# Mario Lovrić



# Senior Data Scientist | Cheminformatician

Data scientist with a PhD degree in cheminformatics and a topic in predictive toxicology. Four years experience in industrial, chemical and medical data science projects. Skilled in Python, predictive modelling and machine learning.

# Professional Experience

▲ 07.2017 – present	Research Lead Life Science (2021+)   Know-Center   Austria  -Project lead across various domains such as traffic, manufacturing and medicine  -Writing scientific papers and funding proposals  -Lead team of 2-3 data scientists  Senior Data Scientist (-2021)   Know-Center   Austria  -Application-oriented research in supervised and unsupervised machine learning  -Project lead across various domains such as traffic, manufacturing and medicine  -Successfully implemented a predictive maintenance procedure causing cost reduction
<b>▼</b> 12.2018 - 05.2020	Biomedical data scientist (part-time)   Children's Hospital Srebrnjak   Croatia -Data analysis and predictive modelling in respiratory diseases -Writing project proposals and scientific papers (H2020, EraPerMed)
<b>▼</b> 03.2015 - 07.2017	Analytical chemist   Teva Pharmaceutical Industries   Croatia -Supervised and trained internists and students in chemical analysis -Developed chemical analysis methods for new active pharmaceutical ingredients (APIs) -Successfully validated and transferred analytical methods to Quality Control -Implemented the Accelerated Stability Assessment Program for pharmaceuticals
<b>▼</b> 02.2014 - 03.2015	Junior scientist   University of Basel   Switzerland -Assisted in practical classes of general and inorganic chemistry -Research project: Development of a miniature microplasma gas chromatography detector for chemical analysis -Developed and tested electric circuits and detector prototypes -Wrote Python programs to drive prototype components
▲ 09.2012 - 09.2013	Junior scientist   AC2T Research   Austria  -Analysed fuels, lubricants and their ageing products with chemical analysis instruments -Presented scientific work at conferences and to customers -Managed work-packages in chemical analysis and mandated projects

#### Research visits

<b>▲</b> 11.2019-12.2019	Institute of Molecular Chemistry   University of Reims   France Data science research project in data analysis of NMR spectra
<b>▲</b> 10.2016-11.2016	Laboratoire de Chémoinformatique   University of Strasbourg   France Data science research project in QSAR analysis of chromatographic parameters

#### Education

<b>►</b> 11.2015 - 06.2021	PhD Cheminformatics Faculty of Science - Chemistry Department   University of Zagreb   Croatia Thesis: Development and application of models for ecotoxicological risk assessment of bioactive chemical compounds
<b>≈</b> 10.2010 - 07.2012	M.Sc. Applied Chemistry Faculty of Chemical Engineering and Technology   University of Zagreb   Croatia
<b>≈</b> 10.2005 - 09.2010	B.Sc. Applied Chemistry Faculty of Chemical Engineering and Technology   University of Zagreb   Croatia

#### Courses & Certificates

Big Data Specialization
Coursera   Introduction to Big Data; Big Data Modeling and Management Systems; Big
Data Integration and Processing; Machine Learning With Big Data; Graph Analytics for
Big Data
Deep Learning Specialization
Coursera   Neural Networks and Deep Learning; Improving Deep Neural Networks: Hyper-
parameter tuning; Regularization and Optimization Structuring Machine Learning Pro-
jects; Convolutional Neural Networks; Sequence Models
Machine Learning course
Coursera

## Languages

$\operatorname{Croatian}$	Native
$\operatorname{German}$	Native
English	$\operatorname{Fluent}$
$\operatorname{French}$	Beginner

#### Soft skills

	Willing to take lead, experience in leading data scientists
Social	Outgoing and communicative personality, familiar to intercultural environments

### Technical skills

Data analysis	Dealt with data engineering, predictive maintenance, forecasting and machine learning
Programming	Linux, Spark, Python, Scikit-Learn, Tensorflow, PyTorch, RDKit
Chemical Laboratory	Used chromatographic, electroanalytical and spectrometric instruments

### Relevant publications

- Lovrić M. et al (2021) Predictive Capability of QSAR Models Based on the CompTox Zebrafish Embryo Assays: An Imbalanced Classification Problem. Molecules 26:1617. https://doi.org/10.3390/molecules26061617
- 2 Lovrić M. et al (2021) Machine learning in prediction of intrinsic aqueous solubility of druglike compounds: Generalization, complexity, or predictive ability? J Chemom 35:e3349. https://doi.org/10.1002/cem.3349
- 3 Lovrić M. et al (2021) Should We Embed in Chemistry? A Comparison of Unsupervised Transfer Learning with PCA, UMAP, and VAE on Molecular Fingerprints. Pharmaceuticals 14:. https://doi.org/10.3390/ph14080758
- 4 Lovrić M. et al (2020) Understanding the true effects of the COVID-19 lockdown on air pollution by means of machine learning. Environ Pollut 115900. https://doi.org/10.1016/j.envpol.2020.115900
- Žuvela P., Lovric M. et al (2020) Ensemble Learning Approaches to Data Imbalance and Competing Objectives in Design of an Industrial Machine Vision System. Ind Eng Chem Res 59:4636–4645. https://doi.org/10.1021/acs.iecr.9b05766