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Biography of Dudley Howard Williams

Statement of Career

Name: Dudley Howard Williams
Date of birth: 25 May 1937
Nationality: British
Education:

Institution	Years	Qualifications gained or position occupied
University of Leeds	1955–1958	B.Sc. (1st Class Hons.)
University of Leeds	1958–1961	Ph.D.

Subsequent career

Stanford University (USA)	1961–1964	Postdoctoral Fellow (Fulbright Scholar)
University of Cambridge	1964–1966	Senior Assistant in Research
Churchill College, Cambridge	1964–	Fellow
Churchill College, Cambridge	1964–1973	College Lecturer in Chemistry
University of Cambridge	1964	M.A.
University of Cambridge	1966–1974	Assistant Director of Research
University of California Irvine	1967	Visiting Professor
Churchill College, Cambridge	1968–1973	Director of Studies in Chemistry
University of Cambridge	1972	Sc.D.
University of Cape Town	1972	Visiting Lecturer
University of Sydney	1972	Nuffield Visiting Lecturer
University of Florida	1973	Visiting Professor
University of Cambridge	1974–1996	Reader in Organic Chemistry
University of Wisconsin	1975	Visiting Professor
University of Copenhagen	1976	Visiting Professor
Australian National University	1980	Visiting Research Fellow
University of California, Irvine	1986	Visiting Professor
University of Cambridge	1988–	Deputy Director, Camb. Centre Mol. Rec.
University of California, Irvine	1989	Visiting Professor
Churchill College, Cambridge	1989	Elected Extraordinary Fellow
University of Queensland	1994	Visiting Professor
University of Cambridge	1996–	Professor in Biological Chemistry
University of California, Irvine	1997	Visiting Professor

Awards, Lectureships, and Societies

The Meldola Medal (Royal Institute of Chemistry, 1966).
The Corday-Morgan Medal and Prize (The Chemical Society, 1968).
Fellow of the Royal Sociey of Chemistry, 1969.
Tilden Medal and Lecturer (The Royal Society of Chemistry, 1983).
Elected Fellow of The Royal Society, 1983.
The Royal Society of Chemistry 1984 Award for Structural Chemistry.
The 1985 Arun Guthikonda Memorial Award Lectureship, Columbia University, New York.
The 1989 Rorer Lecturer, Ohio State University.

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Distinguished Visiting Lecturer, Texas A and M University, 1986.
Member of Academia Europaea.
The 1990 Bader Award for Organic Chemistry, Royal Society of Chemistry.
Pacific Coast Lecturer, 1991.
University of Auckland Foundation Lecturer, 1991.
Steel Lecturer, University of Queensland, 1994.
Leo Friend Award of the American Chemical Society, 1996.
Byvoet Symposium Lecturer, 1998.
Burgenstock Symposium Lecturer, 1999.
Lee Kuan Yew Distinguished Visitor, Singapore, 2000.
Wageningen Symposium Lecturer, Holland, 2000.
Elected Honorary Fellow of the Singapore National Institute of Chemistry, 2000.
Paul Ehrlich Lecture (awarded for "an outstanding contribution in the field of Medicinal Chemistry"), France, 2001.
Marvin Carmack Distinguished Lecturer, Indiana University, 2001.
Merck Distinguished Lecturer, November, 2001.
James Sprague Lecturer, University of Wisconsin, Madison, 2002.
Erasmus Lecturer, University of Neuchatel, Switzerland, 2002.
Merck Research Lectureship 2003, Royal Society of Chemistry.

