Supplement to the Special Issue on Protein Folding and Harold A. Scheraga

Mahesh Narayan¹ · **Lawrence J. Berliner²**

Accepted: 13 March 2021 / Published online: 16 March 2021

© The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2021

Please find three additional articles in tribute to Harold A. Scheraga (HAS; 1921–2020) which follow the October (2020) issue of *The Protein Journal*. As mentioned earlier, HAS initially worked on the physical properties of fibrinogen (size and shape) along with investigations in the mechanism by which thrombin cleaves fibrinogen to form the fibrin clot as earlier proteins were considered to be rigid colloidal particles. He refined these interactions significantly over the years and the design of several anticoagulant drugs are based on these findings.

HAS later became involved in defining noncovalent interactions in the structure of RNase A. HAS was one of the first to point out and “exploit” the role of disulfide bonds in protein folding pathways in molecular detail, using RNaseA and homologs. They could trap folding intermediates and study the intermolecular interactions that led to the native structure. The review article in this installment by Narayan highlights this area. He developed both experimental and computational methodologies to understand the interactions

that guide the folding and stable folded forms of proteins very early ‘in the game.’ The codification of realistic interatomic potentials via ECEPP (Empirical Conformational Energy Program for Peptides), was a major contribution to predicting protein folding. The second article in this supplement highlights modern computational approaches. Lastly, the third article in this special issue highlights the use of several computational approaches to drug development.

We invited several former group members, collaborators, visiting scientists, acquaintances and others influenced by his work to contribute their recent discoveries. Again, we thank these authors for their contributions which exemplify the impact of HAS work to their careers and dedication to the science of protein folding.

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

✉ Mahesh Narayan
mnarayan@utep.edu

Lawrence J. Berliner
Lawrence.Berliner@du.edu

¹ The Department of Chemistry and Biochemistry, The University of Texas At El Paso, El Paso, TX 79968, USA

² The Department of Chemistry and Biochemistry, Denver University, Denver, CO 80208, USA