

# EUROPEAN CURRICULUM VITAE FORMAT



## PERSONAL INFORMATION

Name **MAURIZIO FERMEGLIA**  
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Nationality Italian  
Date of birth October 9th, 1955

## WORK EXPERIENCE

- Dates (from – to) 2016 - 2018
- Name and address of employer Ministry of Research Education and University, Viale Trastevere, Roma - Italy
- Type of business or sector Scientific evaluation of professors (ASN)
- Occupation or position held President of the AN commission for sector 09D2
- Main activities and responsibilities Evaluation of profiles of candidates to professorships at national level
  
- Dates (from – to) 2013 - 2019
- Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
- Type of business or sector Rectorate
- Occupation or position held Rector of the University of Trieste
- Main activities and responsibilities Legal representation and management of the University of Trieste
  
- Dates (from – to) 2011 - 2017
- Name and address of employer DECHEMA, Frankfurt, Germany
- Type of business or sector Member of the EU working party on thermodynamics
- Occupation or position held Member of the working party of the European federation of chemical engineering on thermodynamics and transport properties
- Main activities and responsibilities Coordination of scientific activities
  
- Dates (from – to) 2002 -
- Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
- Type of business or sector Faculty of Engineering, then Department of Engineering and Architecture
- Occupation or position held Full Professor of Chemical Engineering
- Main activities and responsibilities Coordinator of the MOSE (Molecular Simulation Engineering) laboratory of the University of Trieste
  
- Dates (from – to) 2009 - 2013
- Name and address of employer UNEP / MAP- MedPol 48, Vassileos Konstantinou Ave. 11635 Athens - Greece
- Type of business or sector UN agency

- Occupation or position held Consultant on PRTR implementation
  - Main activities and responsibilities Scientific and technical responsibility of PRTR project implementation in developing countries.
- Dates (from – to) 2006 - 2013
  - Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
    - Type of business or sector PhD Schools
    - Occupation or position held Director of the PhD School of Nanotechnology of the University of Trieste
  - Main activities and responsibilities Member of the teachers' board and, as the school director, coordination of the teaching and research activities of its PhD students
- Dates (from – to) 2010 - 2012
  - Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
    - Type of business or sector Faculty of Engineering
    - Occupation or position held Director of the Department of Industrial Engineering and Information Technology (DI3)
  - Main activities and responsibilities Coordination of research activities in industrial engineering, materials engineering and ICT
- Dates (from – to) 2010 - 2012
  - Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
    - Type of business or sector Administration and scientific coordination
    - Occupation or position held President of the 'Council of the scientific structures' of the University of Trieste (CSS)
  - Main activities and responsibilities Coordination of research activities and science administration for the University
- Dates (from – to) 1998 - 2011
  - Name and address of employer ICS – UNIDO, Area Science Park, Padriciano 99, 34012 Trieste - Italy
    - Type of business or sector UN agency
    - Occupation or position held Consultant on process simulation for sustainable industrial development
  - Main activities and responsibilities Training and coordination of activities in the area of sustainable industrial development in developing countries. Project leader of PRTR implementation.
- Dates (from – to) 2009 - 2010
  - Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
    - Type of business or sector Faculty of Engineering
    - Occupation or position held Director of the Department of Materials and Natural Resources (DMRN)
  - Main activities and responsibilities Coordination of research activities in process engineering, materials engineering and environment
- Dates (from – to) 2006 - 2009
  - Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
    - Type of business or sector Faculty of Engineering
    - Occupation or position held Director of the Department of Chemical, Environmental and Raw Materials Engineering (DICAMP)
  - Main activities and responsibilities Coordination of research activities in process engineering, material engineering and environment
- Dates (from – to) 2005 - 2008
  - Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
    - Type of business or sector Industrial Liaison Office (ILO)
    - Occupation or position held Member of the scientific committee of Innovaction the Fair of Innovation, put in charge of the project by an official Rector's act
  - Main activities and responsibilities Member of the scientific committee for Innovaction fair and coordination of the participation of the University to the fair.
- Dates (from – to) 1993 - 2006
  - Name and address of employer Università di Padova, via 8 Febbraio, 2 - 35122 Padova - Italia
    - Type of business or sector Faculty of Engineering
    - Occupation or position held Member of the teachers' board
  - Main activities and responsibilities Member of the teachers' board of the PhD in Chemical Engineering, organized by the Universities of Trieste and Padua. Coordination of PhD projects.

- Dates (from – to) 2004
- Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
  - Type of business or sector Faculty of Engineering
  - Occupation or position held President evaluation committee of CIVR Sector 09 – Industrial Engineering and ICT
- Main activities and responsibilities Selection of research product to be presented for the national university evaluation on Sector 09
  
- Dates (from – to) 1998 - 2003
- Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
  - Type of business or sector Rectorate
  - Occupation or position held Rector's delegate for the digitalization of the University administration offices
- Main activities and responsibilities Coordination of ICT projects: year 2000, Euro, ERP SAP implementation, SAS data warehouse, students ID and e-mail system, directory service, faculty logistics and students data base
  
- Dates (from – to) 1992 -2002
- Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
  - Type of business or sector Faculty of Engineering
  - Occupation or position held Associate Professor of Chemical Engineering
- Main activities and responsibilities Research and teaching activities in Chemical Engineering
  
