte, S. De Seigneux, P.-Y. Martin, J. Schappler, J. Boccard, S. Rudaz, 27<sup>th</sup> *International Symposium on Pharmaceutical and Biomedical Analysis*, November 2016, Guangzhou (China).
12. Best poster award (Phytochemical Society of Europe), 1<sup>st</sup> prize. **Detection and dynamics of volatile/non-volatile metabolite induction in fungal co-culture through a miniaturised MS-based metabolomic approach.** A. Azzollini, L. Boggia, J. Boccard, B. Sgorbini, N. Lecoutre, P. Rubiolo, S. Rudaz, K. Gindro, C. Bicchi, J.-L. Wolfender, 9<sup>th</sup> *Joint Natural Products Conference*, July 2016, Copenhagen (Denmark).
11. Best poster award, 1<sup>st</sup> prize. **Suivi longitudinal de stéroïdes endogènes dans le sérum humain par UHPLC-MS/MS comme outil de détection de l'usage de testostérone dans le sport.** F. Mehl, F. Ponzetto, R. Nicoli, N. Baume, M. Saugy, J. Boccard, S. Rudaz. *Chimiométrie XVII*, January 2016, Namur (Belgium).
10. Best poster award, 1<sup>st</sup> prize. **Analyse métabolomique de l'urine : stratégies de normalisation en UHPLC-QTOF-MS.** Y. Gagnebin, J. Schappler, J. Boccard, S. Rudaz *Chimiométrie XVI*, January 2015, Geneva (Switzerland).
9. Journal Highlight in spectroscopyNOW (Chemometrics & Informatics), February-March 2014. **Harnessing the complexity of metabolomic data with chemometrics.** J. Boccard, S. Rudaz. *Journal of Chemometrics* (2014), 28(1), 1-9.
8. Best poster award, 2<sup>nd</sup> prize. **Analyse métabolomique pour la recherche de biomarqueurs urinaires d'exposition à la dioxine chez l'Homme.** J. Boccard, F. Jeanneret, D. Tonoli, F. Badoud, O. Sorg, J.-H. Saurat, D. Hochstrasser, S. Rudaz. *Chimiométrie 2013*, September 2013, Brest (France).
7. Best poster communication for spectroscopic techniques (Brucker), 1<sup>st</sup> prize. **Analyse multi-tableaux de données UHPLC-QTOF-MS, RMN et FT-MIR : application à la différenciation d'huile essentielle de citron.** F. Mehl, G. Marfi, J. Boccard, L. Marcourt, B. Debrus, P. Merle, E. Delort, L. Baroux, H. Sommer, J.-L. Wolfender, S. Rudaz. *Chimiométrie 2011*, December 2011, Marseille (France).
6. Best poster award, 2<sup>nd</sup> prize. **Profiling of endogenous steroids by UHPLC-QTOF-MS<sup>E</sup>.** F. Badoud, E. Grata, J. Boccard, S. Rudaz, J.-L. Veuthey, M. Saugy. *Congress on Steroid Research*, March 2011, Chicago (USA).
5. Top 25 Hottest articles, October to December 2011, January to March 2012 & January to December 2012 full year, *Forensic Science International*. **Analytical aspects in doping control: Challenges and perspectives.**
4. Top 25 Hottest articles, October to December 2010 & January to March 2011, *Chemometrics and Intelligent Laboratory Systems*. **Standard machine learning algorithms applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in *Arabidopsis thaliana*.**
3. Best poster award, 1<sup>st</sup> prize, **Analyse stéroïdomique dans l'urine par UHPLC-QTOF-MS pour le dépistage anti-dopage,** J. Boccard, F. Badoud, E. Grata, S.S. Ouertani, M. Hanafi, G. Mazerolles, P. Lantéri, J.-L. Veuthey, M. Saugy, S. Rudaz. *Chimiométrie 2010*, December 2010, Paris (France).
2. Hottest Articles in Analytical Chemistry / Top accessed articles during 2010, *Journal of Separation Science*. **Knowledge discovery in metabolomics: an overview of MS data handling.**
1. Top 25 Hottest articles, April to June 2007 & July to September 2007, *Chemometrics and Intelligent Laboratory Systems*. **Multivariate data analysis of rapid LC-TOF/MS experiments from *Arabidopsis thaliana* stressed by wounding.**

## HONORS

### INVITED PROFESSOR

1. **University of Picardy Jules Verne**, 2018, Amiens (France).

