

## ► Aalizadeh Reza

Post-Doctoral Researcher at University of Athens

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### Education

**B.Sc. in Applied Chemistry (2008-2012)**, Azad University, Grade: 18.45/20.00

**M.Sc. in Analytical Chemistry (2013-2015)**, National and Kapodistrian University of Athens (9.57/10.00)

**Ph.D. in Analytical Chemistry (2015-2019)**, National and Kapodistrian University of Athens (Excellent)

**Post-Doctoral research in Analytical Chemistry (2019-present)**, National and Kapodistrian University of Athens

### Research Topics:

**Undergraduate Thesis:** "Development of computational framework for designing Hepatitis C Virus NS5B Polymerase Inhibitors", Chemistry department, Azad University, Iran (2012)

**Master Thesis:** "Development and validation of wide-scope retention time prediction models to support suspect and non-target screening of emerging contaminants in environmental samples", Laboratory of Analytical Chemistry, Chemistry department, University of Athens, Greece (2013-2015)

**Ph.D. Thesis:** "Quantitative Structure-Property Relationships to support non-target LC-HRMS Screening", Laboratory of Analytical Chemistry, Chemistry department, University of Athens, Greece (2015-2019)

**Post-Doctoral Research:** Development of chemometric methods to facilitate the non-target screening of the unknowns in the environmental samples by liquid chromatography high resolution mass spectrometry

### Research Interests

**General research interests:** Metabolomics, High Resolution Mass Spectrometry (HRMS), Chemometrics, Non-target Screening, Development of LC-MS/MS methods, Retention Time mechanism in RPLC & HILIC

#### Projects:

**2018-2021:** Foodomics-GR – Molecular Characterization of Food (funding: EPANEK-NSFR)

**2018-2021:** pHION: Environmental Protection Agency of Germany (UBA): pH effects on toxicity and bioaccumulation of ionic substances. UBA GZ 97 406/0536

**2016-2019:** NORMAN Suspect list exchange (NORMAN Network association)

**2016-2018:** EMBLAS II: United Nations Development Programme: Analysis of water framework priority substances and screening of black sea specific pollutants in water biota and sediment samples obtained during the National Pilot Monitoring Studies and Joint Open Sea Surveys and risk assessment of identified pollutants-EU/UNDP Project: Improving environmental monitoring in the Black Sea.

**2016-2017:** Analysis of WFD and screening of Black Sea Specific Pollutants (UNDP, 2016-12-ITB, 2016)

**2007–2016:** (“KALLIMANIS”): Frozen and processed foodstuff with advanced chemometric tools and LC-HRMS data treatment procedures.

