# CURRICULUM VITAE ET STUDIORUM

## Gennaro ESPOSITO

**Current Affiliations and Contact Data:**

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INBB (Istituto Nazionale Biostrutture e Biosistemi. A network connecting ~ 650 researchers from 24 public Universities and over 80 laboratories across the Italian academic system)
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**Positions Held**

1992 - present – Research Member of INBB (Istituto Nazionale Biostrutture e Biosistemi)
May 2025 – present – Research Professor – Science Div., NYUAD UAE
Nov. 2021- Apr. 2025 – Senior Research Scientist – Science Div., NYUAD UAE
Jan. 2014-Aug. 2021 – Visiting Professor of Chemistry – Science Div., NYUAD UAE
Sept. 2000-Aug. 2018 – Tenured Associate Professor of Applied Physics
with full Professor habilitations (Applied Physics, Biochemistry)
Udine University Medical School – Udine University, Italy
Jun. 2013-Jun. 2013 – Visiting Professor – IPR, Osaka University, Japan
May 2012-Jun. 2012 – Visiting Professor – IPR, Osaka University, Japan
Jul. 2001-Aug. 2001 – Visiting Professor – Chemistry Dept. Univ. J. Fourier, Grenoble, France
May 1990-Aug. 2000 – Tenured Researcher
Udine University Medical School – Udine University, Italy
Sept. 1982-Jan. 1990 – Industrial Laboratory Researcher, ENI-Ricerche, Monterotondo, Italy
Oct. 1980-Aug. 1982 – Chemistry Teacher, VII ITIS, Naples, Italy

**Education and Qualifications**

2016 Habilitation of full Professor in Applied Physics, Italian University Ministry
2014 Habilitation of full Professor in Biochemistry, Italian University Ministry
1979 Legal qualification of professional chemist
1979 Laurea cum laude (MSc with Honour) in Chemistry
1972-1979 Chemistry Courses at University of Naples – Italy

**Summary of Career Highlights**

- ***Awards and professional recognition*:** Gold Medal for NMR research activity – Joint German, Slovenian and Italian Magnetic Resonance Associations (2013); External competitive grants awards for ~30 years from Private Sector, Universities, Italian Government Institutions, National Institutions, European Union. Active member of several Editorial Boards, Invited Advisory Groups and Scientific Review Boards and invited Organizer of many international conferences. Invited reviewer of major scientific journals.
- ***Key achievements***: Developed NMR techniques to measure internuclear distances and dihedral angles for structural determinations. Developed isotope exchange methodology to assess protein thermodynamics at single residue resolution. Developed paramagnetic perturbation techniques to characterize accessible surface and slow-to-intermediate conformational and interaction dynamics of proteins. First published NMR protein structures produced in three different countries, namely human Epidhermal Growth Factor, first NMR structure obtained in UK (1986); human Thryroid Transcription Factor I Homeodomain, first NMR structure obtained in Italy (1993); Nb23 nanobody, first NMR structure obtained in UAE (2021).
- ***Scientific production***: Google Scholar H-index 49; ~ 6,500 citations; 181 publications (peer-reviewed articles or book chapters), first author in 32, second or penultimate author in 43, last and corresponding author in 50.

- ***Mentoriship and training***: Taught University courses of Chemistry, Physics, Physical Chemistry, Analytical chemistry, Biochemistry, Biophysics, Spectroscopy and related fields for over 30 years. Trained over 45 postdoc, PhD, MSc, BSc students.

