

**Name and surname:** Erik LAURINI  
**Current position:** Associate Professor, University of Trieste  
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### Present Positions

2020 - Associate Professor at the Department of Engineering and Architecture of University of Trieste; SSD ING-IND/24.

### Education.

2007 - 2010 PhD in Chemical and Pharmaceutical Sciences and Technologies (University of Trieste).

2001 – 2006 Major Degree in Medicinal Chemistry (University of Trieste).

### Research Experience and Positions

2017 - 2020 Assistant Professor (RTD-B) at the Department of Engineering and Architecture of University of Trieste; SSD ING-IND/24.

2015 - 2017 Assistant Professor (RTD-A) at the Department of Engineering and Architecture of University of Trieste; SSD ING-IND/24.

2010 - 2015 Post-doc Researcher at the MOSE-Lab of the Department of Engineering and Architecture at the University of Trieste in collaboration with the Oncology Institute of Italian Switzerland (IOSI) and Otsuka Pharmaceuticals (project title: "Study of mechanisms of inhibition of STAT3 by computer-aided simulation").

2007 - 2010 Visiting Scientist, Molecular Simulation Engineering Laboratory (MOSE-Lab), University of Trieste, Italy.

## Teaching experience

- 2015 – 2019: Assistant Professor of the course “Molecular Simulation”, MSc in Process and Materials Engineering (University of Trieste).
- 2015 – 2019: Assistant Professor of the course “Thermodynamics”, BSc in Industrial Engineering (University of Trieste).
- 2015 – 2019: Assistant Professor of the course “Organic and Biologic Chemistry”, MSc in Clinical Engineering (University of Trieste).
- 2019 – present: In charge Professor of the course “Molecular Simulation”, MSc in Process and Materials Engineering (University of Trieste).
- 2019 – present: In charge Professor of the course “Organic and Biologic Chemistry for Engineering”, MSc in Clinical Engineering (University of Trieste).
- 2020 – present: In charge Professor of the course “Advance Methods in Molecular Simulation for Nanobiotechnology”, MSc in Process and Materials Engineering (University of Trieste).

Prof. Laurini was supervisor or co-supervisor for more than 100 undergraduate project students in the BSc of Industrial Engineering, in the MSc in Drug Science and in MSc in Process and Materials Engineering of the University of Trieste and for 2 PhD students of the PhD school in Nanotechnology of University of Trieste.

## Research interest

The main research activities of prof. Erik Laurini are focused in computer-aided molecular simulation of biological systems related to drugs, drug resistance in cancer treatment and study of nanocarriers for gene therapy and drug delivery. Moreover, he is also involved in project in the area of multiscale molecular modeling of nanostructured and nanomaterials for material science.

Prof. Erik Laurini is a co-founder of the MolBNL@UniTS, the Molecular Biology and Nanotechnology Laboratory of the Department of Engineering and Architecture (DEA) of the University of Trieste. The scientific mission of MolBNL@UniTS is to develop computer-based molecular simulation techniques and recipes in different sectors: (i) life sciences, and (ii) material sciences. Specifically, for point (i) MolBNL@UniTS is particularly active in the field of computer simulation with specific reference for the following topics:

1) In silico protein-drug, protein-protein and protein/nucleic acid structure and interactions in cancer targeted therapies. The main purposes of this research field are i) in deep characterization - from the structural, chemico-physical and biological perspective - mutant proteins as pathological drivers/hallmarks in major and rare human diseases; ii) prediction/determination of their structure, stability and behavior per se and in complex with e.g., small molecule inhibitors, other proteins and nucleic acids (e.g., binding thermodynamics, kinetics, stability, residence time) via a combined in silico/experimental approach.

2) Computer-assisted design and characterization of nanovectors and nanoparticles for the transport and delivery of small molecules and biologics. The main lines of research in this field are i) computer-assisted design of new and self-assembling multivalent-based nanocarriers for active

molecules, protein and gene delivery; ii) prediction/determination of their structure, critical micelle concentration, active molecules loading/release capacity, and stability per se and in complex with e.g., small molecules proteins and nucleic acids. In particular, we carry out extensive binding thermodynamics, kinetics and stability studies via a combined in silico/experimental approach.

### **Bibliometric Indicators** (January 2021)

(Scopus)

Total number of documents= 114; h index=25; Article total number of citations= 1863

(Web of Science)

Total number of documents= 115; h index=24; Article total number of citations= 1723

(Google Scholar)

Total number of documents= 114; h index=27; Article total number of citations= 2326

### **Scientific Outputs**

Articles:**99**

Review: **6**

Book chapters: **10** (3 in press, February 2021)

### **National/International conference attendance**

Oral presentation:**12**

Poster contribution: **55**

Proceedings contribution: **15**

### **Project coordination and participation in National and International Scientific Project** (most significant)

- (from 01-05-2010 to 30-04-2014) Project: Development of new inhibitors of STAT3 in oncology. Granted by: Otsuka Pharmaceuticals/Oncology Institute of Italian Switzerland (IOSI). Role: junior scientist for the molecular modeling part of the project.
- (from 22-03-2013 to 22-12-2013) Project: IN Silico Description and Prediction of drug resistance in cancer targeted therapy (INSIDER) ID: HP10CEM9ML. Granted by: CINECA. Call: ISCRA - Class C. Role: Principal Investigator.
- (from 01-01-2014 to 31-12-2016) Project: Modelling of morphology development of micro- and nanostructures (MoDeNa) Grant agreement: 604271. Granted by: European Commission Call: FP7 NMP.213.1.4-1. Role: researcher.
- (from 01-01-2016 to 31-12-2018) Project: Novel hot-spot mutations in BCR-ABL1: role in resistance to CML target therapy Grant agreement: Id.17413. Granted by: Associazione Italiana per la ricerca sul cancro. Call: IG 2015. Role: Work Package leader.
- (from 01-01-2017 – 31/12/2020) Project Multi-scale Composite Material Selection Platform with a Seamless Integration of Material Models and Multidisciplinary Design Framework (COMPOSELECTOR). Grant agreement: 721105. Granted by: European Commission. Call: H2020-

NMBP-2016-2017 NMBP-23-2016. Role: scientist in charge for the atomistic and mesoscopic modeling section of the project.

