

Gennaro ESPOSITO  
Naples (ITALY), September 19<sup>th</sup> 1953

#### Education

1972-1979 Chemistry Courses at University of Naples – Italy

1979 Laurea cum laude (MSc with Honour) in Chemistry

#### Professional Qualification

1979 Legal qualification of professional chemist

2014 National habilitation of full professorship in Biochemistry

2016 National habilitation of full professorship in Applied Physics

#### Present position:

Visiting Professor of Chemistry

Science and Mathematics Division – New York University Abu Dhabi

NYUAD Campus, Saadiyat Island, ERB, Abu Dhabi, UAE

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Homepage: <http://nyuad.nyu.edu/en/research/faculty-research/nmr-group.html>

#### Previous Positions

Sept. 2000-Aug.2018 - Associate Professor of Applied Physics – DMIF, Udine University, Italy

Jan. 2014-Aug. 2017 – Visiting Research Professor – ScienceDiv., NYUAD UAE

May 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 – Permanent Researcher – DSTB, Udine University, Italy

Sept. 1982-Jan. 1990 – Industrial Researcher- Physical Chemistry, ENI-Ricerche, Monterotondo, Italy

Oct. 1980-Aug. 1982 – Chemistry Teacher, VII ITIS, Naples, Italy

#### Highlights

- *Scientific production*: out of 148 *in-extenso* publications (articles or book chapters), first author in 30 (6 over last 15 years) , second author in 17, last and corresponding author in 39 (35 over the last 15 years). Google Scholar H-index 35 (21 since 2013) – more than 4,000 citations (about 1,400 since 2013); i10-index 89 (46 since 2013)
- *Activity in international laboratories*: overall more than 5 years, with 32 months in UK, 27 months in UAE, 12 months in Switzerland, 2 months in France and 2 months in Japan
- *National funding*: 15 funded projects, 11 as principal investigator of local or multicenter (INBB consortium) research-unit (RU), 2 as national co-ordinator, 2 as sub-project or collaborating laboratory responsible –overall national funding 717,000 Euros, i.e. about 860,000 US\$ (only for his own RU )
- *International funding*: 2 projects funded by EU as principal investigator of local or multicenter (INBB consortium) RU, 2 New York University Abu Dhabi (NYUAD) research grants as laboratory head – overall international funding 533,000 Euros, i.e. about 638,500 US\$ (only for his own RU )

#### Awards

- Gold Medal for NMR research activity in the joint meeting of the German, Slovenian and Italian Magnetic Resonance Associations (2013)

### **Memberships and Editorial Boards**

Member of Italian Magnetic Resonance Discussion Group (GIDRM) Advisory Board – 1988-1991  
Member of Directive Committee of Istituto Nazionale di Biofisica e Biosistemi (INBB) – 2013 – 2018  
Member of GERAMY (German Amyloid) Advisory Board – 2012–2015  
Member of the Editorial Board of BBA (Protein and Proteomics) – 2013–present  
Member of the Editorial Board of ISRN Structural Biology – 2012–2015  
Member of American Chemical Society – 2014–present

### **Invited presentations and seminars**

23 presentations as invited speaker in national and international conferences. 12 invited seminars.

### **Degree and PhD thesis supervising**

18 Degree theses (BSc or MSc) theses directed or co-directed, 8 PhD theses directed.

### **International scientific and professional experience**

G. Esposito has a vast scientific and professional experience because of the numerous opportunities of scientific contacts and collaborations he had along his carrier. 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), G. 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 scientist as NATO-CNR, NMR laboratory, Lausanne University, Lausanne, Switzerland
- July 2001 – September 2001, temporary professorship, LEDDS (Laboratoire d'Etudes Dynamiques et Structurales de la Sélectivité), J. Fourier University – Grenoble, France
- May 2012 – June 2012, June 2013 visiting associate 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)

### **Conference organization**

Annual conference of Italian Nuclear Magnetic Resonance Society (1987, Rome, Italy; 1991, Trieste, Italy).