- Dates (from – to) 1983 - 1992
- Name and address of employer University of Trieste, Piazzale Europa 1, 34127 Trieste - Italy
  - Type of business or sector Faculty of Engineering
  - Occupation or position held Assistant Professor of Chemical Engineering
- Main activities and responsibilities Research and teaching activities in Chemical Engineering

## EDUCATION AND TRAINING

- Dates (from – to) 2002
- Name and type of organisation providing education and training Italian Ministry of University
- Principal subjects/occupational skills covered Chemical Engineering Principles
  - Title of qualification awarded Full Professor
- Level in national classification
  
- Dates (from – to) 1992
- Name and type of organisation providing education and training Italian Ministry of University
- Principal subjects/occupational skills covered Chemical Engineering Principles
  - Title of qualification awarded Associate Professor
- Level in national classification
  
- Dates (from – to) 1983
- Name and type of organisation providing education and training Italian Ministry of University
- Principal subjects/occupational skills covered Chemical Engineering Principles
  - Title of qualification awarded Assistant Professor
- Level in national classification
  
- Dates (from – to) 1981 - 1982
- Name and type of organisation providing education and training Technical University of Denmark, Lyngby
- Principal subjects/occupational skills covered Chemical Engineering Principles

- skills covered
- Title of qualification awarded Researcher
- Level in national classification
  
- Dates (from – to) 1980 - 1981
- Name and type of organisation providing education and training Italian Ministry of Defense
- Principal subjects/occupational skills covered Military service as on officer of Alpine infantry
- Title of qualification awarded Lieutenant, then Captain
- Level in national classification
  
- Dates (from – to) 1974 - 1979
- Name and type of organisation providing education and training University of Trieste, Faculty of Engineering
- Principal subjects/occupational skills covered Chemical Engineering
- Title of qualification awarded MSc in Chemical Engineering
- Level in national classification
  
- Dates (from – to) 1974
- Name and type of organisation providing education and training Liceo Scientifico G. Oberdan – Trieste, Italy
- Principal subjects/occupational skills covered Scientific curriculum
- Title of qualification awarded High school graduation
- Level in national classification

**PERSONAL SKILLS AND COMPETENCES**

*Acquired in the course of life and career but not necessarily covered by formal certificates and diplomas.*

Mother tongue(s) **ITALIAN**

Other language(s) **ENGLISH, SPANISH, FRENCH**

Self-assessment

*European level (\*)*

**English**

**Spanish**

**French**

**Understanding**

Listening

Reading

**Speaking**

Spoken interaction

Spoken production

**Writing**

C2

C2

C2

C2

C2

B1

B2

A2

A2

A1

A1

A1

A1

A1

A1

(\*) [Common European Framework of Reference for Languages](#)

**SOCIAL SKILLS AND COMPETENCES**

*Living and working with other people, in multicultural environments, in positions where communication is important and situations where teamwork is essential (for example culture and sports), etc.*

I GAINED EXCELLENT MANAGING SKILLS DURING THE EXPERIENCES IN THE MANAGEMENT OF RESEARCH GROUPS, THE MILITARY SERVICE, DIRECTOR OF THE DEPARTMENT AND PHD SCHOOLS AND ABOVE ALL IN THE MANAGEMENT OF THE UNIVERSITY OF TRIESTE FOR 5 YEARS. THE SAME EXPERIENCES ALLOWED ME TO GAIN RELATIONAL SKILLS AND WORKGROUP CAPACITY. IN MORE THAN 15 YEARS OF EXPERIENCE WORKING WITH EU ORGANIZATIONS SPECIFICALLY FOR DEVELOPING AND EMERGING COUNTRIES I GOT SKILLS IN DEALING WITH MULTI LANGUAGE AND MULTI ETHNIC GROUPS.

**ORGANISATIONAL SKILLS AND COMPETENCES**

*Coordination and administration of*

IN MOST OF THE ACTIVITIES CARRIED OUT DURING MY PROFESSION I HAD TO LEAD, ORGANIZE AND MANAGE GROUP ACTIVITIES. DURING THE MILITARY SERVICE I HAD THE RESPONSIBILITY OF SOLDIERS IN OUTDOOR ACTIVITIES IN THE ALPS, IN SPORT ACTIVITY I WAS TRAINER AND PROFESSIONAL PLAYER AND I

people, projects and budgets; at work, in voluntary work (for example culture and sports) and at home, etc.

## TECHNICAL SKILLS AND COMPETENCES

*With specific kinds of equipment, machinery, etc.*

ALSO WAS INSTRUCTOR OF MOUNTAINEERING, LEADING GROUPS OF PEOPLE IN THE MOUNTAINS. I WAS RESPONSIBLE OF ALPINE RESCUE TEAM IN FRIULI REGION IN ITALY, THUS MANAGING THE RESCUE ACTIONS. AT THE UNIVERSITY, I MANAGED RESEARCH PROJECTS AND COORDINATED RESEARCH ACTIVITIES.