**Selected Editorial and Advisory Boards**

Board of the Molecular Medicine PhD School (formerly Biomedical and Biotechnological Sciences) Udine University – 2000-present
Editorial Board of Nanomaterials – 2020-2023
Editorial Board of BBA (Protein and Proteomics) – 2013-present
Directive Committee of Istituto Nazionale Biostrutture Biosistemi (INBB) – 2013-2018
Advisory Board of GERAMY (Amyloid Research Project funded by German University Ministry) – 2012-2015
Editorial Board of ISRN Structural Biology – 2012-2015
Advisory Board of Italian Magnetic Resonance Discussion Group (GIDRM) – 1988-1991

**Selected Professional Memberships**

Member of Mohammed bin Rashid Academy of Scientists (MBRAS),
Category: Natural Sciences – 2021-present
Member of American Chemical Society – 2014-present
Member of Istituto Nazionale Biostrutture Biosistemi (INBB) – 1992-present
Member of Italian Magnetic Resonance Discussion Group (GIDRM) – 1988-present

**Research Grants**

Funding supported research in NMR methodology applied to biopolymers, the study of proteins such as transcription factors, extracellular matrix proteins, amyloidogenic proteins, to mention a few examples. Funding sources have included Italian public institutions such as National Research Council (CNR), University and Research Ministry, Health Ministry, private pharmaceutical industry (Italfarmaco, Cinisello Balsamo, Milan, Italy). Two European Union grants were obtained to study "reversible antibodies" in a project headed by the Swedish company Biacore and to coordinate a consortium of Italian laboratories on the characterization of amyloids and amyloidogenic proteins. In the UAE, seed funding was obtained from NYUAD and ADEK to set up the NMR group and to study the amyloid inhibition of topologically non-trivial metal-organic complexes.
List of funding sources:
ITALFARMACO spa, 1993, 1995
CNR N. 94.00268.CT14, 1994
CNR N. 94.00427.CT12, 1994
CNR N. 96.03069.CT04, 1996
CNR N. 98.00445.CT04, 1998
CNR N. 99.02468.CT04, 1999
MURST (COFIN) N. 9805198429, 1998-1999
EU Associated Contract BIO4-CT98-0502, 1998-2000
Italian Ministry of Health Contract N. ICS 030.4/RA00.57 2001-2004
MIUR (PRIN) N. 2003051399, 2004-2005 (as National Coordinator)
MIUR (PRIN) N. 2006058958, 2007-2008
MIUR (PRIN) N. 20083ERXWS 2009-2010
MIUR (FIRB) N. RBNE03PX83_004, 2005-2007 (as INBB Consortium Coordinator)
EU STREP project N.037625 FP6-2005-LIFESCIHEALTH-6, 2006-2009 (as INBB Consortium Coordinator)
MIUR (FIRB) N. RBRNE07BMCT_003, 2008-2011 (as Joint Investigator - Udine unit)
MIUR (FIRB) N. RBFR109EOS_003, 2012-2015 (as Joint Investigator – Udine unit)
MIUR (PRIN) N. 2012A7LMS3 2013-2015 (as National Coordinator)
NYUAD research grant 2014

NYUAD research grant 2015-2017
ADEK project 2019-2020
NYUAD research grant 2018-2021

(CNR = National Research Council; MURST, MIUR = Italian Education, University and Research Ministry; EU = European Union; PRIN, COFIN, FIRB, STREP = research project specific funding schemes)

**International Scientific and Professional Experience**

Prof. Esposito has a large scientific and professional network because of the numerous opportunities of scientific contacts and collaborations he had throughout his career. Besides the activity in Italian laboratories, in particular at National Research Council (CNR) in Milan and at the Universities of Pavia, Verona, Florence, Naples, Catania, Palermo and Rome, a remarkable amount of his activity took place abroad. In addition to frequent work sessions at the European instrumental facilities in Grenoble (F), Diamond (UK), Utrecht (NL), Lubljana (SLO), Prof. Esposito had the opportunity of spending abroad long time for research and teaching. In the following the most significant periods are listed.