### SCIENTIFIC ADVISORY BOARDS

1. **MEtabolomics Lipidomics Steroidomics Analysis (MELISA) Platform** (since 2017). Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA), ONIRIS, Nantes (France).

2. **Polyphenols Platform** (since 2019), INRAE & SupAgro, Montpellier (France).

### PHD SUPERVISIONS

4. Célie Da Silva (2024-ongoing). **Novel strategies for Omics data integration from multiple sources**. Co-direction Prof. S. Rudaz, University of Geneva (Switzerland).

3. Oriane Strassel (2022-ongoing). **Multitargeted quantification of exposure biomarkers**. Co-direction Prof. S. Rudaz, University of Geneva (Switzerland).

2. Elfried Salanon (2022-2025). **Integrative analysis of multiple study data for the identification of common metabolic syndrome phenotypes**. Co-direction Dre E. Pujos-Guillot, INRAE, University Clermont Auvergne (France).

1. Yoric Gagnebin (2014-2019). **Multiplatform metabolomic characterization of biofluids**. Co-direction Prof. S. Rudaz, University of Geneva (Switzerland).

### PHD JURIES

11. Priyanka Kumari. **Different approaches of Quantitative Structure Retention Relationship of small molecules in Liquid Chromatography (QSRR)** (2024). Scientific direction: P. Hubert and C. Hubert, Liège University, Liège (Belgium).

10. Cécile Tardif. **Développement de stratégies bioanalytiques pour l'étude et la détection de formes dégradées d'anticorps monoclonaux thérapeutiques en milieu hospitalier** (2023). Scientific direction: C. Smadja and E. Jaccoulet, Paris-Saclay University, Paris (France).

9. Denis Werner. **Inférence de source de traces d'essence : étude de la contribution combinée des compositions moléculaire et isotopique** (2023). Scientific direction: O. Delémont, University of Lausanne, Lausanne (Suisse).

8. Nicolas Di Giovanni. **Development of multidimensional approaches for metabolomics** (2021). Scientific direction: J.-F. Focant, Liège University (Belgium).

7. Céline Dalle. **Profilage lipidomique ciblé des oxylipines pour identifier de nouveaux biomarqueurs du syndrome cardiométabolique - Robustesse analytique et pertinence biologique** (2020). Scientific direction: C. Gladine, Clermont Auvergne University (France).

6. Hikmat Ghosson. **Développement d'un nouveau proxy universel pour évaluer le devenir et l'impact environnemental de (bio)pesticides complexes par Métabolomique basée sur la Spectrométrie de Masse** (2020). Scientific direction: C. Bertrand and M.-V. Salvia, University of Perpignan Via Domitia (France).

5. Julian Pezzatti. **Application and evaluation of liquid chromatography – high resolution mass spectrometry in untargeted metabolomics for compound annotations in biological matrices** (2020). Scientific direction: S. Rudaz, University of Geneva (Switzerland).

4. Oriane Moyne. **Approche métabolomique pour l'étude de l'évolution adaptative de Pseudomonas aeruginosa au cours des infections pulmonaires chroniques dans la mucoviscidose** (2019). Scientific direction: B. Toussaint and D. Bicoût, Grenoble Alpes University, (France).

3. Baninia Habchi. **Mise en évidence des perturbations métaboliques liées à l'exposition aux toxiques présents dans l'environnement ou l'aliment par spectrométrie de masse à ultra haute résolution FTMS combinée avec des outils chimiométriques** (2017). Scientific direction: E. Rathahao-Paris and S. Alves, Paris-Saclay University, Paris (France).