MY RESEARCH ACTIVITY IS CARRIED OUT AT THE 'DEPARTMENT OF ENGINEERING AND ARCHITECTURE OF THE UNIVERSITY OF TRIESTE. THE MAIN RESEARCH ACTIVITIES ARE FOCUSED ON MULTISCALE MODELING FOR MANAGING THE COMPLEXITY OF PROCESS – PRODUCT DESIGN, SUSTAINABLE PROCESS DESIGN AND ANALYSIS, THEORY, MODELING AND SIMULATION OF NANOSTRUCTURED MATERIALS, DRUG DESIGN AND DESIGN OF CONTROLLED RELEASE PROCESSES. OTHER FIELD OF INTEREST IS TRANSPORT AND THERMODYNAMIC PROPERTY, THEIR EXPERIMENTAL DETERMINATION, CORRELATION AND PREDICTION. IN THIS FIELD, I HAVE DONE EXPERIMENTAL WORK IN THE DETERMINATION OF PHASE EQUILIBRIA (VAPOR - LIQUID, LIQUID - LIQUID AND GAS -LIQUID) DATA, CORRELATION AND PREDICTION OF EXPERIMENTAL DATA BY MEANS OF DIFFERENT MODELS (EXCESS GIBBS ENERGY MODELS AND EQUATIONS OF STATE), APPLICATION OF THE MODELS TO THE SIMULATION OF CHEMICAL PROCESSES (STEADY STATE AND DYNAMIC PROCESSES).

THE RESEARCH ACTIVITY CAN BE SUMMARIZED IN THE FOLLOWING AREAS:

1. EXPERIMENTAL DETERMINATIONS
  - a. EXPERIMENTAL DETERMINATION OF PHASE EQUILIBRIUM
  - b. DATA COLLECTION
  - c. EXPERIMENTAL DETERMINATION OF TRANSPORT PROPERTIES
2. MULTISCALE MOLECULAR MODELING
  - a. THERMO PHYSICAL PROPERTIES FOR REFRIGERANTS AND ORGANICS
  - b. THERMO PHYSICAL PROPERTIES FOR POLYMERS AND POLYMER SYSTEMS INCLUDING BLENDS
  - c. TRANSPORT PROPERTIES FOR POLYMERS
  - d. NANOTECHNOLOGY AND NANOCOMPOSITES
  - e. CHEMICAL REACTION ENGINEERING
  - f. MOLECULAR MODELING FOR BIOLOGICAL SYSTEMS
3. CHEMICAL ENGINEERING THERMODYNAMICS
  - a. EXCESS GIBBS ENERGY MODELS DEVELOPMENT
  - b. EQUATIONS OF STATE DEVELOPMENT
  - c. THERMODYNAMICS OF POLYMER SYSTEMS AND GELS
4. PROCESS ENGINEERING
  - a. TRADITIONAL PROCESSES
  - b. NON TRADITIONAL PROCESSES

IN COMPUTER SCIENCE, MY MAIN RESEARCH ACTIVITY IS IN THE DATA BASE AND INTERNET FIELDS, WHERE I FOCUSED ON THE DIFFERENT ASPECTS AND POSSIBILITIES OF PUBLISHING DATA BASE INFORMATION IN THE WWW. IN THIS FIELD, I PERFORMED DESIGN AND DEVELOPMENT OF DATA BASE SYSTEMS, WITH PARTICULAR ATTENTION TO DATA BASE OF PHYSICAL PROPERTIES, TOXICOLOGICAL DATA AND POLLUTANT RELEASES.

IN THE AREA OF NANOMATERIALS I WAS THE LOCAL LEADER OF SEVERAL EU FP6, FP7 AND H2020 PROJECTS DEALING WITH MODELING AND SIMULATION. I WAS SCIENTIFIC CONSULTANT OF ICS - UNIDO WITHIN THE SUBPROGRAM 'PROCESS SIMULATION' FROM 1998 TO 2011 AND OF UNEP FOR THE IMPLEMENTATION OF PRTR IN DIFFERENT COUNTRIES.

I AM IUPAC FELLOWS FROM 2003. I AM MEMBER OF THE EUROPEAN WORKING PARTY OF THERMODYNAMICS AND TRANSPORT PROPERTIES.

## COMPUTER SKILLS AND COMPETENCES

FTN JAVA, C#, VISUAL BASIC PROGRAMMER. DATA BASE DEVELOPER. WINDOWS SYSTEM ENGINEER. ADVANCED USER OF PROCESS SIMULATION AND MOLECULAR SIMULATION SOFTWARE. DATA BASE ADMINISTRATOR. COMPUTER NETWORK DESIGN AND COMPUTER SYSTEM ARCHITECTURES DESIGN. DESIGN AND DEVELOPMENT OF APPLICATIONS AND DATA BASES

## ARTISTIC SKILLS AND COMPETENCES

*Music, writing, design, etc.*

I WAS A MEMBER OF A MUSICAL GROUP OF CLASSICAL AND FOLK MUSIC, WHERE I WAS PLAYING STRING INSTRUMENTS.