- June 1983 – December 1983, visiting scientist, NMR laboratory, Biochemistry Department, Oxford University, UK
- March 1985 – September 1986, research assistant, NMR laboratory, Biochemistry Department, Oxford University, UK
- July 1987 – December 1987, research assistant, NMR laboratory, School of Pharmacy, London University, UK
- August 1993 – August 1994, visiting NATO-CNR fellow, NMR laboratory, Lausanne University, Lausanne, Switzerland
- July 2001 – September 2001, visiting professor, LEDDS (Laboratoire d'Etudes Dynamiques et Structurales de la Sélectivité), J. Fourier University – Grenoble, France
- May 2012 – June 2012, June 2013 visiting professor, Institute for Protein Research, Osaka University, Osaka, Japan
- January 2014 – December 2014, visiting professor of Chemistry, NYUAD, Abu Dhabi, UAE (on sabbatical leave from Udine University)
- January 2015 – August 2017, visiting professor of Chemistry, NYUAD, Abu Dhabi, UAE (Spring term leave granted by Udine University)
- September 2018 – August 2021, visiting professor of Chemistry, NYUAD, Abu Dhabi, UAE (resident after retirement from Udine University)

**Research Accomplishments**

i) first NMR-based protein structures obtained respectively in an English, an Italian and an Emirati laboratory
ii) interatomic distance measurements for NMR structural determinations
iii) determination of exposed protein surface by paramagnetic mapping
iv) studies of DNA binding domains of transcription factors and p53
v) measurement of coupling constants from TOCSY spectra intensities
vi) studies of amyloidogenic proteins and their interactions (in particular with small molecules, nanoparticles and nanobodies)
vii) protein folding and unfolding by isotopic exchange
viii) functional mobility in small heat-shock proteins and diffusion studies
ix) equilibrium and non-equilibrium paramagnetic perturbation to map surface accessibility and slow-to-intermediate exchange events in proteins
x) interaction between nanobodies and SARS-CoV2 Nsp9 for antiviral design

**Broad Areas of Expertise**

***General subjects and specific topics of the scientific production***

1. Conformational characterization of amino acid neurotransmitters, and other nervous system effectors by NMR spectroscopy and by molecular mechanics calculations
2. NMR spectroscopy of synthetic oligopeptides and derivatives thereof, and organic molecules in general. NMR, ESR and small angle X-ray scattering of micelle systems
3. NMR structural studies of epidermal growth factor and alamethicin. Characterization of immunoactive natural or modified peptides (immunodominant repeat of circumsporozoite protein, retro-inverso peptides)
4. Characterization of silylated glass coating and functionalized chromatographic stationary phases, by means of silicon NMR spectroscopy in solution and solid state
5. NMR theory and biophysical methodology: paramagnetic perturbation of NMR spectra of biopolymers to determine exposed molecular surface; inter-proton separations from homo and hetero-nuclear correlation spectra; strong coupling effects in HSQC spectra; scalar coupling determination from NMR TOCSY; reconstruction of NMR data by modified self-correlation functions and linear prediction; applications of pulsed field gradients for coherence selection; selective NOESY optimization; non-equilibrium paramagnetic perturbation of protein NMR spectra for structural and dynamic determinations; geometry and force field simplification for conformational calculations; applications of Poisson-Boltzmann equation and generalized Born model for electrostatic contributions in biopolymer modeling; continuum limit simulations of molecular mechanics and dynamics; configurational entropy assessment; evaluation of thermodynamic parameters from isotope exchange experiments
6. Structural and functional NMR and Molecular Dynamics (MD) characterization of biopolymers: antitumoral rutenium oligonucleotide complexes, transcription factor oligonucleotide ligands; retro-inverso analogue of the immunodominant region from foot-and-mouth disease virus; scaffold of template assembled synthetic proteins (TASP); pertussis toxin multiple antigen peptide (MAP); antimicrobial peptide PMAP23; regio-selectively addressable cyclic peptides; phosphorylated metabolites during muscle contraction by $^{31}$P NMR; murine HSP25 (25 kDa heat shock protein); thyroid transcription 1 (TTF1) homeodomain; Pax-8 Paired Box domain; trimeric C1q-like domain of EMILIN1; C-terminal fragment of tau protein; NMR and mass spectrometry metabolomics; determination of phosphorylation sites by mass spectrometry; diffusion NMR measurements for cirrhosis diagnosis; human retinol binding protein; p53 DNA binding domain.
7. Structure and interaction of amyloidogenic proteins: β2-microglobulin and variants thereof; apolipoprotein A-I; amyloidogenic mutants of human lysozyme; Aβpeptide derivatives; acylphosphatase from *E. coli* and *S. sulfataricus*; interaction of amyloidogenic proteins with molecular chaperones, αB-crystallin, tetracyclins, gold nanoparticles, VHH domains from single-chain antibodies (nanobodies); supramolecular complexes; characterization of exopolysaccharides; heart-transplant-related metabolomics; isolated nanobody structure; interaction of nanobodies and SARS-CoV-2 Nsp9.

