Saer Samanipour

PERSONAL DATA

DATE OF BIRTH: 14 January 1984

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RESEARCH EXPERIENCE

From:	Assistant Prof. Van't Hoff Institute for Molecular Science (HIMS), University of Amsterdam
MAY 2020	
То:	Focus: Application of the state-of-the-art machine learning and artificial intelligence in analytical chemistry, with particular focus on
Tenure Track	computational mass spectrometry.
From:	Researcher, Norwegian Institute for Water Research (NIVA).
January 2017	, , , , , , , , , , , , , , , , , , ,
То:	Focus: Development and application of computational mass spectrometry, signal processing, and advanced statistics (i.e. chemometrics) in
April 2020	non-target analysis of complex environmental samples.
From:	Visiting Scientist, Queensland Alliance for Environmental Health Sci-
DECEMBER 2017	ences, Faculty of Health and Behavioural Sciences (QAEHS), University
To:	of Queensland, Australia.
MAY 2018	
	Focus: Comprehensive analysis of co-produced water from coal-seam
	gas production using statistical methods combined with high resolution mass spectrometry.
From:	Postdoc, Norwegian Institute for Water Research (NIVA).
November 2015	
To:	Focus: Chemical characterization of produced water, employing adva-
January 2017	nced chromatography, mass spectroscopy, and chemometric methods.
From:	Research Assistant, Ecole Polytechnique Fédérale de Lausanne (EPFL).
JUNE 2015	
To:	Focus: Non-target analysis of the sediment samples of Lake Geneva,
SEPTEMBER 2015	employing GC×GC-EI-TOFMS.
From:	Doctoral Research, Ecole Polytechnique Fédérale de Lausanne (EPFL).
DECEMBER 2010	This there is investigated the accommon of least and a second paper.
To:	Focus: This thesis investigated the occurrence of legacy and novel PBPs
June 2015	in a deep aquatic system and specifically in Lake Geneva by taking advantage of the resolution power of comprehensive two-dimensional gas chromatography (GC \times GC).

EDUCATION

From: DECEMBER 2010 To: JUNE 2015	PhD in Environmental Analytical Chemistry, EPFL, Switzerland. Thesis: "Overlooked persistent and bioaccumulative pollutants (PBPs) in Lake Geneva: their measurement, occurrence, and concentration distribution in the water and sediments."
	Advisor: Prof. J. Samuel Arey
June 2010	Master of Science (MSc) in Chemistry, University of Camerino, Italy. 110/110 summa cum laude Major: Analytical chemistry Thesis: "Kinetic model, HPLC-DAD method development and optimization of Lycopene extraction from tomatoes." Advisor: Dr. Paolo Passamonti
DECEMBER 2008	Bachelor of Science (BSc) in Chemistry, University of Camerino, Italy. 110/110 summa cum laude Major: Physical chemistry Thesis: "Thermal engines and their efficiency and irreversibility." Advisor: Prof. Bernard Howard LAVENDA

Honors

May 2020	Session Chair SETAC Europe 2020, Dublin Ireland
Nov 2019	Discussion panel member SETAC NA 2019, Toronto Canada
Current	Honorary Research Fellow at the University of Queensland, Australia.
Current	Reviewer for J. Chrom. A., Anal. Chem., Water Res., ES&T Chemosphere, Talanta, and Food. Chem.
Current	Member of American Chemical Society (ACS), Division of Analytical Chemistry.
2010-2015	Member of Swiss Chemical Society (SCS), Division of Analytical Chemistry.

GRANTS AND AWARDS

Current	(AUD 500K) Australian Research Council for a research project in application of HRMS in detection of CECs in environment. (Principal Investigator).
Current	(EUR 20K) NORMAN Network grant for non-target screening activity (Project leader).
2017	(NOK 300K) Internal grant for basic research from NIVA (Project leader)
2016	(NOK 206K) Overseas visit grant from the Research Council of Norwegian (Project leader)
2016	(EUR 500) NORMAN Network, traveling award.
2015	(CHF 500) Swiss Chemical Society (SCS), Analytical chemistry division, traveling award.
2014	(CHF 500) Swiss Chemical Society (SCS) traveling award.
2009-2010	(EUR 22K) Research scholarship based on academic merit, funded by the University of Camerino.