## OTHER SKILLS AND COMPETENCES

*Competences not mentioned above.*

*Page 5/19 - Curriculum vitae of  
Maurizio Fermeglia*

SPORTS PERFORMED: VOLLEYBALL, MOTORCYCLING, TENNIS, CLIMBING SKI, BASKET, ATHLETIC. I WAS MOUNTAINEERING AND SKI INSTRUCTOR FROM 1985 TO 2005. I PARTICIPATED TO DIFFERENT MOUNTAINEERING EXTRA EUROPEAN EXPEDITIONS IN THE EIGHTIES. I WAS A MEMBER OF THE NATIONAL

ALPINE RESCUE TEAM FROM 1982 TO 2000. I AM ACADEMIC MEMBER OF THE ITALIAN ALPINE CLUB.

**DRIVING LICENSE**

LICENSE B (CAR)  
ITALIAN MOUNTAINEERING INSTRUCTOR  
ITALIAN SKI-TOURING INSTRUCTOR

**ADDITIONAL INFORMATION**

I PUBLISHED MORE THAN 200 PEER REVIEWED JOURNAL ARTICLES AND BOOK CHAPTERS AND I MADE MORE THAN 200 CONFERENCE PRESENTATIONS AS INVITED PLENARY, KEYNOTE, ORAL OR POSTER PRESENTER. I HAVE ALSO GIVEN INVITED LECTURES SEMINARS AT NUMEROUS COMPANIES AND ACADEMIC INSTITUTIONS AND ORGANIZED SEVERAL WORKSHOPS ON TOPICS RELATED TO PROCESS ENGINEERING, NANOTECHNOLOGY AND MULTISCALE MODELING. I SUPERVISED DOZENS OF MASTER THESIS IN CHEMICAL ENGINEERING AND COMPUTER TECHNOLOGY AS WELL AS PH.D. PROJECTS AT THE UNIVERSITY OF PADOVA AND AT THE UNIVERSITY OF TRIESTE. IN THE AREA OF NANOMATERIALS I WAS THE LOCAL LEADER OF SEVERAL EU FP6 AND FP7 AND H2020 PROJECTS DEALING WITH MODELING AND SIMULATION. I WAS SCIENTIFIC CONSULTANT OF ICS - UNIDO WITHIN THE SUBPROGRAM 'PROCESS SIMULATION' FROM 1999 TO 2011 AND OF UNEP FOR THE IMPLEMENTATION OF PRTR IN DIFFERENT COUNTRIES FROM 2005 TO 2013.

MORE INFORMATION IN [WWW.MOLBNL.IT](http://WWW.MOLBNL.IT) . H INDEX IN 2019 IS 46; NUMBER OF CITATIONS 7065; I10 INDEX 139; TOTAL NUMBER OF PAPERS 533 (GOOGLE SCHOLAR).

**ANNEXES**

LISTS OF PUBLICATIONS AND RESEARCH PROJECTS ARE AVAILABLE AT [WWW.MOSE.UNITS.IT](http://WWW.MOSE.UNITS.IT)



## Appendix 1: teaching activity

Main teaching activity at the University of Trieste :

- Chemical Engineering principles II from 1990 to 2003
- Chemical reaction engineering from 2002 to 2009
- Chemical and biochemical reaction engineering from 2009 to 2019
- Process simulation from 2003 to 2006.
- Process and product design from 2011 to 2017.
- Data base design from 1994 to 2014
- Advanced Data base design from 2004 to 2009.

## Appendix 2: scientific projects

Main International research projects of the last 10 years:

- Innovative Molecular modeling approach to up grade polymeric materials from post industrial rejects (MoMo), EU STREP - FP6: 2004 – 2006.
- MOMO: Innovative Molecular modeling approach to up grade polymeric materials from post industrial rejects, FP6: 2004 – 2006.
- MULTIPRO: Design of ‘tailor to made’ MULTIfunctional organic material by molecular modeling of structure property relationship, experimentation and PROcessing: FP6: 2006-2008.
- MULTYHYBRID: Innovative sensor-based procesing technology of nanoscrutured multifunctioanl hybrids and composites, FP6: 2006-2009.
- NANOMODEL: Multi-Scale Modelling of Nano-Structured Polymeric Materials: From Chemistry to Materials Performance, FP7, 2008-2011.
- MODENA: MOdelling of morphology DEvelopment of micro- and NAnostructures (MoDeNa), FP7, 2013-2016.
- COMPOSELECTOR: (NMP NMBP-23-2016)— Advancing the integration of Materials Modelling in Business Processes to enhance effective industrial decision making and increase competitiveness, H2020, 2016- 2019.
- Novel direct HRTEM imaging of DNA, DNA/proteins interaction and cell membrane structure, CRG Proposal Framework collaboration KAUST – University of Trieste. 2017 - 2019

