PETAR ŽUVELA

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Multilateral, versatile and results-oriented researcher with more than seven years of experience in data science and a PhD in chemical engineering. Working in the semiconductor industry. Area of interest and expertise includes an array of multidisciplinary research involving methods of **chemometrics/machine learning, mathematical programming and computational chemistry** in fields ranging **from semiconductor industry, separation science, *omics, cancer diagnostics to novel pharmaceutical design and screening**. Communicative and cogent in forming professional relationships with management, peers, and staff.

EXPERIENCE

2019-12-11~

DATA SCIENTIST, ONTO INNOVATION (EX. NANOMETRICS INC.), SINGAPORE

Developing disruptive technologies, products and algorithms in semiconductor metrology powered by machine learning, chemometrics & AI. Actively contributing to the R&D process through (i) **development of novel semiconductor metrology recipes & improvement of existing ones, (ii) troubleshooting and support of the internal & external company stakeholders.** Working in an Agile development (SCRUM) environment.

2017-04-17~2019-12-10

RESEARCH FELLOW, NATIONAL UNIVERSITY OF SINGAPORE, SINGAPORE

Development of quantitative **machine learning models** (regression, classification) focused on **feature engineering, selection and interpretability**. Inference of chemical information from large-scale MD/QM models and simulations. Training and supervising undergraduate and graduate students. Active networking with local and international collaborators.

Key on-going projects:

1. HPLC elution order prediction via machine learning and mathematical programming
2. cross-HPLC column retention time prediction using machine learning and mixture modelling
3. large-scale MD and QM models/simulations for elucidation of binding of zinc to ovalbumin
4. Python(Flask)-powered web platform for GC-MS experimental-based modelling and optimization of (bio-crude) mixtures

Key deliverables:

1. Articles: 8 peer-reviewed research articles published in top-tier research journals, 4 pending
2. Intellectual property: 1 patent granted (KRPTO: *KR-10-2017-0085981*, EU PCT pending), 4 patents pending (USPTO, KRPTO)
3. Student supervision: trained and supervised four FYP students, and one Master student; training
4. Presentations: several invited lectures at PKNU, Busan, Korea; UNIST, Ulsan, Korea, ~10 oral and poster presentations at renowned conferences

2013/10~2017/03

RESEARCHER, PUKYONG NATIONAL UNIVERSITY, BUSAN, KOREA

Development and optimization of high-throughput computational methods to tackle analytical problems. Nature-inspired algorithms for **feature engineering and selection**. Quantitative linear and non-linear **machine-learning models** built from high-dimensional data. Teaching undergraduate experimental chemical engineering labs. Supervision and training of graduate students. **Productive scientific output**. Networking with local and international cooperators.

Key projects:

1. Feature selection in supervised learning in **proteomics**, **spectroscopy**, and **cancer diagnostics**
2. Large-scale **QSRR model development** in proteomics through machine learning
3. Modelling and simulation of lactoferrin-functionalized silver nanoparticles

Key deliverables:

1. Articles: 6 peer-reviewed research articles published in top-tier research journals
2. Presentations: ~30 oral and poster presentations in and outside of Korea

EDUCATION

FEBRUARY 2017

DOCTOR OF PHILOSOPHY, PUKYONG NATIONAL UNIVERSITY, BUSAN, KOREA

Doctoral degree in chemical engineering, with a focus on chemometrics/machine learning and computational chemistry. Thesis title: "**Development and optimization of high-throughput computational methods and their applications in analytical chemistry**". Advisors: Prof. Dr. J. Jay Liu, Prof. Dr. Tomasz Bączek

JULY 2013

MASTER OF SCIENCE, UNIVERSITY OF ZAGREB, ZAGREB, CROATIA

Master's degree in applied chemistry with a focus on chemometrics. Thesis title: "**Ion chromatographic retention modelling using QSPR relationships**". Advisor: Prof. Dr. Šime Ukić.

NOVEMBER 2011

BACHELOR OF SCIENCE, UNIVERSITY OF ZAGREB, ZAGREB, CROATIA

Bachelor's degree in environmental engineering with a focus on scientific software development and chemometrics. Thesis title: "**Development of a computer environment for optimization of ion chromatographic curves**". Advisor: Prof. Dr. Tomislav Bolanča.

