



Prof. Petre T. FRANGOPOL
(1933 – 2020)



IN MEMORIAM PROF. PETRE T. FRANGOPOL
(1933 – 2020)

Ana-Nicoleta Bondar^{a,b}

^aUniversity of Bucharest, Faculty of Physics, Str. Atomîștilor 405, Bucharest-Măgurele 077125, Roumania

^bInstitute for Neuroscience and Medicine and Institute for Advanced Simulations (IAS-5/INM-9), Computational Biomedicine, Forschungszentrum Jülich, 52425 Jülich, Germany

Petre T. Frangopol died at his home in Bucharest in December 2020. Born in May 1933 in Constanța, a beautiful city by the Black Sea, Prof. Frangopol was a pioneer of biophysics in Roumania, a passionate advocate of excellence and integrity in scientific research and University teaching, and an inspiring mentor for his younger colleagues.

Petre Frangopol had a tremendous influence on Roumanian science: His leadership and research were instrumental to establishing the laboratory of organic marker compounds at the Institute of Atomic Physics (IFA) Magurele, with grants awarded in international competitions (AIEA Vienna, Copernicus, Erasmus, The Soros Foundation) –the medical physics and biophysics sections at the University of Iași, with funding from the World Bank –the first implementation in Roumania of the Science Citation Index from the Institute of Scientific Information USA, with funding from the World Bank, the laboratory of atomic force microscopy and thin Langmuir films at the Babeș-Bolyai University. Furthermore, Prof. Frangopol's contributions were essential for establishing at IFA a center for the production of isotopes, and a line to develop radiopharmaceutics.

Petre Frangopol published numerous research papers – according to the records at the Roumanian Academy of Science, where he was a corresponding member for the Chemistry Section. Prof. Frangopol published about 225 scientific papers. He was extremely supportive of the Roumanian journals, in which about 130 of his research papers were published. Indeed, just one issue of *Review Roumaine de Biochimie* from 1991 contains six papers from the Frangopol laboratory, on topics that remained of interest 30 years later –liquid membranes as mimics of biological taste sensors, ion channel gating, interactions between local anesthetics and membranes.

The broad research interests that Petre Frangopol developed during his long academic career included technological chemistry – he established in Roumania the preparation of several radioisotopes, radiobiology, archeometry, biophysics, history of Roumanian science, scientometry and science policy.

In 1985's, Petre Frangopol started what became an extremely productive activity as an editor. He edited the *Seminars in Biophysics* series until 1990 then, from 1992 to 1997, *Current Topics in Biophysics*, which included another topic that remained highly relevant today: biosensors. From 2012 to 2015, Petre Frangopol was the editor of *Revista de Politica Științei și Scientometrie*; throughout the years, Petre Frangopol published tens of articles in *România Liberă* on subjects pertaining to research and teaching in Roumania.

Most recently, Petre Frangopol was editor for an encyclopedic volume on the "Istoria chimiei românești" ("The history of roumanian chemistry"), commissioned by the Roumanian Academy of Sciences. This volume, published in 2018, has 31 chapters that cover all branches of the Roumanian chemistry, from basic science to technological applications. Starting with 2002, Petre Frangopol published and coordinated the series of books on "Mediocritate și Excelență. O radiologie a științei și învățământului în România" ("Mediocrity and Excellence. A radiology of science and teaching in Roumania"). The 7th volume of this series, published at Casa Cărții de Știință in 2019, contains a chapter on the anniversary session, in the Aula of the Roumanian Academy

* Corresponding author: ana.bondar@unibuc.ro; nbondar@fizica.unibuc.ro

of Sciences, on the occasion of the 85th Birthday of Prof. Petre T. Frangopol (the photograph on the cover of this *In Memoriam* Issue of *Revue Roumaine de Chimie* was taken on that occasion). The contributions in this chapter, by fellow Roumanian Academy members, highlight the tremendous influence that Petre Frangopol had on the Roumanian scientific landscape, and the profound appreciation he received for his works.

Petre Frangopol's concluding words to this 7th volume, "Valoarea unui om rezidă în ceea ce dă el și nu în ceea ce este capabil să primească" (A man's value is in what he gives, not in what he is capable of receiving) speak for how Petre Frangopol understood to dedicate his life to science. The presentation Petre Frangopol gave to the audience in the Academy Aula ended with a confession of how deeply grateful he felt to his wife, friend and collaborator Dr. Mioara Frangopol, who was with him for 58 years until her death.