**2012–2015:** “EXCELLENCE”: Transformation products of emerging pollutants in the aquatic environment-TREMEPOL

## Publications in journals and books

1. Gisela A. Umbuzeiro, Anjaina F. Albuquerque, Francine I. Vacchi, Malgorzata Szymczyk, Xinyi Sui, Reza Aalizadeh, Peter C. von der Ohe, Nikolaos S. Thomaidis, Nelson Vinueza & Harold S. Freeman “Towards a reliable prediction of the aquatic toxicity of dyes” *Environmental Sciences Europe*, 2019, Accepted.
2. Konstantina Diamanti, Reza Aalizadeh, Nikiforos Alygizakis, Aikaterini Galani, Marie Mardal, Nikolaos S. Thomaidis “Wide-scope target and suspect screening methodologies to investigate the occurrence of new psychoactive substances in influent wastewater from Athens” *Science of The Total Environment*, 2019, 685, 1058-1065
3. Marilena Dasenaki, Sofia Drakopoulou, Reza Aalizadeh, Nikolaos S. Thomaidis “Targeted and Untargeted Metabolomics as an Enhanced Tool for the Detection of Pomegranate Juice Adulteration” *Foods*, 2019, 8, 212; doi:10.3390/foods8060212.
4. Finnian Freeling, Nikiforos A. Alygizakis, Peter von der Ohe, Jaroslav Slobodnik, Peter Oswald, Reza Aalizadeh, Lubos Cirka, Nikolaos S. Thomaidis and Marco Scheurer “Occurrence and potential environmental risk of surfactants and their transformation products discharged by wastewater treatment plants” *Science of The Total Environment*, 2019, doi: 10.1016/j.scitotenv.2019.04.445
5. Nikiforos A. Alygizakis, Peter Oswald, Nikolaos S. Thomaidis, Emma L. Schymanski, Reza Aalizadeh, Tobias Schulze, Martina Oswaldova and Jaroslav Slobodnik “NORMAN digital sample freezing platform: A European virtual platform to exchange liquid chromatography high resolution-mass spectrometry data and screen suspects in “digitally frozen” environmental samples” *TrAC Trends in Analytical Chemistry*, 2019, 115, 129-137.
6. Pawel Rostkowski, Peter Haglund, Reza Aalizadeh, Nikiforos Alygizakis, Nikolaos S. Thomaidis, Joaquin Beltran Arandes, Pernilla Bohlin Nizzetto, Petra Booiij, Hélène Budzinski, Pamela Brunswick, Adrian Covaci, Christine Gallampois, Sylvia Grosse, Ralph Hindle, Ildiko Ipolyi, Karl Jobst, Sarit L.Kaserzon, Pim Leonards, Francois Lestremau, Thomas Letzel, Jürgen Magnér, Hidenori Matsukami, Christoph Moschet, Peter Oswald, Merle Plassmann, Jaroslav Slobodnik, Chun Yang “The Strength in Numbers: Comprehensive Characterization of House Dust using Complementary Mass Spectrometric Techniques” *Analytical and Bioanalytical Chemistry*, 2019, 411, 10, 1957–1977.
7. Reza Aalizadeh, Maria-Christina Nika and Nikolaos S. Thomaidis “Development and application of retention time prediction models in the suspect and non-target screening of emerging contaminants” *Journal of hazardous materials*, 2019, 363, 277-285.
8. Natasa P. Kalogiouri, Reza Aalizadeh and Nikolaos S. Thomaidis “Application of an advanced and wide scope non-target screening workflow with LC-ESI-QTOF-MS and chemometrics for the classification of the Greek olive oil varieties” *Food Chemistry*, 2018, 256, 53-61.
9. Afshin Saadat, Eslam Pourbasheer, Somayeh Morsali and Reza Aalizadeh “Simultaneous Spectrophotometric Determination of Aspirin and Dipyrindamole in Pharmaceutical Formulations Using the Multivariate Calibration Methods” *Current Pharmaceutical Analysis*, 2018, 14, 419-425.
10. Reza Aalizadeh, Peter C. Von der Ohe and Nikolaos S. Thomaidis “Prediction of acute toxicity of emerging contaminants on the water flea *Daphnia magna* by Ant Colony Optimization–Support Vector Machine QSTR models” *Environmental Science: Processes & Impacts*, 2017, 19, 438-448.
11. Maria Ibáñez, Viola Borova, Clara Boix, Reza Aalizadeh, Richard Bade, Nikolaos S. Thomaidis and Felix Hernández “UHPLC-QTOF MS screening of pharmaceuticals and their metabolites in treated wastewater samples from Athens” *Journal of Hazardous Materials*, 2017, 323, 26-35.
12. Natasa P. Kalogiouri, Reza Aalizadeh and Nikolaos S. Thomaidis “Investigating the organic and conventional production type of olive oil with target and suspect screening by LC-QTOF-MS, a novel semi-quantification method using chemical similarity and advanced chemometrics” *Analytical and Bioanalytical*