JOURNAL PUBLICATIONS

Published work

- 1. **Samanipour, S.**; Reid, M.; Rundberget, T. J.; Frost, T. and Thomas, K. V., Concentrations and distribution of naphthenic acids in the produced water from Norwegian North Sea oilfield, *Environ. Sci. Technol.*, **2020** (*forthcoming*).
- 2. Ahmed, F.; Tscharke, B.; O'Brien, J. W.; Thompson, J.; Samanipour, S.; Choi, P.; Li, J.; Mueller, J. F.; Thomas, K. V., Wastewater-based estimation of the prevalence of gout in Australia, *STOTEN.*, 2020.
- 3. Okoffo, E., D.; Ribeiro, F.; O'Brien, J. W.; O'Brien, S.; Tscharke, B.; Gallen, M.; Samanipour, S.; Mueller, J. F.; Thomas, K. V., Identification and quantification of selected plastics in biosolids by pressurized liquid extraction combined with double-shot pyrolysis gas chromatography-mass spectrometry, *STOTEN.*, 2020.
- 4. Choi, P.; Tscharke, B.; **Samanipour, S.**; Hall, W. D.; Gartner, C. E.; Thomas, K. V.; Mueller, J. E.; O'Brien, J. W., Social, demographic and economic correlates of chemical consumption measured by wastewater based epidemiology, *Proc. Natl. Acad. Sci.*, **2019**, 116 (43), 21864–21873.
- 5. Samanipour, S.; O'Brien, J.; Reid, M.; and Thomas, K. V., A self-adjusting algorithm for non-targed feature detection of LC-HRMS data, *Anal. Chem*, 2019, 91 (16), 10800–10807.
- 6. **Samanipour, S.**; Martin, J; Lamoree, M; Reid, M.; and Thomas, K., Optimism for Nontarget Analysis in Environmental Chemistry, *Environ. Sci. Technol.* **2019**, 53 (10), 5529–5530.
- 7. Gallen, C.; Heffernan, A. L.; Kaserzon, S.; Dogruer, G.; Samanipour, S.; Gomez-Ramos, M. J.; and Mueller, F. J., Integrated chemical exposure assessment of coastal green turtle foraging grounds on the Great Barrier Reef, STOTEN 2019, 657, pp 401–409.

- 8. Samanipour, S.; Kaserzonb, S.; Vijayasarathy, S.; Jiang, H.; Choi, P.; Reid, M.; Mueller, J.; and Thomas, K. V., Machine Learning Combined with Non-targeted LC-HRMS Analysis for a Risk Warning System of Chemical Hazards in Drinking Water, *Talanta*, 2019 195, pp 426–432.
- 9. **Samanipour, S.**; Hooshyari, M; Baz-Lomba, J. A.; Reid, M.; Casale, M.; and Thomas, K. V., The Effect of Extraction Methodology on the Recovery and Distribution of Naphthenic Acids of oilfield Produced Water, *STOTEN* **2019**, 652, 1416-1423.
- 10. **Samanipour, S.**; Baz-Lomba, J. A.; Reid M. J.; Ciceri, E.; Rowland, S.; Nilsson, P.; and Thomas, K. V., Assessing sample extraction efficiency in the analysis of complex unresolved mixtures: A comprehensive non-target approach, *Anal. Chim. ACTA*, **2018** (1025) 92-98.
- 11. **Samanipour, S.** et al. Exploring the potential of a global emerging contaminant early warning network through the use of retrospective suspect screening with high-resolution mass spectrometry, *Environ. Sci. Technol.* **2018**, 52 (9), pp 5135–5144.
- 12. **Samanipour, S.**; Reid M. J.; Baek, K.; and Thomas, K. V., Combining a deconvolution and a universal library search algorithm for the non-target analysis of data independent LC-HRMS spectra, *Environ. Sci. Technol.* **2018**, 52 (8), pp 4694–4701.
- 13. **Samanipour, S.**; Reid, M. R.; and Thomas, K. V., Statistical Variable Selection: An Alternative Prioritization Strategy during the Nontarget Analysis of LC-HR-MS Data. *Anal. Chem.*, **2017**, 89 (10), 5585-5591.
- 14. **Samanipour, S.**; Baz-Lomba, J. A.; Alygizakis, N. A.; Reid, M. R.; Thomaidis, N. S.; and Thomas, K. V., Two stage algorithm vs commonly used approaches for the suspect screening of complex environmental samples analyzed via liquid chromatography high resolution time of flight mass spectroscopy: A test study. *J. Chromatogr. A*, **2017**, Volume 1501, Pages 68-78.
- 15. **Samanipour, S.**; Dimitriou-Christidis, P.; Nabi, D.; Arey, J. S., Elevated Concentrations of 4-Bromobiphenyl and 1,3,5-Tribromobenzene Found in Deep Water of Lake Geneva Based on GC×GC- μ ECD and GC×GC-ENCI-TOFMS *ACS Omega* **2017**, 2 (2), pp 641-652.
- 16. **Samanipour, S.**; Langford, K; Reid M. J.; and Thomas, K. V., A two stage algorithm for target and suspect analysis of produced water via gas chromatography coupled with high resolution time of flight mass spectrometry. *J. Chromatogr. A* **2016**, 1463, 153-161.
- 17. Dimitriou-Christidis, P.; Bonvin, A.; **Samanipour, S.**; Hollender, J.; Rutler, R.; Westphale, J.; Gros, J. and Arey, J. S., GC×GC quantification of priority and emerging nonpolar organic micropollutants in all types of wastewater streams: analysis methodology, chemical occurrence, and partitioning. *Environ. Sci. Technol.* **2015**, 49 (13), 7914-7925.
- 18. **Samanipour, S.**; Dimitriou-Christidis, P.; Grange, A.; Gros, J.; Arey, J. S., Analyte quantification with comprehensive two-dimensional gas chromatography: Assessment of methods for baseline correction, peak delineation and matrix effect elimination. *J. Chromatogr. A* **2015**, 1375, 123-139.
- 19. Alibabaei, L.; Giovannetti, R.; **Samanipour, S.**, Structure investigations of binary azeotrope of diethyl amine-acetone by FT-IR and H-NMR spectroscopy. *Spectrochim. Acta A* **2009**, 72, 390-393.