Industrial and public appointments

Consultant to SmithKline Beecham, UK, 1966–1998.
Consultant to Kratos Inc., Manchester, 1970–1988.
Consultant to Lepetit, Milan, 1983–1986.
Member of the Editorial Advisory Board for "Methods in Stereochemical Analysis" (J. Wiley and Sons Inc.), 1981–.
Consultant to Napp Laboratories, 1984–1989.
Consultant to The Upjohn Company, Kalamazoo, USA, 1984–1992.
Member of the Royal Society Sectional Committee for Chemistry, 1985–1988.
Member of SERC Chemistry Committee, 1981–1985.
Member of the Royal Society Research Grant Board for Chemistry, 1987–1989.
Consultant to Xenova Limited, London, 1987–1989.
Chairman of the 1989 Gregynog European Symposium on Bio-organic Chemistry.
Member of the Scientific Advisory Board, Xenova, London, 1989–1999.
Member of the Editorial Board of Accounts of Chemical Research, American Chemical Society, 1988–1992.
Member of the Editorial Board of Protein Science, Journal of the Protein Society of the USA, 1990–1992.
Member of the Editorial Board of The Journal of Antibiotics, Tokyo, 1990–to date.
Member of the Advisory Board of the "Tables Rondes Roussel Uclaf" and of the "Symposia Pharmaco-Cliniques Roussel Uclaf", 1990–1995.
Member of the Organising Committee, Gregynog European Symposia on Bio-Organic Chemistry, 1989–2002.
Chairman, Scientific Advisory Board of Xenova plc, 1993–1999.
Consultant to Astra, UK (Astra Charnwood), 1995–1997.
Consultant to Unilever, Port Sunlight, UK, 1995–1998.
Member of the Royal Society Research Grant Board for Chemistry, 1996–1998.
Member of the Scientific Advisory Board, RiboTargets, Cambridge, UK, 1997–2000.
Member of the Scientific Advisory Board, TerraGen, Vancouver, Canada, 1999–2000.
Member of the International Advisory Board of "Current Organic Chemistry", 2000–
Consultant to RiboTargets, Cambridge, UK, 2000–2002.
Member of the International Carbohydrate Symposium (July, 2004, University of Warwick) Advisory Committee.

University, college and society duties

Approximately 500 invited lectures, presented at major universities, and/or conferences (including some 60 main or plenary lectures), and/or major companies based upon organic chemistry, and/or chemistry-based learned societies of the following countries:

United Kingdom, Eire, France, Belgium, Holland, Denmark, Norway, Sweden, Germany, Italy, Singapore, Spain, Switzerland, Poland, United States, Canada, South Africa, Bulgaria, former Yugoslavia, Australia, New Zealand, Japan, Israel, India and Pakistan.

Normal teaching duties to all three (or later, four) undergraduate years, including the organisation of practical classes, in the period 1964–present. Supervised the Ph.D. theses of ca. 65 graduate students, and the work of ca. 35 post-doctoral fellows and visiting scholars. Former member of the Departmental Teaching Committee, the Appointments Committee of the Faculty Board of Physics and Chemistry, and the Biotechnology Syndicate. Former member of the Faculty Board of Physics and Chemistry (1991–1999), Degree Committee of the Faculty Board of Physics and Chemistry (1991–1999), and associated Discretionary Payments Committee (1995–1999) and Appointments Committee (1993–1997). Chairman of the Chemistry Appeal Steering Committee and Member of the Chemistry Appeals Advisory Board (1995–2000). Over the period 1964–present, a recipient of numerous major grants from SERC, EPSRC, BBSRC, and the Wellcome Trust for the provision of post-doctoral fellowships, and instrumentation in mass spectrometry and nuclear magnetic resonance for the University Chemical Laboratory and CCMR. Deputy Chairman of the Cambridge Centre for Molecular Recognition (1988–2002). Member of the Management Committee of the East Anglian Structural Biology Initiative (2000–2003).

Supervision of undergraduates for Churchill College in the period 1964–1996 and, at various times, member of the College's Council, Fellowship Electors, Finance Committee, Building Committee, and Committee for Statutes, Ordinances, and Regulations, and Fellows' Research Committee. Member of Churchill College Investment Committee.

Organiser of courses on Spectroscopic Methods in Organic Chemistry for the Royal Institute of Chemistry, 1965–1967, and course presenter for the American Chemical Society Course "Frontiers of Organic Chemistry" at University of Wisconsin and Stanford University, 1984–2001.

Highlights of research achievements

DHW has supervised the Ph.D. theses of ca. 70 graduate students and the work of 40 post-doctoral fellows. The research programme has led to the publication of some 460 original papers and 70 review papers. As a result of the work carried out in the period 1961–1967, seven books were published in the period 1964–67. The purpose of these books was to guide the organic chemist in the use of MS and NMR; the Institute for Scientific Information listed one of these books (no. 7) as a "citation classic" [1].

In the 1960s, the dependency of vicinal proton–proton coupling constants on the electronegativity of attached substituents was demonstrated. This work had wide implications since such coupling constants are used to deduce the solution conformations of organic molecules. In the same period, books were published that summarised the outcome of researches on the proton NMR spectra of steroids, and on the mass spectra of organic compounds. In 1969, an inorganic chemist, C.C. Hinckley, published a paper showing that $Eu(DPM)_3{\cdot}(pyridine)_2$ caused marked shifts in the proton NMR spectrum of cholesterol. It was proposed by DHW that $Eu(DPM)_3$ alone would be a much superior "shift reagent". This proved to be the case, and two papers published on this shift reagent became "citation classics" [2,3]. One was the most cited 1971 paper in the Natural Sciences in the period 1971 and 1972 [4]. Shift reagents became commercially available as important tools to aid the interpretation of NMR spectra.