SKILLS

- **Inter-personal skills:** Strong **networking**, **managerial** and **communication** skills (both oral and written), leadership and teaching
- **Coding skills: MATLAB** - strong, **Python** (numpy, pandas, scipy, matplotlib, keras, tkinter, Flask, etc.) -strong, **Bash** - intermediate, **Mathematica** - basic, **R**- basic **(> 11 years of experience)**
- **Machine learning / chemometric methods**: Strong understanding of PCA, MLR, PLS, PLS-LDA, ANNs, CNNs, SVM/SVR, kPLS, kNN, single- and multi-objective optimization, non-linear programming
- **Statistical analysis and data visualization:** Strong grasp of statistics and data visualization. Software: **OriginPro**, Tableau, Simca-P, Statistica, Minitab, ProMV, **Python (matplotlib)**
- Comfortable in both **Windows and Linux** platforms, experienced in the use of **high-performance computing (HPC)**
- **Molecular modelling, simulation, and visualization: DFT, semiempirical, MD, molecular docking, Monte Carlo**. Software: **Gaussian**, Gromacs, NAMD, HyperChem, **VMD**, Avogadro, ChemSketch, Dragon
  Image Processing: Adobe Photoshop – intermediate
- **MS Office Tools (365):** strong proficiency in all the Office programs
- **Research, searching and organizing literature**
- **Professional scientific paper preparation and writing**

PUBLICATIONS

Nineteen research articles published and about 40 presentations given at world-renowned conferences. Key publications listed below. Please refer to my website and Google Scholar profile (http://www.petar-zuvela.com/Publications; http://scholar.petar-zuvela.com) for a full bibliography.

RESEARCH ARTICLES

1. **Žuvela, P.**; Lin, K.; Shu, C.; Zheng, W.; Lim, C. M.; Huang, Z. **Fiber-optic Raman Spectroscopy with Nature-inspired Genetic Algorithms Enhances Real-time In Vivo Detection And Diagnosis of Nasopharyngeal Carcinoma**. *Anal. Chem.* **2019**, *91*, 8101-8108.
2. **Žuvela, P.**; Skoczylas, M.; Liu, J. J.; Bączek, T.; Kaliszan, R.; Wong, M. W.; Buszewski, B. **Column selection and characterization systems in reversed-phase liquid chromatography.** *Chem. Rev.* **2019**, *119*, 3674-3729.(**strong impact**)
3. Brigljević B.; **Žuvela, P.**; Liu, J. J.; Woo, H. C., Choi, J. H. **Development of an automated method for modelling of bio-crudes originating from biofuel production processes based on thermochemical conversion.** *Appl. Energy* **2018**, *215*, 670-678. (**strong impact**)
4. **Žuvela P.**; David J.; Wong. M.W. **Interpretation of ANN-based QSAR models for prediction of antioxidant activity of flavonoids.** *J. Comput. Chem.* **2018**, *39*, 953-963.
5. Pomastowski, P.; Sprynskyy, M.; **Žuvela, P.**; Rafińska, K.; Milanowski, M.; Liu, J. J.; Yi, M.; Buszewski, B. **Silver-Lactoferrin Nanocomplexes as a Potent Antimicrobial Agent.** *J. Am. Chem. Soc.* **2016**, *138*, 7899–7909. (**strong impact**)
6. **Žuvela, P.**; Liu, J. J.; Macur, K.; Bączek, T. **Molecular Descriptor Subset Selection in Theoretical Peptide Quantitative Structure–Retention Relationship Model Development Using Nature-Inspired Optimization Algorithms.** *Anal. Chem.* **2015**, *87*, 9876–9883.

PATENTS

1. Liu, J. J.; Brigljević, B.; **Žuvela, P.** **Method for simultaneous modeling and complexity reduction of bio-crudes for process simulation**. KR-10-20-73856B1, **2020**.
2. Liu, J. J.; Yi, M.; **Žuvela, P.** **Methods for target-based drug screening through numerical inversion of quantitative structure-drug performance relationships and molecular dynamics simulations.** KR-10-2017-0085981, **2019**.

AWARDS AND GRANTS

AWARDS

Highest distinction awarded by the Rector of Nicolaus Copernicus University, in Toruń, Poland for group contributions to science and research. (**October 2018, September 2017, December 2016**)

Two silver medals and a gold medal at international innnovation fairs in recognition of excellent and creative efforts to invent: **"OptIC - computer software for development and optimization of chromatographic methods**" (**September 2018, November 2016**)

Award for best oral presentation at the KiCHE Busan-Gyeongnam Branch conference (**December 2014)**

Dean's award for exceptional science paper: "Development of software for optimization of chromatographic analyses" (**September 2010)**

GRANTS

Medical University of Gdańsk research visit support grant (**June~September 2016)**

HPLC 2015 conference travel grant (**May 2015**).

CEEPUS III grant for study at Nicolaus Copernicus University in Toruń, Poland (**March~June 2013**)

REFERENCES

References available upon request.