***General areas of current interest***

1. *C. elegans* metabolomics and functional biochemistry
2. Structural and functional characterization of biomolecules by NMR spectroscopy, in particular for amyloidogenic proteins and their interactions, and for nanobodies
3. Theory and methodology of NMR spectroscopy
4. Protein folding and misfolding. Applications of isotopic exchange and NMR relaxation to protein folding studies
5. NMR and mass spectrometry for *in vitro*, *in situ* and *in vivo* metabolomics
6. Conformational analysis of biopolymers by molecular mechanics and dynamics
7. Mass spectrometry, main applications in biophysics and proteomics; QCMD

**University Teaching**

- from 1990 to 2018 – Term courses of Physics, Chemistry, Biophysics, Physical Chemistry, Nuclear Magnetic Resonance Imaging for Medical School, Medical Radio-diagnostics Specialty School, Biotechnology Degree, Physiotherapy Degree, Radiology Technician Degree, Biomedical and Biotechnological Sciences PhD School – Udine University, Italy;
- from 2014 to 2021 – Term courses of NMR Spectroscopy, Analytical Chemistry, Biochemistry, Physical Chemistry Lab. for Chemistry Program – New York University Abu Dhabi, UAE

**Teaching for Post-graduate Training Schools**

-Nuclear Magnetic Resonance School, Siena University, Siena, 1988
-Chemical Synthesis School - Milan University, Milan, 1989
-IV Protein Science National School, Pontignano (Siena), 1990
- Nuclear Magnetic Resonance School, Siena University, Siena, 1990
-V Protein Science National School, Pontignano (Siena), 1991
- Nuclear Magnetic Resonance School, GDRM, Pontignano (Siena), 1991
-Courses on Molecular Genetics, ISAS and ICGEB, Trieste, 1992
-Advanced COMETT Course on Protein NMR, UETP-Tuscany and Siena University, Pontignano (Siena), 1992
- Nuclear Magnetic Resonance School, GDRM and Parma University, Parma, 1993
- Nuclear Magnetic Resonance School, GDRM and Verona University, Verona, 2001;
- Nuclear Magnetic Resonance School, GDRM and Turin University, Turin, 2006, 2010, 2012, 2016, 2018

**Supervising Activity**

20 postdoctoral researchers, 10 PhD students, 18 BSc or MSc students

**Selected Conference organization**

Annual conference of Italian Nuclear Magnetic Resonance Society (1987, Rome, Italy; 1991, Trieste, Italy).
1st Italian-Japanese workshop 'Dialysis-related amyloidosis: from molecular mechanisms to therapies' (2004, Pavia, Italy).
XII International Symposium on Amyloidosis (2010, Rome, Italy).
NYUAD Chemistry Faculty Meetings – Protein Amyloid Degeneration: still an open challenge (2014, Abu Dhabi, UAE)
Towards a cure for amyloid diseases: a successful example of precision and translational medicine (2019, Pavia, Italy)