In 1971, the structure of 1,25-dihydroxyvitamin D_3 was determined in collaboration with Kodicek and his colleagues at the Dunn Nutritional Laboratory. This substance is the key metabolite of Vitamin D_3; hydroxylation of the vitamin occurs consecutively in the liver and the kidney to produce a hormone that is essential for calcium absorption at levels appropriate for the production of healthy bones. Since this hormone is utilised in humans, synthetic 1,25-dihydroxycholecalciferol is now used in human therapy. It is manufactured by the pharmaceutical company Roche in the United States, and is essential for survival of patients with renal failure.

Also in the 1970s, a strategy was developed for the sequence determination of peptides by mass spectrometry (in collaboration with a post-doctoral fellow in my group, now Professor Howard Morris, FRS). The power of this strategy was later demonstrated by Morris when he used it to determine the structures of the enkephalins, the brain's natural opiates (using material provide by Hughes and Kosterlitz). In this period, the release of kinetic energy in some gas phase eliminations of H_2 were shown to be a consequence of the symmetry forbidden nature of these reactions, and potential energy profiles (with predictive power) were constructed for the gas phase reactions of simple organic ions.

Between the years 1975 and 1984, the structure and mode of action of the antibiotic vancomycin were determined. This work appears to have been the first use of the inter-molecular nOe to establish the binding site of a drug to its receptor. It is now used in this way on a world-wide basis, and is arguably the most powerful method for the determination of the molecular basis of biological recognition at atomic resolution in solution. Vancomycin group antibiotics are now of great commercial importance. Vancomycin is the most commonly used antibiotic in the treatment of serious infections due to methicillin resistant *Staphylococcus aureus* (MRSA), and in this sense is the successor to the penicillins in treating serious hospital infections. Such infections ("super bugs") are a major world-wide threat in hospitals, and although many thousands of lives are lost annually due to these infections, vancomycin is a life-saving drug in an enormous number of cases.

In 1984, the structure determination of teicoplanin, another glycopeptide antibiotic that has now established its place as a clinically important antibiotic, was achieved. The clinical impact of these antibiotics cannot be over-emphasised; combined world-wide sales of teicoplanin and vancomycin are currently running at ca. US$ 1 billion per annum.

In 1982, it was shown by fast atom bombardment mass spectrometry that the N-terminal group of calcineurin B is blocked by myristic acid. This was only the third report of a fatty acid group blocking the N-terminus of a protein. Since that

time, this feature has proved to be not uncommon, providing in many cases the physical basis for membrane association of a protein, and thereby for localisation of an important signalling function. Calcineurin is the most widespread synaptic Ca^{2+}/calmodulin-dependent phosphatase, with an important role in terminating the process of synaptic transmission, and in T-cell activation.

In 1983, a novel neuropeptide was isolated from mammalian spinal chord. This material was named substance K (since it was located by its cross-reaction with antibodies raised against the frogskin peptide kassinin), and shown to contain methionine. Its complete sequence was subsequently determined by others who showed it to be coded for by the same gene that codes for the biosynthesis of the neuropeptide substance P. The human receptor for substance K (also known as one of the neuromedins) has now been cloned by others. Substance K is now established as a neuropeptide of major importance.

Another area of research has been concerned with the interaction of drugs with DNA. In the first part of this programme, we used proton nOes to assign the spectra, and characterise the right-handed helical structures, of small self-complementary fragments of DNA, and of RNA/DNA hybrids. This was a new idea, and one that was conceived independently by, and published concurrently with, work of a group in Holland and one in the USA. In the second part of the programme, the molecular interactions involved in binding the antibiotic actinomycin D to a DNA duplex in solution were determined. This appears to have been the first work in which the binding of a second molecule to DNA was examined by nOes; and an enormous body of work has used this method since that time.

In 1984, the structure of the toxin that is produced by algal blooms of *Microcystis aeruginosa* was determined. This is a structure of importance for two reasons. First, the toxin is a serious threat to both human and wildlife populations in many parts of the world because the algal blooms can cover lakes and reservoirs. Second, the toxin is now used as a classical inhibitor of intracellular phosphatases (these enzymes play crucial roles in intracellular signalling—see also later).