1<sup>st</sup> 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)

### **Research grants**

All funding applications were based on original research projects concerning, for instance, the NMR methodology applied to biopolymers, the study of transcription factors, extracellular matrix proteins, amyloidogenic proteins, to mention the most relevant subjects. The successful applications were typically addressed to Italian public institutions such as National Research Council (CNR), University and Research Ministry, Health Ministry, and in a couple of cases also a private pharmaceutical industry (Italfarmaco, Cinisello Balsamo, Milan, Italy). Particularly rewarding were the two grants obtained from European Union. A first time, in 1998, G. Esposito’s laboratory was funded in a project on reversible antibodies headed by the Swedish company Biacore. Subsequently, in 2006, the Udine research unit co-ordinated a consortium of Italian laboratories that was funded in the EURAMY project, a proposal addressing the characterization of amyloids and amyloidogenic proteins. Lastly, from 2014 to 2017, G. Esposito received fundings from NYUAD to set up the NMR group, hire postdocs, support visiting collaborators and thesis students, besides consumable supplies (overall some 300,000 US\$).

In the following the list is reported of the fundings received as research-unit principal investigator (unless otherwise indicated). The overall net amount of grants obtained for Udine and Abu Dhabi laboratories is about 1,200,000 Euros, i.e. about 1,440,000 US\$

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

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

### **Scientific activity**

The scientific activity of G. Esposito is hereby described in terms of general subjects and specific topics along which his work has been developing, with a final listing of the areas that are currently pursued.

Among the scientific results G. Esposito obtained or contributed to, it is worth mentioning (the number in parenthesis indicates the relative publication, according to the appended scientific production list):

- i) first protein structure by NMR obtained by an Italian laboratory (30, 44)
- ii) first protein structure by NMR obtained by an English laboratory (6)
- iii) interatomic distance measurements for NMR structural determinations (10, 21)
- iv) determination of exposed protein surface by paramagnetic mapping (18, 20, 25, 27, 32, 49, 63)
- v) study of amyloidogenic proteins and intermediates (58, 65, 69, 72, 83, 88, 98, 101, 122) e di loro interattori (79, 104, 120, 130, 135, 136)
- vi) protein folding and unfolding by isotopic exchange (50, 110, 112)
- vii) functional mobility in small heat-shock proteins (34, 57)

#### *General subjects and specific topics*

1. Conformational characterisation of aminoacid 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 alamthicin. Characterisation of immunoactive natural or modified peptides (immunodominant repeat of circumsporozoite protein, retro-inverso peptides)
4. Characterisation of silylated glass coating and functionalised 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; interproton separations from homo and heteronuclear 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; 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 MD characterization of biopolymers (immunodominant repeat of circumsporozoite protein; retro-inverso peptides; 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; regioselectively addressable cyclic peptides; phosphorylated metabolites during muscle contraction by  $^{31}\text{P}$  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 metabolomics; determination of phosphorylation sites by mass spectrometry; diffusion NMR measurements for clinical diagnostics; human retinol binding protein

7. Structure and interaction of amyloidogenic proteins:  $\alpha$ 2-microglobulin and variants thereof; apolipoprotein A-I; human lysozyme amyloidogenic mutants;  $\text{A}\beta$  peptide derivatives; acylphosphatase from *E. coli* and *S. sulfataricus*; interaction of amyloidogenic proteins with molecular chaperones,  $\alpha$ -crystallin, gold nanoparticles, VHH domains from single-chain antibodies (nanobodies); supramolecular complexes

*General areas of current interest*

- Structural and functional characterization of biomolecules by NMR spectroscopy, in particular for amyloidogenic proteins and their interactions. Theory and methodology of NMR spectroscopy
- Protein folding and misfolding. Applications of isotopic exchange and NMR relaxation to protein folding studies
- NMR and mass spectrometry metabolomics
- Conformational analysis of biopolymers by molecular mechanics and dynamics
- Mass spectrometry, main applications in biophysics and proteomics
- Biophysical applications of FT-IR, CD, fluorescence and UV spectroscopy