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Editorial:

Changing Shape of Molecules

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It is with great pleasure that we have collated this Special Issue to honour the long and steadfast guidance of Peter Wright as Editor-in-Chief of the Journal of Molecular Biology (JMB). Peter is the third and longest serving Editor-in-Chief of JMB since the journal was inaugurated in 1959, following Sir John Kendrew and Sydney Brenner (25 years and 6 years, respectively). Over his 33 years as Editor-in-Chief, Peter has overseen the publication of 1280 issues of JMB, containing 21,372 articles that have accumulated 1,417,488 citations as we write this piece. A total of 58 of these articles were authored by our Editor-in-Chief. On behalf of the Editorial Board and the readers of JMB, we offer our most sincere and heartfelt gratitude!

During Peter's 33 years at our helm, the field of molecular biology has changed dramatically and now includes a breadth of topics and techniques that were unimaginable 33 years ago. O'mics methods, cryoEM, Alphafold predictions, single molecule and single cell experiments are but a few new and expanding areas, and the seamless synergy of *in vivo*, *in vitro* and *in silico* approaches described within a single study is now commonplace. These advances have led to new understanding of molecular mechanisms and new functional insights into macromolecular and cellular behaviour. Yet, the remit of the journal, "to publish high quality, comprehensive studies in all areas of molecular biology" and "use complementary experimental and computational approaches to address challenging biological questions" have not changed.

What is "molecular biology?" Clearly the topic is much more than cloning and PCR! After some debate (1), the consensus is that the term "molecular biology" was first coined by Warren Weaver in 1938, two decades before JMB was launched, with the term defined as "a new field in which delicate modern techniques are being used to investigate ever more minute details of certain life processes" (1). Bill Astbury, a physicist by training, who worked at the University of Leeds from 1928, was also an early pioneer and protagonist of the field of 'molecular biology', popularising the 'new science of molecular biology' (2). His approach was also to combine disciplines, in his case applying X-ray diffraction to study protein and nucleic acid fibres, and later using EM to investigate the structures of cells, cancerous cells and flu virus "to understand the complexity of living systems by studying the three-dimensional structure of the molecules from which they were made" (2,3). Today, the remit of JMB remains true to these early definitions, combining physical and biological approaches to understand biological mechanisms, including how cells work, how macromolecules control and choreograph key biological process from transcription to metabolomics, and how loss of control gives rise to deleterious biological outcomes and disease. JMB remains a favourite "go-to" for authors and readers seeking out the very best of science and the most exciting of discoveries in the field of molecular biology.

The topic “Changing Shape of Molecules” was chosen for this special issue to honour the major contributions that Peter Wright has made to this area of biology, with his ground breaking studies of how proteins fold, how their structures change when they assemble on nucleic acids, and how proteins that do not need to fold, so-called ‘intrinsically disordered proteins’, shape shift to carry out their important functions. With an impressive 453 papers to date that have amassed more than 57,000 citations, Peter has transformed our understanding of protein folding and dynamics, protein-nucleic acid recognition, and what is meant by ‘disorder’ and ‘folding on binding’. Peter stands out not only for his contributions to science, but also for his mentoring and service to our community. He has been a positive and supportive influence to our community and has given generously of his time, selflessly helping the field to grow. He leaves the journal at an exciting point in time, when new computational approaches and artificial intelligence promise to more rapidly produce and refine diverse paradigms and as the scientists who are conducting forefront research are themselves more diverse. Because of Peter’s leadership, JMB is now well positioned to support generations of scientists who will push boundaries and explore new frontiers in molecular biology.

In the pages that follow you will find 11 articles and 4 reviews that describe current topics and new discoveries that impact our understanding of the Changing Shape of Molecules. The topics span NMR studies of massive (300 kDa) AAA+ unfoldases (4), use of high pressure NMR to expose ‘invisible’ protein conformations (5), cryoEM structural studies of amyloid-specific PET ligands (6) and combined cryoEM/NMR structural analysis of temomerase:LARP7 protein complex involved in chromosome maintenance (7). New insights into virus structure and assembly are described, including the effect of Inositol hexakisphosphate on HIV -1 particle production (8), NMR validation of the X-ray crystal structural ensemble of SARS COV-2 protease (9), and a marvellous review on the importance of IDPs in virus assembly (10). Four articles come from the field of protein folding and amyloid formation: a fantastic review of functional amyloid (11), new insights into bacterial biofilm formation (12), the roles of chaperone recycling in flagellar assembly (13), and the fascinating action of the E3 ubiquitin ligase, CHIP/STUB1 in tau misfolding and assembly (14). Two articles focus on force: the use of single molecule force spectroscopy to understand membrane protein folding (15) and feeling the force in mechanobiology of chromatin structure and the epigenome (16). Lipids and biological membranes are also included, with an inspiring article showing the synergy of NMR and MD applied lipid dynamics in the cell membranes of *S. aureus* and *E. coli* (17). Last, and certainly not least, a sparkling review updates readers on the conserved features and function of intradimeric Walker A ATPases (18).

We hope you enjoy reading this special issue as much as we have enjoyed assembling it. We thank Peter Wright for his care and wisdom in guiding JMB for the last 33 years. We look forward to reading more of the great science from all of you working in the exciting field of molecular biology in future issues of Journal of Molecular Biology.

Sheena Radford and Mike Summers
Associate Editors of Journal of Molecular Biology, April 2023

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