- Chemistry, 2017, 409, 5413–5426.
13. Reza Aalizadeh, Nikolaos S. Thomaidis, Anna Bletsou and Pablo Gago Ferrero “QSRR Models to Support Non-target High Resolution Mass Spectrometric Screening of Emerging Contaminants in Environmental Samples” *Journal of Chemical Information and Modeling*, 2016, 56, 1384-1398.
  14. Christophoros Christophoridis, Maria-Christina Nika, Reza Aalizadeh and Nikolaos S. Thomaidis “Ozonation of ranitidine: Effect of experimental parameters and identification of transformation products” *Science of The Total Environment*, 2016, 557-558, 170–182
  15. Vasiliki G. Beretsou, Aikaterini K. Psoma, Pablo Gago-Ferrero, Reza Aalizadeh, Kathrin Fenner, Nikolaos S. Thomaidis “Identification of biotransformation products of citalopram formed in activated sludge” *Water Research*, 2016, 103, 205-214.
  16. Natasa P. Kalogiouri, Nikiforos A. Alygizakis, Reza Aalizadeh and Nikolaos S. Thomaidis “Olive oil authenticity studies by target and nontarget LC-QTOF-MS combined with advanced chemometric techniques” *Analytical and Bioanalytical Chemistry*, 2016, 408, 7955–7970.
  17. Reza Aalizadeh “Interactions Study of Non-Nucleoside Inhibitors with Hepatitis B Virus E Antigen toward Better Design of New Inhibitors Based on Molecular Docking and Pharmacophore Methods” *Journal of Hepatology*, 2016, 64, S600.
  18. Eslam Pourbasheer and Reza Aalizadeh “3D-QSAR and molecular docking study of LRRK2 kinase inhibitors by CoMFA and CoMSIA methods” *SAR and QSAR in Environmental Research*, 2016, 27, 385–407
  19. Pablo Gago-Ferrero, Emma L. Schymanski, Anna A. Bletsou, Reza Aalizadeh, Juliane Hollender and Nikolaos S. Thomaidis “Extended Suspect and Non-Target Strategies to Characterize Emerging Polar Organic Contaminants in Raw Wastewater with LC-HRMS/MS” *Environmental Science and Technology*, 2015, 49, 12333–12341.
  20. Reza Aalizadeh, Eslam Pourbasheer and Mohammad Reza Ganjali “Analysis of B-Raf V600E inhibitors using 2D and 3D-QSAR, molecular docking and pharmacophore studies” *Molecular Diversity*, 2015, 19, 915–930.
  21. Eslam Pourbasheer, Reza Aalizadeh, Hamid Mohammad Shiri, Alireza Banaei and Mohammad Reza Ganjali “2D and 3D-QSAR analysis of pyrazole-thiazolinone derivatives as EGFR kinase inhibitors by CoMFA and CoMSIA” *Current Computer - Aided Drug Design*, 2015, 11, 292-303.
  22. Eslam Pourbasheer, Reza Aalizadeh, Mohammad Reza Ganjali and Parviz Norouzi “Prediction of superoxide quenching activity of fullerene (C60) derivatives by genetic algorithm-support vector machine” *Fullerenes, Nanotubes and Carbon Nanostructures*, 2015, 23, 290-299.
  23. Eslam Pourbasheer, Alireza Banaei, Reza Aalizadeh, Mohammad Reza Ganjali, Parviz Norouzi, Javad Shadmanesh and Constantinos Methenitis “Prediction of PCE of fullerene (C60) derivatives as polymer solar cell acceptors by genetic algorithm–multiple linear regression” *Journal of Industrial and Engineering Chemistry*, 2015, 21, 1058-1067.
  24. Eslam Pourbasheer, Mahdi Aghbolagh Shahmohammadi and Reza Aalizadeh “Investigation of residuals responsible for binding of triazolo-pyrimidine inhibitors with HBsAg based on molecular docking and pharmacophore methods for designing potent HBsAg inhibitors” *Journal of Hepatology*, 2015, 62, S570.
  25. Eslam Pourbasheer, Samira Shokouhi Tabar, Vijay H. Masand, Reza Aalizadeh, Mohammad Reza Ganjali “3D-QSAR and docking studies on adenosine A2A receptor antagonists by the CoMFA method” *SAR and QSAR in Environmental Research*, 2015, 26, 461-477.
  26. Eslam Pourbasheer, Sadat Vahdani, Reza Aalizadeh, Alireza Banaei, Mohammad Reza Ganjali “QSAR study of prolylcarboxypeptidase inhibitors by genetic algorithm: Multiple linear regressions” *Journal of Chemical Sciences* 2015, 127, 1243-1251.
  27. Eslam Pourbasheer, Reza Aalizadeh, Mohammad Reza Ganjali and Parviz Norouzi “QSAR study of  $\alpha 1\beta 4$  integrin inhibitors by GA-MLR and GA-SVM methods” *Structural Chemistry*, 2014, 25, 355-370
  28. Eslam Pourbasheer, Reza Aalizadeh, Mohammad Reza Ganjali and Parviz Norouzi “QSAR study of IKK $\beta$  inhibitors by the genetic algorithm: multiple linear regressions” *Medicinal Chemistry Research*, 2014, 23, 57-66.
  29. Eslam Pourbasheer, Reza Aalizadeh, Mohammad Reza Ganjali, Parviz Norouzi and Alireza Banaei, “QSAR study of mGlu5 inhibitors by genetic algorithm-multiple linear regressions” *Medicinal Chemistry Research*, 2014, 23, 3082-3091.