## Appendix 3: publications

### Scopus summary table (May 2020)





## Publication list (2008 – 2019 from Scopus).

1. Marson, D., Laurini, E., Aulic, S., Fermeglia, M., Pricl, S.; Unchain my blood: Lessons learned from self-assembled dendrimers as nanoscale heparin binders; *Biomolecules*; 2019; 9; 8; 10.3390/biom9080385
2. Marson, D., Laurini, E., Aulic, S., Fermeglia, M., Pricl, S.; Evolution from covalent to self-assembled PAMAM-based dendrimers as nanovectors for siRNA delivery in cancer by coupled in silico-experimental studies. part I: Covalent siRNA nanocarriers; *Pharmaceutics*; 2019; 11; 7; 10.3390/pharmaceutics11070351
3. Laurini, E., Marson, D., Aulic, S., Fermeglia, M., Pricl, S.; Evolution from covalent to self-assembled PAMAM-based dendrimers as nanovectors for siRNA delivery in cancer by coupled in silico-experimental studies. Part II: Self-assembled siRNA nanocarriers; *Pharmaceutics*; 2019; 11; 7; 10.3390/pharmaceutics11070324
4. Marson, D., Laurini, E., Aulic, S., Fermeglia, M., Pricl, S.; Self-assembling Nanotechnology for Cancer Personalized Medicine; *Chemical Engineering Transactions*; 2019; 74; 1549; 1554; 10.3303/CET1974259
5. Laurini, E., Marson, D., Aulic, S., Mio, A., Fermeglia, M., Pricl, S.; Integrating multiscale simulations for composite materials with industrial business decision: The EU H2020 composelector project experience; *Chemical Engineering Transactions*; 2019; 74; 619; 624; 10.3303/CET1974104
6. Carta, A., Bua, A., Corona, P., Piras, S., Briguglio, I., Molicotti, P., Zanetti, S., Laurini, E., Aulic, S., Fermeglia, M., Pricl, S.; Design, synthesis and antitubercular activity of 4-alkoxy-triazoloquinolones able to inhibit the M. tuberculosis DNA gyrase; *European Journal of Medicinal Chemistry*; 2019; 161; 399; 415; 10.1016/j.ejmech.2018.10.031
7. Piras, S., Sanna, G., Carta, A., Corona, P., Ibba, R., Loddo, R., Madeddu, S., Caria, P., Aulic, S., Laurini, E., Fermeglia, M., Pricl, S.; Dichloro-phenyl-benzotriazoles: A new selective class of Human Respiratory Syncytial Virus entry inhibitors; *Frontiers in Chemistry*; 2019; 7; MAR; 10.3389/fchem.2019.00247
8. Marson, D., Laurini, E., Fermeglia, M., Smith, D.K., Pricl, S.; Mallard Blue binding to heparin, its SDS micelle-driven de-complexation, and interaction with human serum albumin: A combined experimental/modeling investigation; *Fluid Phase Equilibria*; 2018; 470; 259; 267; 10.1016/j.fluid.2017.11.005
9. Ziouziou, H., Andrieu, C., Laurini, E., Karaki, S., Fermeglia, M., Oueslati, R., Taieb, D., Camplo, M., Siri, O., Pricl, S., Katsogiannou, M., Rocchi, P.; Correction: Targeting Hsp27/eIF4E interaction with phenazine compound: A promising alternative for castration-resistant prostate cancer treatment [Oncotarget. 2017; 8:77317-77329]doi 10.18632/oncotarget.20469; *Oncotarget*; 2018; 9; 47; 28797; 28797; 10.18632/oncotarget.25683
10. Mio, A., Limleamthong, P., Guillén-Gosálbez, G., Fermeglia, M.; Sustainability Evaluation of Alternative Routes for Fine Chemicals Production in an Early Stage of Process Design Adopting Process Simulation along with Data Envelopment Analysis; *Industrial and Engineering Chemistry Research*; 2018; 57; 23; 7946; 7960; 10.1021/acs.iecr.7b05126
11. Laurini, E., Marson, D., Fermeglia, M., Pricl, S.; Multimodel approach for accurate determination of industry-driven properties for Polymer Nanocomposite Materials; *Journal of Computational Science*; 2018; 26; 28; 38; 10.1016/j.jocs.2018.03.002
12. Karimi, M., Marchisio, D., Laurini, E., Fermeglia, M., Pricl, S.; Bridging the gap across scales: Coupling CFD and MD/GCMC in polyurethane foam simulation; *Chemical Engineering Science*; 2018; 178; 39; 47; 10.1016/j.ces.2017.12.030
13. Loddo, R., Francesconi, V., Laurini, E., Boccardo, S., Aulic, S., Fermeglia, M., Pricl, S., Tonelli, M.; 9-Aminoacridine-based agents impair the bovine viral diarrhoea virus (BVDV) replication targeting the RNA-dependent RNA polymerase (RdRp); *Bioorganic and Medicinal Chemistry*; 2018; 26; 4; 855; 868; 10.1016/j.bmc.2018.01.001
14. Carta, A., Sanna, G., Briguglio, I., Madeddu, S., Vitale, G., Piras, S., Corona, P., Peana, A.T., Laurini, E., Fermeglia, M., Pricl, S., Serra, A., Carta, E., Loddo, R., Giliberti, G.; Quinoxaline derivatives as new inhibitors of coxsackievirus B5; *European Journal of Medicinal Chemistry*; 2018; 145; 559; 569; 10.1016/j.ejmech.2017.12.083