This special issue dedicated to the memory of Prof. Petre T. Frangopol showcases research by distinguished colleagues and their collaborators. The distinguished authors of the papers included in the special *In Memoriam* issue are former collaborators, co-workers, or colleagues of Petre T. Frangopol, or they have visited the laboratory of Petre T. Frangopol. Their contributions, which made possible this special *In Memoriam* issue, reflect the broad interests of Petre T. Frangopol in modern biophysics and biophysical chemistry.

Mocanu and colleagues contribute an article on experimental investigations of the interaction between the local anesthetic procaine and a lipid bilayer. Thermodynamic studies are combined with atomic force microscopy to explore the depth at which procaine molecules insert themselves into the membrane, and to present a mechanism that explains how drug penetration occurs. The response of the membrane to procaine binding includes enhanced membrane fluidity. An increased lateral surface could impact ion channels that are sensitive to lateral pressure.

Benga reviews historical research, and fundamental aspects of electron spin resonance (ESR) studies in biology and of the spin label methodology. As a close collaborator of Petre Frangopol at the Babes-Bolyai University of Cluj Napoca, Benga discusses how compounds needed for ESR studies were synthesized at IFA-Magurele, collaborations with the laboratories of Vasile Morariu and colleagues from Roumania and abroad, and seminal work including the discovery in a human membrane of the first water channel, later named aquaporin.

Smith, Petridis, Elkins, Nuckels, Katsaras and Smith, present an overview of microbial membranes from the perspective of the challenges for bioenergy. Key experiments and theory on the structure of the plasma membrane are reviewed, together with a discussion of recent progress on deciphering the effects of amphiphilic solvents on microbial membranes. The combined experimental and theoretical approach discussed in the review article reveals fundamental aspects of microbial membranes, and suggests strategies to optimize microbes for biofuel production.

Stone, Ray and Andricioaei present the applicability of enhanced sampling molecular dynamics scheme to studies of the association and dissociation of the trypsin-benzamidine complex. The well tempered meta-eABF method gives free energy values within 2-3kcal/mol from the experimental counterparts, and unbinding rate constant values close to those obtained from significantly longer computations. The approach presented could be used to screen protein-ligand interactions for applications in drug design.

The article by Al-Shammari and colleagues presents experiments that probe antifungal properties of zein nanoparticles with and without a load of transition metal ions. These nanoparticles are of interest at potential drug delivery systems, and findings presented in the article suggest that, when loaded with copper or chromium ions, zein nanoparticles show antifungal activities against three *Candida* strains.

Vanderweyen, Tuck and Oprisan numerical investigations to find out how a single-compartment Hodgkin-Huxley type model neuron responds to stimuli. They find the neuron's response is linear with respect to the amplitude of the stimulus, but non-linear with respect to duration. The amplitude and duration of the stimulus determine the amount of injected charge, which largely governs transient changes of neurons firing periods. The shape of the stimuli influences how neurons respond.

Caiali, Moldovanu and David present reversed-phase liquid chromatography experiments using eight different mobile phases containing methanol and an aqueous component to evaluate enthalpy-entropy compensation. These studies suggest that the hydrophobicity of the alcohol in the mobile phase influences the standard enthalpy and entropy changes for the transfer of a solute from the mobile to the stationary phase.

Suciu, Lupa and Silaghi-Dumitrescu rely on computational chemistry approaches to evaluate redox isomerism in a series of palladium adducts. Structures of various compounds were subjected to energy minimizations, and energy considerations used to evaluate relative stabilities of the isomers and redox isomerism.

Karathanou and Bondar present applications of graph-based algorithms to dissect the role of hydrogen-bond networks in conformational dynamics of a model motor protein. Graph-based analyses of dynamic hydrogen-bond networks enable long-distance transient connections between remote sites of the protein to be identified, which could be used as guidance to select groups for further study with site-directed mutagenesis.

Note. Independent of this special *In Memoriam* issue hosted by the *Revue Roumaine de Chimie*, Profs. Maria Tomoaia-Cotișel and Aurora Mocanu and have organized a special *Petre T. Frangopol In Memoriam* issue hosted by *Studia Universitatis Babeș-Bolyai Chimia*, volume 3, 2021.

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