Harold A. Scheraga [1921–2020]: Eminent Researcher, Mentor, Teacher, Friend

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Harold Abraham Scheraga (HAS), known to many simply as Harold, passed away on August 1st, 2020; a couple of months short of his 99th birthday (Fig. 1). He was preceded in January of the same year by Miriam, his wife of ~77 years. A product of Brooklyn and upstate NY and its educational systems, he spent his graduate years at Duke simultaneously working on projectile motions (for the Manhattan project) and with Fritz London/John Edsall on Van Der Waals and hydrophobic interactions in aminoacids, peptides and proteins. Invited by Peter Debye to Cornell in 1947, HAS would spend the next 73 years (till Saturday, Aug 1 2020!) in the Baker Laboratory of Chemistry and Chemical Biology working on the structure of water, the hydrophobic effect and “the protein folding problem” among other scientific areas.

HAS had an illustrious career as a biophysicist. A contemporary of Anfinsen and Pauling, he began his adventure with proteins when they were largely unknown objects represented only as ellipsoids (or everything is a “spherical cow/billiard ball” analogy). Equally fluent in experiment and computation, he was instrumental in the discovery and characterization of the helix–coil transition in proteins, the development of the ECEPP force-field via the united residue approach, the detailing of hydration and its applications, an understanding of the role of the hydrophobic effect, the folding pathways of proteins, ab initio predictions, etc., etc., etc. (Scheraga, H. A. (2011) *Respite, Adspice, and Prospice Annual Review of Biophysics* 40:1, 1–39; Scheraga H. A. (2015) *My 65 years in protein chemistry. Quarterly reviews of biophysics*, 48(2), 117–177) (Fig. 2).

Though an atheist, HAS was a strong supporter of the Jewish cause. Whether it be working to revoke Yasser Arafat’s Nobel Peace Prize (a controversial issue), or writing the

famous Science piece with Carl Sagan, Hans Bethe and others for the release of an imprisoned Argentine scientist (<https://science.sciencemag.org/content/197/4307/938.2.long>), HAS remained the activist for the causes that he felt were just. I am not sure what his thoughts were when, in 2006, Debye himself became controversial as an alleged Nazi sympathizer. Some demanded that Debye’s Nobel Prize be revoked and his name expunged from its association with Cornell. It created quite a tumult on the Hill (actually the

Fig. 1 Prof. Harold A. Scheraga (1921–2020). Courtesy of Cornell University/Frank DiMeo

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Fig. 2 Prof. Scheraga with CCNY President Vince Boudreau (left) and CCNY Professor David Jeruzalmi (middle) in 2018 while receiving an honorary degree from The City College of New York for seven decades of research at Cornell University. Photo courtesy of Cornell University/Patrick Shanahan and CCNY

statues of the Nobel Foundation prohibit revoking a Nobel Prize).

A man of principles and ethics, he stopped accepting PhD students when he turned 70. Who knew he would march on, almost 30 years on, surviving many a former student and postdoctoral associate. He wound down his experimental group in the mid-2000's citing hassles related to Environmental Health and Safety/OSHA regulations. Nevertheless, he still retained a group of 15–22 researchers, mostly postdocs, which spoke to his funding. The last 10 years saw him completely focus on theory; the last few years confined to a wheelchair; with his last paper reading: Curvature and Torsion of Protein Main Chain as Local Order Parameters of Protein Unfolding. (June 4th 2020) *The Journal of Physical Chemistry. B*. PMID 32392067. <https://doi.org/10.1021/acs.jpcb.0c01230>. This was his 4th publication this year and there are still several in the pipeline.

Many will remember that HAS visited the Department of Chemistry and Biochemistry, UTEP in 2006. He insisted on coming in on a Monday. The uncanonical Tuesday afternoon seminar was house-full; drawing people from NMSU and around.

In memory, Dr. Nobihura Go writes from Japan: “.... when I joined his group as a postdoc from Japan 53 years ago.”....giving us insight into the time-frame HAS spanned.

And Dr. No states: “*He was the brightest lighthouse in my academic and life voyage.*”

The research that started together in 1987 was finalized with a paper last year, and I tried to deliver it to Harold in Ithaca, but the corona virus forced me to cancel the plan. It is a pity that I missed the last chance to meet him. He was a big master in protein science in the twentieth century.”

Harold was as passionate about teaching as he was about research. I have heard that he would wear a bow tie and a suit to teach his class (Protein Chemistry). In those days, respect to the student, the course, the pedagogical profession and the topic was offered sartorially among other mechanisms, such as third-decimal punctuality (always arriving a few minutes before the class hour, he would jump onto a chair and advance the clock so that he could start). Getting yelled at by him in public was another matter and had to be swallowed; nothing to complain about for it was never personal. He never held a grudge, but just conveyed his sentiments there and then smiled at you.

His discussions/debates at our group meetings on the free energy of transfer of amino acids from water to octane with colleague Prof. Ben Widom (a statistical mechanics wizard himself, National Academy of Science member and a math team lead/champ of Stuyvesant High School in New York City), or the amyloidogenic trajectories of prion-like proteins, were always logical, insightful and enthralling and entertaining.

I, for one, learned the most while in his lab; a mecca for thought and debate. The 22 papers I have co-authored with HAS and with some of the brightest undergraduates and fellow postdocs I have ever met, reflect approximately a mere 1.5% of his output. His H-index at last count was 126; quite remarkable given the fundamental work he was involved in and coupled with the fact that stalwart journals like J

Phys Chem B, Biophysical Journal, J. Mol. Biol., and the ACS flagship Biochemistry where HAS frequently published continue to only command impact factors between 2.5 and 5.....the same metric from the 1980s and 1990!

In closing, I remain indebted to this great seer, insatiable seeker, master preceptor, unparalleled perceiver and formidable Pundit of Protein Folding.

Sincerely,

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El Paso, Texas

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