Unpublished work

1. Choi, P.; Tscharke, B.; Hall, W. D.; Gartner, C. E.; Thomas, K. V.; Mueller, J. F.; O'Brien, J. W.; Samanipour, S., Machine learning for prediction of consumption behavior based on socioeconomical parameters, *Nature*, 2020 (*submitted*).

Technical reports

- Screening Programme 2017 AMAP Assessment Compounds, https://brage.bibsys.no/xmlui/handle/11250/2569237.
- 2. Marine Monitoring Program: Annual report for inshore pesticide monitoring 2016-2017, http://hdl.handle.net/11017/3399.

Conferences

Oral contributions

- 1. **Samanipour**, **S.**; Reid M. J.; and Thomas, K. V., A Novel High-Resolution Mass Spectrometry Toolbox for Unravelling the Chemical Exposome, SETAC North America, **November 2019**, Toronto Canada. (**Invited Speaker**)
- 2. **Samanipour, S.**; Reid M. J.; Frost, T. K.; and Thomas, K. V., Quantification of Naphthenic Acids in Produced Water from Norwegian Offshore Oil Platforms in the North Sea, Produced Water Workshop, **June 2019**, Aberdeen Scotland. (**Invited Speaker**)
- 3. **Samanipour**, **S.**; Baz-Lomba, J. A.; Reid M. J.; Ciceri, E.; Rowland, S.; Nilsson, P.; and Thomas, K. V., Application of a non-targeted HR-MS approach for comprehensive recovery assessment of complex unresolved mixtures. EmCon2018 **June 2018**, Oslo, Norway.
- 4. Samanipour, S.; Reid M. J.; and Thomas, K. V., Naphthenic acids in produced water: origin, current status and potential environmental impact, Produced Water Workshop, April 2018, Aberdeen Scotland. (Invited Speaker)
- 5. **Samanipour**, S.; Reid M. J.; and Thomas, K. V., Application of statistical sample classification in non-target analysis of complex environmental samples analyzed via LC-HR-QTOFMS. 15th Scandinavian Symposium on Chemometrics, **June 2017**, Naantali, Finland.
- 6. **Samanipour, S.**; Langford, K; Reid M. J.; and Thomas, K. V., Application of the unique ion extractor and dot product in suspect and target analysis of produced water. non-Target2016 **June 2016**, Ascona, Switzerland.
- Samanipour, S.; Reid M. J.; and Thomas, K. V., Comprehensive chemical characterization of unresolved petrogenic components of Produced Water. Waters 4th Nordic Symposium on Convergence Chromatography May 2016, Gothenburg, Sweden. (Invited Speaker)
- 8. **Samanipour, S.**, Nabi, D.; Gros, J.; Dimitriou-Christidis, P.; and Arey, J. S., Application of GC×GC for detection, quantification, and partitioning property estimation of overlooked bioaccumulative brominated pollutants. EMEC16 **December 2015**, Torino, Italy.
- 9. Samanipour, S.; Mallios, A.; Camilli, R.; and Arey, J. S., Hydrophobic organic pollutant concentrations exhibit strong spatial variability in the deep water column of Lake Geneva. EMEC16 December 2015, Torino, Italy.
- 10. **Samanipour, S.** and Arey, J. S., Pollutant distributions between sediments and the benthic water column in a deep lake: Application of passive sampling and GC×GC to less-studied and legacy halogenated contaminants in Lake Geneva. ContaSed **March 2015**, Ascona, Switzerland.
- 11. Samanipour, S.; Nabi, D.; Arey, J. S., Concentration and trends of novel brominated hydrocarbons in the water column and sediments of Lake Geneva (Switzerland): de-

