Gianfranco Bocchinfuso was born in Cosenza (Italy) the October 18, 1970. He graduated in Industrial Chemistry in 1995 (summa cum laude) and, in 1999 he received the PhD degree in Chemistry at University of Rome La Sapienza.

He worked as researcher at the Chemistry Department in the Flight Experimental Centre of the Italian Air Force (Pratica di Mare Airport – Pomezia (RM)) and then as Laboratory Chief in the 6th Control Laboratory of the Italian Air Force in Trapani.

Since 2002 he works as a Researcher (permanent position) at the University of Rome Tor Vergata. At present, the main scientific interest of Gianfranco Bocchinfuso is the modeling of the structural properties of biological molecules, by means of a combined approach of molecular dynamics simulations and spectroscopic techniques. In particular, his work is focused on:

- antimicrobial peptides, in homogeneous and heterogeneous solutions, to clarify their mechanism of action and also other peculiar features that make these molecules promising materials;

- modified carbohydrates to be used in the formulation of tablets for drug release; his activity in this field is the evaluation of the structural perturbation induced by the introduction of functional chemical groups;

- protein mutants involved in different pathologies, to evaluate the perturbation induced by mutations on the enzyme structure and activity;

Further scientific interests concern the design of chemoreceptor molecules for pesticides and food toxins, the physico-chemical characterization of materials used in artworks, and, more recently, the QM investigation of molecules useful for OLED production.

The results of these researches are resumed in more than 100 works comprising papers on international journals, chapters in books, and congress proceedings, furthermore, they have been presented in many national and international congresses (posters and oral presentations, also as invited speaker).

Grants and Awards:

-2013: Italian SuperComputing Resource Allocation – (ISCRA Award -Class C, 1500000 h/cpu) from CINECA for the project "Alternative regulatory mechanisms of the tyrosine phosphatase protein SHP-2 investigated by means of molecular dynamics simulations." HP10CSICD5 (PI)

-2013: from EU. FP7—OCEAN—2013: Sensing toxicants in Marine waters makes Sense using biosensors-SMS (Project Number 613844), (Unit Member)

-2013 Italian SuperComputing Resource Allocation – (ISCRA Award Class C, 50000 h/cpu) from CINECA for the project "Molecular Dynamics techniques applied to the interaction of Antimicrobial Peptides and Lipopolysaccharides" HP10CDZNA9

- 2012: Paper of the week from "The Journal of Biological Chemistry" for the paper Martinelli S. et al. Counteracting effects on the allosteric control of SHP2's function drive selection of the recurrent Tyr62Asp and Tyr63Cys substitutions in Noonan syndrome. J Biol Chem. 2012; 287: 27066-27077

- 2012: Italian SuperComputing Resource Allocation – (ISCRA) Award (Class C, 250000 h/cpu) from CINECA for the project "Peptide-membrane interactions investigated by means of Molecular Dynamics simulations" HP10CA881J (PI)

- 2012: Standard HPC Grant (100000 h/cpu) from CASPUR for the project "Enhanced Sampling in Molecular Dynamics Simulations of biological system" (PI)

- 2012: Joint Projects for the exchange of researchers within the Executive Programme of Scientific and Technological Cooperation between Italian Republic and Republic of India. supported by the Italian Ministry of Foreign Affairs

- 2011: Best paper Awards 2011 of the Journal of Peptide Science for the paper: G. Bocchinfuso G. et al. Different mechanisms of action of antimicrobial peptides:insights from fluorescence spectroscopy experiments and molecular dynamics simulations. J.Pept.Sci. J. Pept. Sci. 2009; 15: 550–558.

-2011: Standard HPC Grant (80000 h/cpu) from CASPUR for the project "In-silico obtaining of thermodynamic parameters in complex systems of biological interest." (PI);

- 2010: Honorable Mentions from the European Peptide Society, Copennhagen (Denmark) 2010 for the poster: Effect of helix kink on the activity and selectivity of an antimicrobial peptide;

- 2010: Standard HPC Grant (80000 h/cpu) from CASPUR for the project "Coarsegrained and metadynamics simulations to study biological molecules"; (PI)

- 2009: Standard HPC Grant (20000 h/cpu) from CASPUR for the project "Molecules in Action: Simulations of the lipid bilayer permeabilization by antimicrobial peptide aggregates"; (PI)

- 2008: PRIN-2008 "Charge transport in membrane systems controlled by polypeptide molecules and applications thereof" supported by the Italian Ministry of University and Research;

- 2007: Bilateral project Italy/South-Korea "Natural peptides and synthetic analogs as novel antibiotic drugs" ("Progetto di grande rilevanza") supported by the Italian Ministry of Foreign Affairs;

- 2007: "Bando B-2007" grant (15000 h/cpu) from CASPUR for the project "Study of the interaction between the antimicrobial peptide PMAP23 and membrane model using molecular dynamics simulations"; (PI)

- 2006: PRIN-2006 "Inclusion of peptides in membrane model: biological activity, charge transport and molecular sensor" supported by the Italian Ministry of University and Research;

- 2005-2006: Grant from CASPUR for the project "Molecular basis of the Noonan and Leopard Syndrome: Molecular dynamics simulations of mutants of the protein SHP-2" ("Progetti di ricerca nel campo del calcolo ad alte prestazioni 2005");

- 2004-2008: Integrated project BIOCOP (Grant No. IP-FOOD-CT-2004-06988) supported by Framework Program 6 (FP6) of EC. His activity concerned the design (in silico) of an artificial receptor able to bind organochlorine pesticides;

- 2004-2008: Project AFLARID supported by the Italian Ministry of Agriculture to design (in silico) an artificial receptor for aflatoxins;

- 2004-2006: Grant from Telethon (GGP04172) for the project "Molecular Bases of Noonan Syndrome and related disorders "

- Minor grants from the Rome Tor Vergata University.

Didactical Activity:

He has been temporary professor of many academic courses in the Rome Tor Vergata University:

2002-2010 Teacher of 'Laboratorio di Chimica Computazionale e Progettazione Molecolare' for undergraduate students (Computational Chemistry, mainly focused on Molecular Dynamics Simulations) 2003-2005 Teacher of 'Laboratorio di Programmazione' for undergraduate students (Basic lessons in informatics).

2006-2010 Teacher of 'Informatica' for undergraduate students (Basic lessons in informatics).

2005-2010 Teacher of 'Chimica Fisica per Scienze dei Beni Culturali (Mod B)' for undergratuate students. (The physical chemistry applied to the conservation of cultural heritage);

2007-2008 Teacher of 'Esercitazioni di Chimica Fisica I' for undergraduate students (Theoretical lessons and laboratory on the kinetic of the chemical reactions).

since 2008 Teacher of 'Esercitazioni di Chimica Fisica II' for undergraduate students (Theoretical lessons and laboratory on rotovibrational and electronic spectroscopies).