15. Briguglio, I., Laurini, E., Pirisi, M.A., Piras, S., Corona, P., Fermeglia, M., Pricl, S., Carta, A.; Triazolopyridinyl-acrylonitrile derivatives as antimicrotubule agents: Synthesis, in vitro and in silico characterization of antiproliferative activity, inhibition of tubulin polymerization and binding thermodynamics; *European Journal of Medicinal Chemistry*; 2017; 141; 460-472; 10.1016/j.ejmech.2017.09.065
16. Colombo, C., Belfiore, A., Paielli, N., De Cecco, L., Canevari, S., Laurini, E., Fermeglia, M., Pricl, S., Verderio, P., Bottelli, S., Fiore, M., Stacchiotti, S., Palassini, E., Gronchi, A., Pilotti, S., Perrone, F.;  $\beta$ -Catenin in desmoid-type fibromatosis: deep insights into the role of T41A and S45F mutations on protein structure and gene expression; *Molecular Oncology*; 2017; 11; 1495-1507; 10.1002/1878-0261.12101
17. Laurini, E., Posocco, P., Fermeglia, M., Pricl, S.; Multiscale Molecular Modeling of Clay-Polymer Nanocomposites; *Clay-Polymer Nanocomposites*; 2017; 83; 112; 10.1016/B978-0-323-46153-5.00003-3
18. Laurini, E., Marson, D., Fermeglia, M., Pricl, S.; 3D homology model of sigma1 receptor; *Handbook of Experimental Pharmacology*; 2017; 244; 27-50; 10.1007/164\_2017\_35
19. Kokornaczyk, A.K., Schepmann, D., Yamaguchi, J., Itami, K., Laurini, E., Fermeglia, M., Pricl, S., Wünsch, B.; Thiazole-Based  $\sigma$  Receptor Ligands: Diversity by Late-Stage C-H Arylation of Thiazoles, Structure-Affinity and Selectivity Relationships, and Molecular Interactions; *ChemMedChem*; 2017; 12; 1070-1080; 10.1002/cmdc.201700166
20. Ferkl, P., Toulec, M., Laurini, E., Pricl, S., Fermeglia, M., Auffarth, S., Eling, B., Settels, V., Kosek, J.; Multi-scale modelling of heat transfer in polyurethane foams; *Chemical Engineering Science*; 2017; 172; 323-334; 10.1016/j.ces.2017.06.035
21. Ziouziou, H., Andrieu, C., Laurini, E., Karaki, S., Fermeglia, M., Oueslati, R., Taieb, D., Camplo, M., Siri, O., Pricl, S., Katsogiannou, M., Rocchi, P.; Targeting Hsp27/eIF4E interaction with phenazine compound: A promising alternative for castration-resistant prostate cancer treatment; *Oncotarget*; 2017; 8; 77317-77329; 10.18632/oncotarget.20469
22. Perfetti, V., Laurini, E., Aulic, S., Fermeglia, M., Riboni, R., Lucioni, M., Dallera, E., Delfanti, S., Pugliese, L., Latteri, F.S., Pietrabissa, A., Pricl, S.; Molecular and functional characterization of a new 3' end KIT juxtamembrane deletion in a duodenal GIST treated with neoadjuvant Imatinib; *Oncotarget*; 2017; 8; 56158-56167; 10.18632/oncotarget.19341
23. Petrescu, L., Fermeglia, M., Cormos, C.-C.; Life Cycle Analysis applied to acrylic acid production process with different fuels for steam generation; *Journal of Cleaner Production*; 2016; 133; 294-303; 10.1016/j.jclepro.2016.05.088
24. Laurini, E., Marson, D., Posocco, P., Fermeglia, M., Pricl, S.; Structure and binding thermodynamics of viologen-phosphorous dendrimers to human serum albumin: A combined computational/experimental investigation; *Fluid Phase Equilibria*; 2016; 422; 18-31; 10.1016/j.fluid.2016.02.014
25. Chen, C., Posocco, P., Liu, X., Cheng, Q., Laurini, E., Zhou, J., Liu, C., Wang, Y., Tang, J., Col, V.D., Yu, T., Giorgio, S., Fermeglia, M., Qu, F., Liang, Z., Rossi, J.J., Liu, M., Rocchi, P., Pricl, S., Peng, L.; siRNA Delivery: Mastering Dendrimer Self-Assembly for Efficient siRNA Delivery: From Conceptual Design to In Vivo Efficient Gene Silencing (Small 27/2016); *Small*; 2016; 3604; 10.1002/sml.201670131
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## Appendix 4: invited talks (2008-2019)

Year	Conference - Event	Organizer	Place	Period	Title
2008	18th European Symposium on Computer Aided Process Engineering	ELSEVIER	Lyon, F	June 1-4, 2008	Multiscale molecular modeling: a tool for the design of nano structured materials.
	Drug Design and Discovery for Developing Countries	ICS-UNIDO	Trieste, I	July 3-5, 2008	Multiscale molecular strategies for drug delivery
	5th Chemical Engineering	University of	Cetraro, I	May 24-29,	Multiscale molecular modeling for