30. Eslam Pournbasheer, Reza Aalizadeh, Mohammad Reza Ganjali, Parviz Norouzi, Javad Shadmanesh and Constantinos Methenitis "QSAR study of Nav1.7 antagonists by multiple linear regression method based on genetic algorithm (GA-MLR)" *Medicinal Chemistry Research*, 2014, 23, 2264-2276.
31. Eslam Pournbasheer, Reza Aalizadeh, Samira Shokouhi Tabar, Mohammad Reza Ganjali, Parviz Norouzi and Javad Shadmanesh "2D and 3D quantitative structure-activity relationship study of hepatitis C virus NS5B polymerase inhibitors by comparative molecular field analysis and comparative molecular similarity indices analysis methods" *Journal of chemical information and modeling*, 2014, 54, 2902-2914.
32. Mahdi Shahmohammadi Aghbolagh, Eslam Pournbasheer and Reza Aalizadeh " Interactions study of HCV NSB5 polymerase inhibitors with NSB5 non-structured proteins toward better design of new inhibitors based on molecular docking and pharmacophore methods" *Journal of Hepatology*, 2015, 62, S687.
33. Eslam Pournbasheer, Reza Aalizadeh, Jamal Saffar Ardabili and Mohammad Reza Ganjali "QSPR study on solubility of some fullerenes derivatives using the genetic algorithms—Multiple linear regression" *Journal of Molecular Liquids*, 2015, 204, 162-169.
34. Eslam Pournbasheer, Reza Aalizadeh, Amin Ebadi and Mohammad R Ganjali "3D-QSAR analysis of MCD inhibitors by CoMFA and CoMSIA" *Combinatorial chemistry & high throughput screening*, 2015, 18, 751-766.
35. Eslam Pournbasheer, Reza Aalizadeh, Mohammad Reza Ganjali, Parviz Norouzi and Javad Shadmanesh "QSAR study of ACK1 inhibitors by genetic algorithm-multiple linear regression (GA-MLR)" *Journal of Saudi Chemical Society*, 2014, 18, 681-688.

## Conferences Presentations

1. Sofia K. Drakopoulou, Marilena E. Dasenaki, Reza Aalizadeh, Adamantia-Eleni G. Manola, Konstantinos N. Nikolakis, Nikolaos S. Thomaidis, "Un-Targeted Metabolomics Approach for the Characterization, Classification and Mapping of Bioactive Compounds in Greek Extra Virgin Olive Oil", 11th International Conference on "Instrumental Methods of Analysis" (IMA-2019), 22-25 September 2019, Ioannina, Greece
2. A. Tzachristas, M.E. Dasenaki, K. Pasvanka, G. Koulis, S. Drakopoulou, R. Aalizadeh, N. S. Thomaidis and C. Proestos, "Development of a wine metabolomics approach for the varietal discrimination of selected Greek wines", 2nd Food Chemistry Conference: Shaping the Future of Food Quality, Safety, Nutrition and Health, 17-19 September 2019, Seville, Spain
3. Nikolopoulou V.I., Nika M.C., Aalizadeh R., Alygizakis N., Thomaidis N.S. "Screening thousands of emerging contaminants in Asopos river basin by UPLC-QToF-MS", 16th International Conference on Environmental Science and Technology, 4- 7 September 2019, Rhodes, Greece.
4. Reza Aalizadeh and Nikolaos S. Thomaidis, "AUTONONTARGET: An R package to perform automatic non-target screening", 16th International Conference on Environmental Science and Technology, 4- 7 September 2019, Rhodes, Greece.
5. Nikolopoulou V.I., Nika M.C., Aalizadeh R., Miskaki P., Kaloudis T., Deftereos N.T., Avagianos C., Thomaidis N.S., "Determination of emerging contaminants in surface water resources
6. of EYDAP following wide-scope Target and Non-Target Screening", 16th International Conference on Environmental Science and Technology, 4- 7 September 2019, Rhodes, Greece.
7. Damalas D.E., Panagopoulou E., Aalizadeh R., Schweizer M., Heid C., Köhler H., Ohé P.V.D., Triebkorn R., Thomaidis N.S., "Influence of pH on the toxicity, uptake and biotransformation
8. potential of citalopram in zebrafish (*Danio rerio*) embryos", 16th International Conference on Environmental Science and Technology, 4- 7 September 2019, Rhodes, Greece.
9. Marios Kostakis, Reza Aalizadeh, Marilena Dasenaki, Nikolaos Thomaidis, "Exploring data quality of multivariate HRMS data in food authenticity research", Eurachem 14-18 May 2018, Dublin, Ireland, (Best poster award).
10. Emma Schymanski, Reza Aalizadeh, Nikolaos S. Thomaidis, Juliane Hollender, Jaroslav Slobodnik and Antony Williams, "Curating" suspect lists" for international non-target screening efforts". Abstracts of papers of the American Chemical Society. 2018. Amer. Chemical. Soc. 1155 16th st, NW, Washington, dc 20036 USA.
11. Marios Kostakis, Anthi Panara, Giorgos Gkotsis, Reza Aalizadeh, Nikolaos S. Thomaidis "Metabolic Fingerprint of *Sideritis Scardica* by a Novel LC-QTOF-MS Workflow" 11th Aegean Analytical Chemistry Days (AACD2018), Chania, Crete, Greece, 25-29 September 2018.

