

Obituary: Claus-Wilhelm von der Lieth (1949–2007)

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On November 16, 2007, Dr. rer. nat. Claus-Wilhelm (Willi) von der Lieth died unexpectedly, a victim of cancer, at the age of 58. He was born on June 13, 1949 in Bremervörde, Germany, studied chemistry at the Technical University of Hannover from 1969 to 1977, and received his diploma under Prof. H. Seidel with a thesis entitled *Nitrates of metals with valence I and II: preparation and vibrational spectroscopy*. Willi then pursued further studies in theoretical chemistry at the University of Heidelberg under Prof. H.-H. Eysel and received his doctoral degree in 1980 with a thesis on *Single-crystal Raman bandshape analysis of sodium nitrite: studies of order–disorder phenomena through the interpretation of the relative intensities of the internal vibrations of the nitrite ion*. In that same year Willi joined the staff of the German Cancer Research Center (DKFZ) in Heidelberg as a research scientist in the Central Spectroscopy service group initiated by Prof. E. Hecker and began the development of a computer-based spectroscopic information system for NMR, MS, and IR spectra. In 1984 Willi was a Guest Scientist at the University of Lund, Sweden, and worked



with Prof. R. E. Carter and Dr. T. Liljefors on the structure elucidation of organic molecules by force-field calculations and the development of software for the generation and display of 3D structures. Upon his return to Heidelberg, Willi introduced the techniques of molecular modeling as a research tool and central service in the DKFZ. From 1986 to 1987, a further sabbatical in Lund was used to learn the techniques of molecular dynamics simulations of peptides and proteins and to pursue several research projects in the field of Computational Chemistry. For the last 20 years Willi headed the Molecular Modeling group within the Central Spectroscopy Dept. at the DKFZ, where he introduced a wide variety of modeling services and open-access software, conducted courses in modeling techniques, collaborated with many diverse research groups, and organized the development of sophisticated 3D structure and spectroscopy data banks as well as Internet-based educational and research applications in

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modeling. These activities culminated in the Glycosciences.de website, Willi's main avenue of pioneering research, long before Glycomics became a common keyword. In recent years Willi was very active in international efforts to consolidate Glycobiology data bases, as evidenced by his active participation in the Consortium for Functional Glycomics (USA) and the Human Disease Glycomics/Proteome Initiative (HGPI/HUPO) and his function as Coordinator of the EU-funded EuroCarbDB Consortium. Willi von der Lieth served as Treasurer of the German Chapter of the Molecular Graphics Society and as Referee for several journals, was a member of the Editorial Board of Carbohydrate Research, and contributed over 100 journal articles and book chapters in the fields of molecular modeling, computer-based information systems and glycoscience.

Conformational analysis of oligosaccharides

In the late 1980s Willi von der Lieth entered the glycosciences field via an intensive collaboration with Prof. Dr. Janusz Dabrowski from the Max-Planck Institute for Medical Research in Heidelberg concerning the analysis of carbohydrate structures on the basis of NMR data and computational methods (*e.g.*, molecular mechanics, molecular dynamics, distance mapping). Willi's software tools provided information complementary to the NMR data obtained at the MPI, and this pioneering approach demonstrated that the conformational space of oligosaccharides could be explored in great detail by a strategic combination of experimental and theoretical methods.

Protein–oligosaccharide interactions

The next logical step was the *in silico* analysis of protein–oligosaccharide interactions based on the combination of experimental data and computational techniques. NMR spectroscopic as well as X-ray crystallographic data provided the basis for modeling of ligand–receptor interactions. Willi applied his computational tools in intensive collaborations with research groups led by J. F. G. Vliegthart, H.-J. Gabius, and J. Jiménez-Barbero to visualize the conformational dynamics of oligosaccharides and carbohydrate-lectin docking processes. These modeling studies provided key information,

which facilitated the analysis of the experimental data obtained by NMR.

Modeling services in cancer research and tumor therapy

Willi von der Lieth personally provided valuable molecular modeling services to many research groups at the DKFZ for a wide variety of topics, *e.g.*, development of targeted cancer therapies based on glycoconjugates (M. Wiessler), understanding host–virus interactions (M. Pawlita, J. A. Kleinschmidt), and development of contrast agents and molecular imaging techniques for visualizing tumors by MRI.

SWEET DB—an internet data base for the glycosciences

In 1998, as the Internet was becoming a major instrument for the exchange of information in many fields and especially in bioinformatics, Willi von der Lieth introduced SWEET DB, a data base for the interactive construction and 3D modeling of oligosaccharides. In the years that followed a whole ensemble of powerful modeling tools, data bases and useful links have been assembled in the glycosciences website (<http://www.glycosciences.de/>) at the DKFZ. This extremely popular website provides a legacy of Willi's visionary contribution to the glycosciences. The collection of tools and data bases developed under his guidance by many talented coworkers deserve our thankful recognition. It is up to us to provide encouragement and support for the continued maintenance of this website.

Willi von der Lieth was an exceptional personality; his boundless enthusiasm, creativity, and active interest in so many research areas was contagious. His uncomplicated interactions with colleagues and students revealed his openness, modesty and generosity—truly a *primus inter pares*. One could always turn to him for beneficial advice—in scientific as well as personal matters. His sudden departure reminds us of the fragility of life and leaves us with a painful vacuum and sadness that will remain long with us. Therein, we must find the inspiration to continue and build upon his work.