

Marvin L. Vestal, in Remembrance

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Marvin L. Vestal died peacefully on August 17, 2022, at the Metrowest Hospital in Framingham, MA. He was 87 years old. One of the true giants in the field of mass spectrometry, Marvin was still innovating, still inventing, up until just 2 weeks before his death. He will be sorely missed not only by those close friends and associates who surrounded him in his last days but also by the many friends and colleagues from the mass spectrometry community at large who have learned from him, benefited from his work, and enjoyed his company over a career that spanned some 60 years.

During his long and illustrious career Marvin stayed true to one guiding principle: to drive his innovations to commercial products in furtherance of scientific research. As one old friend recently observed, Marvin sometimes likened himself to Thomas Edison in that his research was always focused on

the practical. In Marvin's mind, however, he did Edison one better: his discoveries and inventions were solidly grounded in a mathematical framework. Edison was not a mathematician.

Marvin's early life and career are well documented in both an oral history interview conducted by Mike Grayson in 2010¹ and a focus editorial in JASMS in 2011 on the occasion of his receiving the ASMS Distinguished Contribution to Mass Spectrometry award.² Born and raised in Pendleton, Indiana, Marvin received his bachelor's and master's degrees in Engineering Sciences from Purdue University. Afterward, he joined Johnston Laboratories in Lafayette Indiana, where his introduction to theoretical chemistry could hardly have been more auspicious. His first two collaborators, Henry Rosenstock and Merrill Wallenstein, had invented quasi-equilibrium theory (QET) while students of Austin Wahrhaftig and Henry Eyring. With Rosenstock, Marvin developed a coincidence time-of-flight (TOF) mass spectrometer³ and invented a secondary electron multiplier that vastly improved performance and became a standard in its day. With Wallenstein, he corrected a major problem with QET and applied the theory to what was at the time thought to be a large molecule: propane, C₃H₈.

As would become the case with other companies of which Marvin was a part, Johnston Laboratories and then Scientific Research Instrument Corporation (SRIC, the company Marvin founded with Bill Johnston, Gordon Fergusson, and Bob Jones in 1967) were major stops on any scientist's quest to acquire the latest and greatest in new analytical instrumentation in the 1960s. Their work was supported by the Air Force Aeronautical Research Laboratory and Air Force Cambridge, later the Air Force Geophysical Laboratory, with Jean Futrell and John Paulson the respective monitors. While at SRIC, Marvin built the first commercial chemical ionization source at the request of Henry M. (Hank) Fales at the National Institutes of Health (NIH).

In 1970, Marvin began a Ph.D. program in Chemical Physics at the University of Utah under the auspices of Jean Futrell and Austin Wahrhaftig. During his tenure as a graduate student, he built a crossed-beam apparatus as well as the first tandem quadrupole mass spectrometer to study photodissociation

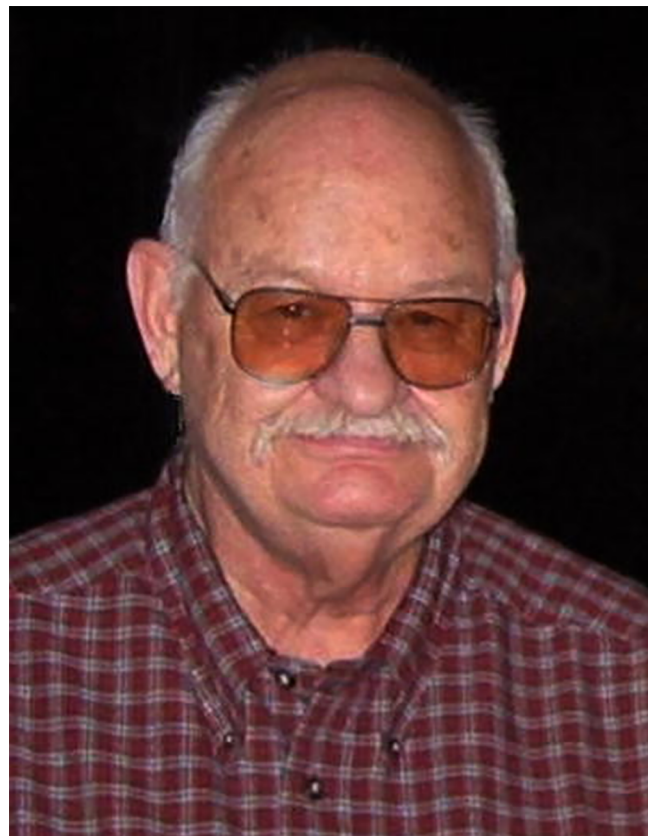


Figure 1. Marvin L. Vestal. (reprinted from ref 2, p. 949).

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mechanisms, formulated new theories of ion–molecule reactions, and expanded his network of scientific friends and collaborators.

In the middle 1970s, toward the end of his stay in Utah, Marvin began to tackle one of the knottiest problems in mass spectrometry: designing and building a successful interface between a liquid chromatograph and a mass spectrometer. For the growing field of mass spectrometry to expand into the nonvolatile and polar realms of pharmaceutical and biological chemistry, a means of connecting the two media-antithetical instruments was essential. Thermospray, which proved to be not only a way of vaporizing large molecules but of ionizing them as well, became a critical innovation in analytical chemistry in the early 1980s. Never content to rest on his laurels, Marvin made constant improvements to the instrumentation but managed along the way to pause long enough to demonstrate the power of Thermospray LC/MS for online sequencing of a peptide.^{4–6} The thermospray interface was commercialized and made available to the scientific community by Vestec, the company Marvin and his University of Houston colleagues founded in 1982.