	Conference for Collaborative Research in Eastern Mediterranean Countries	Cosenza		2008	nanostructured materials
	DPD: addressing deficiencies and establishing new frontiers - CECAM	CECAM	Lausanne, CH	July 16-18, 2008	Message –passing multiscale molecular modeling: mapping atomistic to mesoscale simulation
	International Seminar on Multiscale Modeling of Polymer Materials	National Technical University of Norway	Trondheim, N	October 13-14, 2008	Multiscale molecular modelling of nanostructured polymer systems of industrial interest
<b>2009</b>	Proceedings of the IUTAM Symposium	SPRINGER-VERLAG	Aalborg, DK	May 19-22, 2008	Multiscale molecular modelling of dispersion of nanoparticles in polymer systems of industrial interest
	Accelrys Science Forum 2009	Accelrys	Paris, F	July 2, 2009	Molecular modeling for nanostructured polymer systems of industrial interest
<b>2010</b>	AIChE Annual Meeting 2010, American Institute of Chemical Engineering,	AICHE	Salt Lake City, US	November 7-12, 2010	Multiscale Molecular Modeling of Polymer/Silica Nanocomposites
	6th Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries	Sabancı University, Istanbul	Antalya, T	March 7-12, 2010	Multiscale molecular modeling for nanostructured and hybrid inorganic/organic materials
<b>2011</b>	SimMolMod 2011	DECHEMA	Dortmund, D	September 15-16, 2011	Nano tools for macro problems: multiscale molecular modeling of polymer nanocomposites
	MULT-EU-SIM satellite Workshop at TNT2011	TNT 2011, Phantoms Foundation	Tenerife, S	November 21-25, 2011	Nano tools for macro problems: multiscale molecular modeling of nanostructured systems
	Towards a multi-scale, multi-phenomena modelling-simulation-design-engineering environment & tools	DG Research and Innovation, European Commission	Brussels, B	September 22, 2011	Opportunities and challenges from HPC and research
	POZNAN 2011: Summer Symposium on Nanomaterials and their application to Biology and Medicine	Adam Mickiewicz University	Poznan, P	June 13-16, 2011	Multiscale molecular modelling for the design of nanostructures in materials and life sciences
<b>2012</b>	2nd Nanosymposium on Nanomaterials.	Adam Mickiewicz University,	Poznań, PL	June 20-24, 2012	Multiscale molecular modeling: a virtual microscope for material and life science
	7th Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries	FORTH/ICE-HT	Corfu Island GR	April 27-May 1, 2012	Multiscale molecular modeling for the design of materials in the nano-bio-based economy
<b>2013</b>	3rd Summer Symposium on Nanomaterials and their application to Biology and Medicine	Adam Mickiewicz University,	Poznan, PL	16-19 June 2013	Nano tools for macro problems: multiscale molecular modeling for nano-bio-technology
	3 Int. Elsevier Conference on Multifunctional, Hybrid and Nanomaterials	Elsevier	Sorrento, I,	4-7 March 2013	Nano tools for macro problems: multiscale molecular modeling of functional hybrid nanomaterials
	J.C. Maxwell meeting 2013	Kings College	London, UK	11 June 2013	The role of Multiscale Modeling in Horizon 2020
	Chemelot Colloquium 2013	Dutch School of Mines, NL	Geleen, NL	26 April 2013	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
<b>2014</b>	Material Challenges in Devices for Fuel Solar Production and Employment	ICTP	Trieste, I	19-23 May 2014	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	Workshop on geothermal energy: Status and future in the peri-adriatic- area	ICTP	Losinj, CRO	25 agosto 2014	Workshop on geothermal energy: Status and future in the peri-adriatic-area
<b>2015</b>	Italy meets Asia: scientific	Italian	Kyoto, JAP	1 April 2015	Nano tools for macro problems:

	venue in Kyoto 2015 – Marco Polo award	Embassy in Japan			multiscale molecular modeling of nanostructured polymer systems
	Sharif University meetings	Sharif University, Tehran	Tehran, IRAN	18 April 2015	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	Eurofillers Polymer Blends 2015	University of Montpellier	Montpellier, F	26-30 April 2015	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	5° Summer Symposium on Nanomaterials and their applications to biology and medicine	Adam Mickiewicz University In Poznań	Zakopane, P	14-18 June, 2015	Theory modeling and simulation: a fundamental tool for nano – bio – med research
	CERMODEL 2015 – Modelling and simulation meet innovation in ceramics technology	University of Trento	Trento, I	1-3 July 2015	Materials by design: multiscale molecular modeling of nanostructured materials
	Modellistica molecolare per la soluzione di problemi industriali	Politecnico di Milano	Milano, I	18 Settembre 2015	Materials by design: multiscale molecular modeling of nanostructured materials
	ATMAR: Next generation medicine: an integrated approach at Cattinara university hospital 40 years later	CCIAA TS	Trieste, I	8 – Jun 2015	Nano-bio-med: a strategic area of scientific and technological development
<b>2016</b>	TU HH – seminar serie	TU Hambrug	Hamburg, D	13 January, 2016	Materials by design: multiscale molecular modeling of nanostructured materials
	From intermolecular forces to frontiers in nanoscience and nanomedicine. In honor of Giacinto Scoles	ICTP	Trieste, I	22 Jan, 2016	Materials by design: multiscale molecular modeling of nanostructured materials
	KAUST seminar series	KAUST	Gedda, Saudi Arabia	4 Feb 2016	Materials by design: multiscale molecular modeling of nanostructured materials
	Geotermia e idrotermia per il riscaldamento e il raffrescamento	FIT	Grado, I	20 May 2016	La grande sfida dell'energia: come evitare la 'tempesta perfetta
	College on multiscale computational modeling of materials for energy applications	ICTP	Trieste, I	11 July 2016	Mesoscopic simulation for the prediction of macroscopic properties of nanostructured systems.
	ICNN 4 – international conference on nanomechanics and nanocomposites	UNIPD	Vicenza, I	14 – 17 Sept. 2016	Materials by design: multiscale molecular modeling of nanostructured materials
	International conference on SESAME	ESAC	Lussino, CRO	30 Aug 2016	The role of University as a catalyst for science, technology and society: the Trieste science system
<b>2017</b>	Celebration of Josef Stefan's birthday 2017	Josef Stefan Institute	Lubiana, SLO	20 Mar 2017	Materials by design: multiscale molecular modeling of nanostructured materials
	International festival of Science and Education 2017	University of Novi Sad	Novi Sad SRB	13 May 2017	The role of University as a catalyst for science, technology and society
	Malnisio Science Festival	Pordenone Turismo	Malnisio (PN)	7 Oct 2017	Energia, cibo, acqua e cambiamenti climatici: la tempesta perfetta
	Kyoto Institute of Technology Scientific events	KIT	Kyoto (Jap)	30 Oct 2017	Materials by design: multiscale molecular modeling of nanostructured materials
	University of Palermo	UNIPA - DIC	Palermo	30 Nov 2017	Materials by design: multiscale molecular modeling of nanostructured materials
	Seminario internazionale Pestalozzi: diritto ed economia a scuola: un volano per la democrazia	Liceo Dante-Carli	Trieste	12 Dec 2017	Quale ruolo per le scienze umane e sociali nelle sfide globali che ci attendono?

<b>2018</b>	Italy Slovenia Business forum	Italian Embassy in Slovenia	Ljubljana	13 Feb 2018	Distributed science in Italy: the role of University as a catalyst for science, technology and society
	Energia e Ambiente – Convegno AEIT 2018	AEIT Trieste	Trieste	11 May 2018	Energia e Ambiente Cosa possiamo fare oggi?
	Elektromobility – University of Tarnow	University of Tarnow	Tarnow (PL)	18 May 2018	The planet in 2030 and beyond: the effect of digitalization and decarbonization
	Mappe del futuro - Tra immaginazione e realtà: Dialoghi fra discipline 2018 / 2019	Stazione Rogers, Trieste	Trieste	10 June 2018	Terra 2030 e oltre: digitalizzazione e decarbonizzazione
	Conference on Processes and Procedures of Accreditation and Quality Self-Assessment in Higher Education	University of Hanoi	Hanoi (Vietnam)	29 July 2018	An overview of the European Standards and Guidelines (ESG 2015): a framework for Quality Assurance in Higher Education
	XVIII International Conference on Science, Arts and Culture: transnational cooperation in cultural heritage science	ICTP	Losinj, CRO	24 Sept.. 2018	Science and Higher Education in an international context: the role of the University of Trieste
	Multiscale Materials Modeling 2018	Osaka University	Osaka (Japan)	29 Sept 2018	In silico design of self – assembly nanostructured polymer systems by multiscale molecular modeling.
<b>2019</b>	La società sostenibile del futuro: il ruolo dell'ingegneria chimica	AIDIC - GRICU	Roma	29 Jan 2019	L'ingegneria chimica e il suo ruolo nella transizione energetica
	EMUNI conference: Recognition of Higher Education Qualifications.	EMUNI	Barcellona (S)	12 April 2019	Recognition of foreign qualifications as a tool for increased mobility, youth employability and regional integration in the Mediterranean
	Inaugurazione dell'anno accademico 2019-20	Universidad Católica Santo Toribio de Mogrovejo,	Chiclayo (Perù)	23 April 2019	Reflexiones sobre el futuro que nos espera: envejecimiento, nuevos oficios y desarrollo tecnológico
	Festival dello Sviluppo Sostenibile	TWAS	Trieste	14 May 2019	Lavori del futuro ... legati alla sostenibilità
	Evento CORICHEM	Corichem	Vicenza	8 giugno 2019	Riflessioni sul futuro che ci attende: invecchiamento, nuovi mestieri, sviluppo tecnologico
	University of Tarnow	University of Tarnow	Tarnow	26 April 2019	In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling
	Congresso nazionale del gruppo ricercatori d ingegneria chimica	GRICU	Mondello (PA)	3 Jul 2019	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	Malnisio Science Festival	Pordenone Turismo	Malnisio (PN)	5 Oct. 2019	Digitalizzazione e creatività: armonia o ostilità?
	Chinese Academy of Science	CAS	Beijing (Cina)	30 Oct. 2019	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	Chinese Academy of Science	University of Tsinghua	Beijing (Cina)	1 Nov 2019	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	Chinese Academy of Science	Politecnico pechino	Beijing (Cina)	2 Nov 2019	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems
	Energia e Clima: sfide, opportunità, scuola lavoro	AIET	Udine	22 Nov 2019	La grande sfida dell'energia: come evitare la tempesta perfetta