2. Samar Azzi Ahtouky. **Etude de l'évolution du profil aromatique des moûts de Syrah issus de deux régions libanaises au cours de la fermentation par analyse GC-MS et chimiométrie** (2014). Scientific direction: D. Rutledge, AgroParisTech, Paris (France) and N. Ouaini, Holy Spirit University of Kaslik, Beirut, (Lebanon).

1. Samia Samar Ouertani. **Méthodologie statistique pour un traitement différentiel des données métaboliques** (2014). Scientific direction: M. Hanafi, ONIRIS, Nantes (France) and S. Rudaz, University of Geneva (Switzerland).

#### PHD ADVISORY COMMITTEES

12. Carla Remy. **Recherche de marqueurs hépatiques, plasmatiques et caecaux de l'exposition d'animaux d'élevage aux PCBs par une approche multi-omique** (2024 & 2025). Scientific direction: E. Engel, INRAE, Clermont-Ferrand (France) and C. Canlet, INRAE Toulouse (France).

11. Carla Chehade. **Genetic and environmental factors in CYP3A modulation: Implications for ophthalmology and steroids** (2024). Scientific direction: H. Abouzeid and C. Samer, University of Geneva (Switzerland).

10. Pedro Febrer Martinez. **From cryptic pockets to nanobodies: advanced modelling and simulation approaches for novel therapeutics** (2023). Scientific direction: F.L. Gervasio, University of Geneva (Switzerland).

9. Anouar Mejait. **Evaluation du devenir environnemental et de l'impact de biopesticides en utilisant une approche innovante de multiomique couplant métabolomique et métabarcoding** (2022, 2023 & 2024). Scientific direction: M.-V. Salvia and C. Clerissi, University of Perpignan (France).

8. Méliá Lacaze. **Recherche de marqueurs hépatique et plasmatique de l'exposition d'animaux d'élevage aux PCBs** (2021). Scientific direction: E. Engel, INRAE & Clermont Auvergne University (France) and C. Canlet, INRAE Toulouse (France).

7. Maxime Delmas. **Prédiction d'effets pathologiques liés à l'exposition à des xénobiotiques par comparaison de signatures métaboliques** (2020 & 2021). Scientific direction: F. Jourdan and C. Frainay, University Toulouse III - Paul Sabatier, Toulouse (France).

6. Denis Werner. **Inférence de source de traces d'essence : étude de la contribution combinée des compositions moléculaire et isotopique** (2019). Scientific direction: O. Delémont, University of Lausanne, Lausanne (Switzerland).

5. Katy Dinis. **Development of new applications in food authenticity analysis by liquid chromatography coupled to high resolution mass spectrometry** (2019 & 2020). Scientific direction: V. Camel, AgroParisTech, Paris (France) and F. Thomas, Eurofins, Nantes (France).

4. Thibaut Dumas. **Investigation des effets de contaminants émergents chez le bivalve marin *Mytilus galloprovincialis* à travers l'approche métabolomique** (2018 & 2019). Scientific direction: F. Courant and E. Gomez, University of Montpellier, Montpellier (France).

3. Stéphanie Monnerie. **Apport de la modélisation pour une meilleure stratification des populations à risque – Application à la caractérisation du syndrome métabolique chez la personne âgée** (2018 & 2019). Scientific direction: E. Pujos-Guillot, INRAE, Clermont-Ferrand (France) and P. Gaudreau, University of Montréal, Montréal (Canada).

2. Jihéne Bouhlel. **Determination of volatile organic compounds as markers to back trace food chain exposure to micropollutants** (2016). Scientific direction: E. Engel, INRAE, Clermont-Ferrand (France) and D. Rutledge, AgroParisTech, Paris (France).

1. Bénédicte Yanibada. **Recherche de marqueurs de la production de méthane chez la vache laitière par une approche métabolomique multiplateforme** (2015 & 2017). Scientific direction: H. Boudra and D. Morgavi, INRAE, Clermont-Ferrand (France).