As revolutionary as it was at the time, however, by the late 1980s the thermospray interface had given way to softer and more stable interfaces like electrospray ionization (ESI) and matrix assisted laser desorption ionization (MALDI). Seeing

the MALDI spectrum of β -galactosidase (MW 116,900) shown by Karas and Hillenkamp at the 1988 Bordeaux International Mass Spectrometry meeting, Marvin immediately sensed the potential of MALDI as an interface for a TOF mass spectrometer. He and his Vestec colleagues built the first commercial MALDI-TOF instrument in 1990.

When the company merged with PerSeptive (later Applied Biosystems Inc., ABI), Marvin moved his operations to Massachusetts and assembled a research group with a mission to address what he saw as fundamental limitations to the commercial success of MALDI-TOF: poor resolving power, imprecise mass measurement, and lack of MS/MS capability. Marvin's abilities as a theoretician to the fore, within a year he had analyzed velocity distributions to optimize focus (and thus performance) and had designed the first of a family of instruments that would incorporate the delayed extraction technique. Voyager MALDI-TOFs boasted a resolving power >10,000 and mass accuracy with <10 ppm mass errors. Once again bringing his theoretical insights to bear, Marvin next tackled the lack of sensitivity of MS/MS in TOF instruments. In analyzing and addressing the problem of metastable decay, Marvin's work brought forth a new family of TOF-TOF instruments that found application in a wide variety of research areas from proteomics, glycomics, and cell signaling to structural biology, organelle imaging, and polymer science.

In his last company, Virgin Instruments (later Simultof), which he cofounded in 2005 with his long-time collaborator and wife theoretical chemist Christina Hsieh Vestal, Marvin continued to pursue what had become his holy grail: ever greater mass resolution for TOF instruments. With the constant curiosity and eternal optimism that had characterized his entire scientific career, Marvin and co-workers continued to design and build TOF instruments that used first-principles of physics to push back the resolution frontier. And on one spectacular day in 2013, his two-story high prototype TOF instrument achieved a whopping 100,000 resolution.

Marvin was kind and generous to a fault with young scientists. Each of the authors of this remembrance recounts his or her own early encounter with Marvin as follows:

Familiar with breakdown curves Marvin had developed for methane, ethane and propane, P.J.G. timidly approached "Dr. Vestal" at the 1974 Philadelphia ASMS conference to ask where she might find published versions of the data. "Oh," he laughed, "I never bothered to publish those. If they're useful to you, feel free to put them in your thesis." But he quickly added, "On one condition." Terrified as to the nature of that condition, she worked up her courage to ask, "And what would that be?" His answer boomed out over the conference venue: "That you immediately stop calling me Dr. Vestal!"

Marvin was a great mentor to H.-Y.K. When she had just started her graduate study at the University of Houston, Marvin was developing LC/MS techniques which she found fascinating. She earnestly wanted to join Marvin's team. Although academically she was a top tier student in the Chemistry Department, Marvin immediately turned down her application, saying that no funds were available to support an additional graduate student. Having graduated from a pharmacy school with a thesis in biochemistry, her background and skills at the time were obviously not well suited to his research on instrumental and theoretical development for cutting-edge mass spectrometric techniques. After a week of contemplation, she went back and told him that she still wanted to join his team and that he did not need to support



Figure 2. Marvin installing a thermospray ion source in the Fenselau Laboratory at Johns Hopkins University ca. 1985 (courtesy of Catherine Fenselau Cotter).

her. To her surprise, this time he accepted her with a big smile and, by the way, with full support! That motivated her to work harder and complete all additional courses she felt necessary for understanding and catching up his ongoing research. To utilize her background properly, Marvin went out of his comfort zone and put her on the project to develop a peptide sequencing method using the then still evolving Thermospray LC/MS technique. This endeavor proved successful in demonstrating the capability of Thermospray LC/MS in practical analyses of biological samples. At the time, according to Marvin, she twisted his arm badly, but later he admitted he was very happy that she had and thanked her. In reality, she says, it is she who is ever grateful for his open-mindedness and for his trusting her with an opportunity to grow as a competent scientist.

S.M. met Marvin for the first time in the early 1980s while he was still a graduate student, and he continued to stay abreast of Marvin's innovative techniques as he began his professional career. His long-time collaboration with Marvin started in earnest in the 1990s when, out of the blue, Marvin asked him to join his team. Marvin had been pioneering a new type of mass spectrometer at Vestec (in Houston TX) and was joining forces with PerSeptive Biosystems (in Framingham, MA). Originally, S.M. said no: he was enjoying his career...and perhaps, he thinks, might have lapsed into a risk-averse mindset. That soon changed, as did the trajectory of his career. As many know, Marvin was not only a visionary in mass spectrometry; he was also extremely persistent and persuasive.

Marvin's life illustrated the maxim by which he lived: if you want to have an impact, you need to be first-person in action with a passion to succeed. Marvin was always first-person, showing that success comes from taking risks to drive innovation. Failure was never, ever an option for Marvin; his many scientific contributions drove science forward and changed our world. As much as we will all miss him, we are comforted by the last words he left with us, "...I will not have died. I have only gone with my dear friends and great mass spectroscopists."⁷

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- (7) "Remember Me", a popular funeral poem variously attributed to Christina Rossetti, Margaret Mead, et al.