tection and quantification using $GC \times GC - \mu ECD$ and $GC \times GC - ENCI-TOFMS$. Presented at EuCHeMS **September 2014**, Istanbul, Turkey.

Poster contributions

- 1. **Samanipour, S.**; O'Brien, J.; MacDonald, S.; Kaserzon, S.; Reid, M.; and Thomas, K. V., A cloud based non-targeted approach for identifying emerging contaminants in wastewater. EmCon 2018 **June 2018**, Oslo, Norway.
- 2. **Samanipour**, S.; Kaserzon, S.; Vijayasarathy, S.; Jiang, H.; Choi, P.; Reid, M.; Mueller, J.; and Thomas, K. V., Machine Learning Combined with Non-targeted LC-HRMS Analysis for a Risk Warning System of Chemical Hazards in Drinking Water. WaterJPI 2018, **April 2018**, Helsinki Finland.
- 3. **Samanipour**, **S.**; Cecchi, T. and Passamonti, P., Lycopene extraction kinetic model. CF2010: Il XXXIX congresso nazionale di chimica fisica, **September 2010**, Stresa, Italy.
- 4. **Samanipour**, **S.**; Cecchi, T. and Passamonti, P., Optimization of Lycopene extraction by design of experiment. XXII convegno nazionale della divisione di chimica analitica della società chimica Italiana, **September 2010**, Como, Italy.

Other contributions

- 1. O'Brien, J.; Samanipour, S.; Kaserzon, S.; Tscharke, B; Mueller, J.; Reid, M.; and Thomas, K. V., A novel non-targeted approach for identifying emerging contaminants in wastewater. EmCon 2018 June 2018, Oslo, Norway.
- 2. Reid M. J.; Samanipour, S.; and Thomas, K. V., A deconvolution and library search algorithm for comprehensive non-target analysis using LC-HR-MS data independent acquisition, 16th International Conference on Chemistry and the Environment, June 2017, Oslo, Norway.
- 3. Arey, J. S.; Samanipour, S.; Nabi, D.; Dimitriou-Christidis, P. and Gros, J., Advances in trace detection, quantification, and partitioning property estimation of bioaccumulative pollutants with GC×GC. Presented at SETAC Europe 25th Annual Meeting, May 2015, Barcelona, Spain.
- 4. Mallios, A.; Pizarro, O.; Arey, J. S.; **Samanipour, S.** et al., Synoptic identification of greenhouse gas sources and sinks in Lake Léman. Aquatic Sciences Meeting, **February 2015**, Granada, Spain.
- 5. Arey, J. S.; Samanipour, S.; Nabi, D.; Dimitriou-Christidis, P. and Gros, J., Detection, quantification, and partitioning property estimation of less-studied bioaccumulative pollutants in aquatic environments using $GC \times GC \mu ECD$ and $GC \times GC ENCI-TOFMS$. Presented at The 6th Multidimensional Chromatography Workshop, January 2015, Toronto, Canada.

TEACHING EXPERIENCE

2018 | Main teacher for "Workshop of Statistics", UQ. 2014 | Teaching assistant for "Fate and behavior of organic pollutants", EPFL. 2012-2013 | Teaching assistant for "Quantitative methods II", EPFL. 2012 Teaching assistant for "Numerical analysis II", EPFL.

2011 | Teaching assistant for "Water and wastewater treatment", EPFL.

RELEVANT INFORMATION

Programming Matlab, julia, Python, and R languages June 2013 "Summer school in environmental systems analysis", EAWAG, Switzerland. October 2012 | "Training for GC×GC", **ZOEX**, Amsterdam, Netherlands. November 2009 | "Design of Experiment", Basic level, S-in, Vicenza, Italy.

LANGUAGES

Mother tongue PERSIAN:

ENGLISH: Fluent Fluent ITALIAN: NORWEGIAN: Basic

REFERENCES

· Prof. Kevin Thomas

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Earth Space Technical Ecosystem Enterprises (ESTEE), Switzerland

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