- (from 02-01-2017 – 01-01-2019) Project: Combined in silico/in vitro study of biomechanical and molecular alterations induced by mutations of Lamin A/C protein and identification of specific miRNAs as biomarkers for idiopathic dilated cardiomyopathy. Call: FRA 2016 project. Granted by: University of Trieste. Role: Principal Investigator.
- (from 01-04-2017 – 01-01-2019) Project: Novel direct TEM imaging of DNA, DNA proteins interaction and cell Membrane structure. Call: King Abdullah University of Science and Technology's Competitive Research Grant Program-Round 5 (CRG5). Granted by: King Abdullah University of Science and Technology, Thuwal (Saudi Arabia). Role: Work Package leader.
- (from 08-04-2017 - 08-05-2019) Project: Plastic Cover For Marine Engine (PlastiCo). Call: POR FESR 2014 - 2020 - Attività 1.3.b – Ricerca e sviluppo. Granted by: Regione Autonoma Friuli Venezia-Giulia. Role: Work Package leader.
- (from 07-12-2018 - 07-09-2019) Project: Atomistic Simulation for the Prediction of the frictional behavior of Aluminum Surface (ASPAS) ID: HP10CTBMUT. Granted by: CINECA. Call: ISCRA - Class C Projects. Role: Principal Investigator.
- (from 01-11-2018 – present) Project: Cancer Nanomedicine - from the bench to the bedside (Nano2Clinic). ID: CA17140. Granted by: European Commission – COST project. Role: participant.
- (from 06-05-2019 – present) Project: Studio dell'oncogene BRAF e delle sue mutazioni per la selezione di pazienti affetti da melanoma eleggibili per le terapie mirate con inibitori specifici (NO-Mel). Granted by: Regione Autonoma Friuli Venezia Giulia. Call: Bando 2017 per la concessione di contributi per la ricerca clinica, traslazionale, di base, epidemiologica, e organizzativa, art. 15, comma 2, lett. b), legge regionale 17/2014. Role: Work Package leader.

### **Organization and Coordination activities**

- Organising committee of the First COST Action 17140 Training School on Cancer Nanomedicine: from the bench to the bedside – Nano2Clinic” – 8-11 Aprile 2019, Università degli Studi di Trieste.

### **Scientific Awards (Last 5 years)**

- Cover page of “Journal of the American Chemical Society” volume 140 (47) for the publication “A Dual Targeting Dendrimer-Mediated siRNA Delivery System for Effective Gene Silencing in Cancer Therapy”, Oct 2018.
- Finanziamento delle Attività Base di Ricerca (FFABR - 2017) Granted by: Ministero dell'Istruzione, dell'Università e della Ricerca (MIUR). Grant obtained on the basis of a national ranking by results achieved during the research activity.
- "Best young communication award" at "2018 Conference on Foundations of Molecular Modelling and Simulation (FOMMS 2018, Delavan, WI, USA)" for the communication entitled “In silico/in vitro Combined Study of the Biomechanical and Molecular Alterations Induced by Lamin A/C Protein Mutations”, USA.
- NVIDIA GPU Grant Program 2018

## **National and International Collaboration (most significant)**

- Dr. Silvana Pilotti, Laboratory of Molecular Pathology, Department of Pathology, Fondazione IRCCS Istituto Nazionale dei Tumori, Milano, (Italia). Research topic: characterization through combined computational/experimental approach of mutated forms of oncological proteins and their interactions with specific inhibitors.
- Prof. Ling Peng, CNRS director, Centre Interdisciplinaire de Nanoscience de Marseille, Aix-Marseille Université, Marseille (France). Research topic: design, synthesis, characterization and in vitro/in vivo tests of nanovectors for the transport and controlled release of drugs and genetic material.
- Prof. Antonio Carta, Dipartimento di Chimica e Farmacia, Università degli Studi di Sassari, Sassari (Italia). Research topic: synergistic computational/experimental approach for the development of new and more efficient oncological and antiviral drugs.
- Prof. Bernhard Wuensch, Institute of Pharmaceutical and Medicinal Chemistry, University of Muenster, Muenster (Germania). Research topic: design, synthesis, quantitative structure-activity relationships (QSAR) and thermodynamic aspects of the interaction of new chemical entities such as sigma1 transmembrane receptor ligands.
- Prof. Daniele Marchisio, Department of Applied Science and Technology, Politecnico di Torino, Torino (Italia). Research topic: multiscale modeling approach for the study and the properties prediction of polyurethane-based polymer.
- Prof. Igor Balaz, Laboratory for Biophysics, Physics and Meteorology, University of Novi Sad, (SRB). Research topic: synergistic computational/experimental approach for the development of nanoparticles for loading/release of active molecules.
- Prof. David K. Smith, Department of Chemistry, University of York, (UK). Research topic: self-assembling nanotechnology systems such as nanovectors and/or multivalent ligands for polyanions of biomedical interest (e.g., nucleic acids and heparin).