In 1987, the structures of two 23 residue peptides, isolated from frog skin, were determined; these peptides were shown to cause cell membranes to burst. These peptides were also subsequently isolated and sequenced at the National Institutes of Health in Bethesda, MD, and renamed the magainins. The peptides have antimocrobial and antifungal activity. The discovery of the peptides and their activities was hailed as a major breakthrough by NIH (Nature, News and Views, August, 1987; C&E News, 17 August 1987; New York Times, the International Herald Tribune, and the Washington Post, 31 July 1987). Magainins Inc. was formed in the United States to exploit them commercially.

In 1988, using material provided by Professor P. Cohen (University of Dundee), mass spectrometry was used to determine unambiguously the phosphorylation pattern of the enzyme glycogen synthase. The method allows the determination of the pattern of phosphorylation of proteins. It thus allows an entry to determination of the molecular basis of a key method of intra-cellular signalling, and to understanding of reaction cascades which control intra-cellular responses.

In work carried out in 1994 and 1995, the structures of two peptides that are responsible for the transport of iron into two species of mycobacteria were deduced. This work opens possibilities for the design of drugs that could be useful in treating tuberculosis and leprosy.

In recent work, the role of secondary metabolites in aiding the survival of the producing organisms has been emphasised. This role is supported by findings (of others) that up to ca. 10% of the DNA of a microorganism may be used to code for secondary metabolite biosynthesis. The sophistication of the mode of action of the vancomycin group antibiotics supports the hypothesis. Indeed, it was established in work carried out between 1990 and 1994 that the sugar epitopes of the antibiotics strongly support their dimerisation, and that this dimerisation is used to promote their mode of action. Teicoplanin has been shown to be more efficient in its antibacterial action by virtue of the presence of a membrane anchor, which allows it to attach to bacterial cell membranes. A key 1995 paper in *Antimicrobial Agents and Chemotherapy* established that glycopeptide antibiotics which use the devices of membrane anchoring, or dimerization, are much more active against bacteria than expected on the basis of their solution binding constants to bacterial cell-wall analogues. The pharmaceutical company Eli Lilly submitted for clinical trials a semisynthetic glycopeptide that is potently active in vivo against against vancomycin resistant entercocci (VRE). These enterococci are severe clinical pathogens, and it is accepted that the new antibiotic exercises its remarkable activity by the devices of membrane anchoring and dimerization, as proposed by DHW. The new antibiotic is 100 to 1000 times more active than vancomycin against many serious pathogens in a mouse model.

DHW's research in the period 1997–2002 has seen the determination of the sequence of 72 kilobases of DNA which code for the biosynthesis of a glycopeptide antibiotic—the first such sequence to be determined. Following from this work, a large number of enzymes of the biosynthetic pathway have been cloned, and their biosynthetic functions established. The major achievements of the DHW group in the field of the vancomycin group of antibiotics (both determinations of structures and modes of action) were summarised in a 1999 review in Angewandte Chemie.

A 1998 paper in *Science* (416) demonstrated how a cooperative binding energy can arise other than at the interface which is made in the binding process through a "tightening" of the receptor structure. In 2003, these concepts were extended to show (using ESI mass spectrometry) that the binding energy of ligands for receptors, and of transition states to enzymes, can be enhanced by volume reductions within receptors, and enzymes, respectively. These volume reductions occur with a benefit in enthalpy and a cost in entropy. Thus, a novel source of catalytic efficiency of enzymes is proposed. Since volume contractions

in large structures can provide a major source of binding energy, this novel source of binding energy suggests why enzymes must be relatively large structures.

DHW was elected a Fellow of The Royal Society in 1983, an Extraordinary Fellow of Churchill College in 1989, and a member of the Academia Europaea in 1990. He was Lee Kuan Kew Distinguished Visitor to Singapore in April, 2000. The Institute for Scientific Information listed DHW as the world's most cited organic chemist outside the United States in the period 1965–1978 (5591 citations, at an average of 27 citations per paper) [5]. He was also the most cited scientist in the University of Cambridge in that period, and the most cited chemist in the United Kingdom. The work published in the period 1981–2001 has received over 6200 citations (an average of 30 citations per paper), and the total research programme has received more than 13,000 citations.

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[3] A. Thackray, in: E. Garfield (Ed.), Contemporary Clasics in Physical, Chemical, and Earth Sciences", ISI Press, 1986, p. 272.
[4] E. Garfield, Current Contents, No. 44, 5 (October, 1973).
[5] E. Garfield, Current Contents, No. 41, 5 (October, 1981).