12. Anthi Panara, Marios Kostakis, Giorgos Gkotsis, Reza Aalizadeh, Nikolaos S. Thomaidis "Characterization of Chemical Profile of Pelargonium Sidoides Rhizome Using LC-QTOF/MS" 11th Aegean Analytical Chemistry Days (AACD2018), Chania, Crete, Greece, 25-29 September 2018.
13. M.C. Nika, D. Damalas, G. Koulis, N. Alygizakis, V. Nikolopoulou, S. Drakopoulou, A. Psoma, M. Kostakis, R. Aalizadeh, P. Oswald, J. Slobodnik, N.S. Thomaidis "Extended Monitoring of Legacy Pollutants and Emerging Contaminants in the Marine Environment of Black Sea" 11th Aegean Analytical Chemistry Days (AACD2018), Chania, Crete, Greece, 25-29 September 2018, (Best Poster Award).
14. M.C. Nika, G. Koulis, D. Damalas, K. Diamanti, A. Bletsou, A. Psoma, S. Attiti, R. Aalizadeh, N. Alygizakis, M. Dasenaki, K. Kasiotis, P. Oswald, J. Slobodnik and N. Thomaidis "Determination of legacy pollutants and emerging contaminants in the marine environment of Black Sea" CEST 2017, September 2017, Rodos Palace, Rhodes, Greece.
15. Maria-Christina Nika, Reza Aalizadeh and Nikolaos S. Thomaidis, "Removal and transformation of citalopram and four of its biotransformation products during ozonation experiments", CEST 2017, September 2017, Rodos Palace, Rhodes, Greece
16. Reza Aalizadeh, Emma L. Schymanski and Nikolaos S. Thomaidis, " AutoSuspect: an R package to Perform Automatic Suspect Screening based on Regulatory Databases", CEST 2017, September 2017, Rodos Palace, Rhodes, Greece.
17. Reza Aalizadeh, Emma L. Schymanski, Juliane Hollender, Martin Krauss, Maria Ibáñez Martínez, Nikolaos S. Thomaidis "Development and Prediction of Liquid Chromatographic Retention Time Indices (RTI) to facilitate non-target identification", ICCE 2017, June 2017, Oslo, Norway.
18. Emma L. Schymanski, Andrew McEachran, Reza Aalizadeh, Nikolaos S. Thomaidis, Jaroslav Slobodnik, Jon R. Sobus, Juliane Hollender, Antony J. Williams "International Suspect Screening: NORMAN Suspect Exchange meets the US EPA CompTox Chemistry Dashboard", ICCE 2017, June 2017, Oslo, Norway.
19. Reza Aalizadeh and Nikolaos S. Thomaidis, "RetTrAMS: SMILES based retention time prediction in RPLC/HILIC-(+/-)ESI-LC-HRMS screening", Non-target 2016, May 2016, Ascona, Switzerland (Travel costs awarded).

## Awards and Honors

1. 2017-2018: Scholarship from ELIDEK for Ph.D. studies.
2. 2016-2017: Funded projects by NORMAN Network association (Joint Activity Proposals).
3. 2015-2016: Award: Young Investigators Bursary granted by European Association for the Study of the Liver (EASL).
4. 2013-2015: Scholarship from State Scholarships' Foundation of Greece (I.K.Y.) for M.Sc. studies.
5. 2013: Award: Officially granted the membership by Iran National Elites Foundation (INEF).
6. 2012: Award: Graduated in the Bachelor of Science (Applied Chemistry) with "Second Class Honour".

## Professional Affiliations

Iran National Elites Foundation, 2012-Present

NORMAN Network Association, 2015-Present

European Association for the Study of the Liver (EASL), 2014-2016

## Contact information

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