

CURRICULUM VITÆ

Gianluca Del Frate

Personal Details

Birth date and place: August 01, 1989, Lucca, Italy

Nationality: Italian

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Current Position

PhD Student

SMART@SNS Laboratory

Scuola Normale Superiore, Piazza dei Cavalieri, 7 - 56126

Research Interests

- Force fields development for classical Molecular Dynamics simulations
- Structural and dynamical properties of chemical probes in condensed phases
- Molecular modeling and simulations of biochemical systems
- Virtual screening of potential lead molecules

Education

- Date November 2014 - present
- Name of education institute Scuola Normale Superiore, Pisa (Italy)
- Title of activity PhD Student.
PhD Program: *Methods and Models for Molecular Sciences*
Subject: Computational Chemistry
Supervisors: Prof. Vincenzo Barone, Dr. Giordano Mancini

- Date December 2013
- Name of education institute Department of Pharmacy, University of Pisa (Italy)
- Title of qualification achieved State Examination for Professional Qualification

- Dates (from – to) October 2008 - October 2013
- Name of education institute Department of Pharmacy, University of Pisa (Italy)
- Title of qualification achieved MD in Chemistry and Pharmaceutical Technology
Marks: 110/110 *summa cum laude*.
Supervisors: Prof. T. Tuccinardi, Prof. A. Martinelli

- Date September 2010
- Name of education institute Italian Association for Informatics and computer calculation (AICA)
- Title of qualification achieved European Computer Driving License (ECDL)

- Date 2003 - 2008
- Name of education institute High School, Liceo Scientifico Ettore Majorana, Capannori, Lucca, Italy
- Title of qualification achieved High school diploma

Work Experience

- Dates (from – to) May 2014 - October 2014
 - Name and address of employer A.C.R.A.F. Angelini S.p.a., Piazzale della Stazione - 00040 S. Palomba - Pomezia (Roma) - Italia. www.angelini.it
 - Type of business or sector Pharmaceutical Industries, Research and Development
 - Occupation or position held Computational Chemistry Laboratory, Internship
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- Dates (from – to) October 2013 - 30 June 2014
 - Name and address of employer Scuola Superiore Liceo Scientifico Majorana | Istituto Tecnico Benedetti, ISS Piana di Lucca - Via Roma, 121 – Porcari (LU)
 - Type of business or sector High School
 - Occupation or position held Chemistry Lab Teacher

Personal Skills and Competences

- Mother Tongue Italian
- Other Languages English (Level B2, certified by Centro Linguistico Interdipartimentale, CLI, Pisa)
- Computer Science
- Operating systems: Linux and Windows operating systems
 - MS Office, LibreOffice, LaTeX
 - Pipeline/data flows development (KNIME)
 - Programming languages: Python, Fortran 77/90, Shell scripting
- Chemistry
- Computational Chemistry: classical and *ab initio* Molecular Dynamics (Gromacs, Amber, CP2K), Quantum chemistry (Gaussian), Docking (GOLD, Glide, DOCK, AUTODOCK), Molecular visualizers (Chimera, VMD, GaussView), Molecular Modeling and Drug Discovery (Omega, Phase, ROCS)
 - Synthetic and organic chemistry
 - Technologies used in pharmaceutical formulations

Publications

A. Salvadori, [G. Del Frate](#), M. Pagliai, G. Mancini, V. Barone. Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data. *Int. J. Quantum Chem.*, 2016, **116**: 1731–1746. DOI: 10.1002/qua.25207

[G. Del Frate](#), F. Bellina, G. Mancini, G. Marianetti, P. Minei, A. Pucci, V. Barone. Tuning of dye optical properties by environmental effects: a QM/MM and experimental study. *Phys. Chem. Chem. Phys.*, 2016, **18**, 9724-9733. DOI: 10.1039/C6CP00841K

C. Granchi, A. Capecchi, [G. Del Frate](#), A. Martinelli, M. Macchia, F. Minutolo, T. Tuccinardi. Development and Validation of a Docking-Based Virtual Screening Platform for the Identification of New Lactate Dehydrogenase Inhibitors. *Molecules*, 2015, **20**, 8772-8790; DOI: 10.3390/molecules20058772

Schools and Conferences

IV Congresso Nazionale delle Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, Scuola Normale Superiore, Pisa, October 3-5, 2016.

Poster presentation: "Computational Investigations on the Structural and Optical Properties of Fluorophores within a Sunlight Harvesting Device".

X European Workshop in Drug Design, Siena, Certosa di Pontignano, May 17-22, 2015.

Other Information

Hobbies: Music, playing the guitar, travels, sport activities, cinema.

Driving Licence.

November, 2016