Books

1. Interpretation of Mass Spectra of Organic Compounds.
   Holden-Day, San Francisco, 1964
   by H. Budzikiewicz, C. Djerassi, D.H. Williams
2. Structure Elucidation of Natural Products by Mass Spectrometry.
   Vol. 1. Alkaloids.
   Holden-Day, San Francisco, 1964
   by H. Budzikiewicz, C. Djerassi, D.H. Williams.
3. Structure Elucidation of Natural Products by Mass Spectrometry.
   Vol. 2. Steroids, Sugars, Terpenes.
   Holden-Day, San Francisco, 1964
   by H. Budzikiewicz, C. Djerassi, D.H. Williams.
4. Application of NMR in Organic Chemistry: Illustrations from the Steroid Field.
   Holden-Day, San Francisco, 1964
   by N.A. Bhacca, D.H. Williams.
5. Spectroscopic Methods in Organic Chemistry.
   McGraw-Hill, London, 1966
   by I. Fleming, D.H. Williams.
6. Spectroscopic Problems in Organic Chemistry.
   McGraw-Hill, London, 1967
   by I. Fleming, D.H. Williams.
7. Mass Spectrometry of Organic Compounds.
   Holden-Day, San Francisco, 1967
   by H. Budzikiewicz, C. Djerassi, D.H. Williams.
8. Principles of Organic Mass Spectrometry.
   McGraw-Hill, London, 1973
   by I. Howe, D.H. Williams.
9. Spectroscopic Methods in Organic Chemistry.
   McGraw-Hill, London, 1980 (third ed.)
   by D.H. Williams, I. Fleming.
10. Mass Spectrometry: Principles, Applications.
    McGraw-Hill, New York, 1981
    by I. Howe, D.H. Williams, R.D. Bowen.
11. Spectroscopic Methods in Organic Chemistry.
    McGraw-Hill, London, 1987 (fourth ed.)
    by D.H. Williams, I. Fleming.
12. Spectroscopic Methods in Organic Chemistry.
    McGraw-Hill, London, 1995 (fifth ed.)
    by D.H. Williams, I. Fleming.

Research papers

1960

1. Calciferol and its relatives. Part V. Epicalciferol.
   J. Chem. Soc., 1960, 5176.
   I.T. Harrison, B. Lythgoe, R.A.A. Hurst, D.H. Williams.

1962

2. A new route to 1-oxygenated steroids.
   J. Org. Chem., 1962, 27, 2205.
   C. Djerassi, D.H. Williams, B. Berkoz.

1963

3. A study of the hydrogen transfer reactions accompanying fragmentation processes of 11-keto steroids. Synthesis of deuteriated androstan-11-ones.
   J. Am. Chem. Soc., 1963, 85, 2061.
   D.H. Williams, J.M. Wilson, H. Budzikiewicz, C. Djerassi.
4. Unusual chemical shifts in the NMR spectra of 7- and 11-keto steroids.
   J. Am. Chem. Soc., 1963, 85, 2810.
   D.H. Williams, N.S. Bhacca, C. Djerassi.
5. Spin–spin coupling between hydrogen and angular methyl protons.
   J. Am. Chem. Soc., 1963, 85, 2861.
   D.H. Williams, N.S. Bhacca.
6. Presence of impurity in halothane.
   Science, 1963, 141, 899.
   E.N. Cohen, J.W. Belleville, H. Budzikiewicz, D.H. Williams.
7. Formation of olefins on desulphurisation of ethylene thioketals by raney nickel.
   J. Am. Chem. Soc., 1963, 4046.
   C. Djerassi, D.H. Williams.
8. Synthesis of tachysterol$_3$.
   Tetrahedron Lett., 1963, 1413.
   R.S. Davidson, O.H. Littlewood, T. Medcalfe, S.M. Waddington-Feather, D.H. Williams, B. Lythgoe.
9. Mass spectra of ethylene ketals and thioketals.
   Steroids, 1963, 2, 475.
   G.V. Mutzenbecher, Z. Pelah, D.H. Williams, H. Budzikiewicz, C. Djerassi.

1964

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11. Mass spectrometric fragmentations of isohexyl bromide and five deuterated derivatives.
    J. Am. Chem. Soc., 1964, 86, 877.
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    Monatsh., 1964, 95, 166.
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13. Mass spectrometric fragmentation behaviour of isohexyl cyanide and its deuterium analogs.
    J. Am. Chem. Soc., 1964, 86, 1386.
    R. Beugelmans, D.H. Williams, H. Budzikiewicz, C. Djerassi.
14. Mass Spectrometry in structural and stereochemical problems. A study of the hydrogen transfer reactions accompanying fragmentation processes in 1-keto steroids. Synthesis of deuteriated 5α-androstan-1-ones.
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    D.H. Williams, N.S. Bhacca.
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1965

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