#### MASTER SUPERVISIONS

3. Christian Peralta Viteri. **A data-driven workflow to enrich biomarkers annotation in untargeted metabolomics** (2022), University of Geneva (Switzerland).

2. Marion Brandolini-Bunlon. **Comparaison d'analyses multi-blocs pour l'intégration de données métabolomiques et épidémiologiques** (2017). Clermont Auvergne University (France).

1. Eva-Marie Golder. **Prédiction du temps de rétention des stéroïdes glucuroconjugués** (2016). University of Geneva (Switzerland).

#### MASTER JURIES

15. Yousra Souani. **Pathogenic mechanisms and Zinc responsiveness of Gao (A221D) variant causing GNAO1 encephalopathy** (2025). Scientific direction: V. Katanaev, University of Geneva (Switzerland).

14. Jannate Majdi. **Isolement et caractérisation de métabolites antibactériens naturels et non naturels issus de champignons filamenteux** (2025). Scientific direction: E. Ferreira Queiroz, University of Geneva (Switzerland).

13. Sudarat Bréchon. **Utilisation de la LC-HRMS pour l'identification et la caractérisation des métabolites de phase II de la solanidine** (2025). Scientific direction: A. Thomas, University of Lausanne (Switzerland).

12. Sermin Ekiztas. **Caractérisation phytochimique de trois espèces du genre Potamogeton par métabolomique computationnelle** (2025). Scientific direction: G. Glauser, University of Neuchâtel (Switzerland).

11. Marie-Amélie Girardet. **Recherche de nouveaux composés bioactifs par la biotransformation du xanthohumol par des laccases de *Trametes versicolor*** (2024). Scientific direction: E. Ferreira Queiroz, University of Geneva (Switzerland).

10. Etienne Lim Houn Tchen. **Molecular dynamics of Benzene - Studying the effects of parameter changes in protein force fields** (2023). Scientific direction: F. Gervasio, University of Geneva (Switzerland).

9. Lukas Müller. **Determination of nicotinic acid and nicotinamide in human serum using liquid chromatography-tandem mass spectrometry** (2023). Scientific direction: S. Rudaz, University of Geneva (Switzerland).

8. Carla Hentsch. **Metabolomic analysis of *Epicoccum nigrum* and *Botrytis cinerea* strains GIK1 and 1238 for the identification and isolation of antibacterial compounds** (2022). Scientific direction: J.-L. Wolfender, University of Geneva (Switzerland).

7. Pranavy Sundaralingam. **Segregation and weight variation impacts due to sticking tendency and encapsulate operating conditions in various formulations and modeling using non API based material** (2022). Scientific direction: E. Allémann, University of Geneva (Switzerland).

6. Ruth Suissa. **Understanding BRaf paradoxical activation** (2022). Scientific direction: F. Gervasio, University of Geneva (Switzerland).

5. Ezgi Çokatak. **Analyse phytochimique de la décoction d'*Argemone mexicana* utilisée traditionnellement pour traiter le paludisme** (2022). Scientific direction: E. Ferreira Queiroz, University of Geneva (Switzerland).

4. Youssef Hellioui. **Etude du lien entre l'alimentation et les maladies basé sur une analyse statistique de biomarqueurs** (2021). Scientific direction: S. Guerrier, University of Geneva (Switzerland).

3. Niruthi Sinnathurai. **Essais de traitements photothermiques pour le traitement du cancer** (2021). Scientific direction: E. Allémann, University of Geneva (Switzerland).

2. René Nellen. **Simultaneous determination of progestins and steroid profiles in plasma by HPLC-MS** (2018). Scientific direction: H. Henry, University of Lausanne (Switzerland).

1. Vadym Mozgovoy. **Metropolis-Hastings MCMC for univariate and bivariate Bayesian Lasso Regression in the steroid detection context** (2017). Scientific direction: M.-O. Boldi, University of Geneva (Switzerland).