

nature Structural biology

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molecular form & function

Journal evolution

The appearance, for the first time, of the strap-line “molecular form and function” on the cover of the October issue, as well as on the home page of our Web site, is unlikely to have gone unnoticed by regular readers of the journal. A brief 10 months after having initiated a spurt of journal ‘speciation’¹, the strap-line heralds a new and more significant phase of growth and development for *Nature Structural Biology*: the breadth of research considered for publication in the journal will be expanded to cover a much wider range of molecular and cellular biology, biochemistry and biophysics.

Our new policy of “considering any and all studies that provide insight into the molecular function of biological macromolecular systems” is essentially a paraphrasing of our old policy, except that under the new rubric the insight does not have to be provided in the form of high resolution structures — indeed, the structural insight may be much more indirect. At the same time, we are adding an increased number of pages per issue, as well as additional staff, to ensure that broadening of the editorial content does not affect our present eclectic mix of biomolecular structural biology, but rather adds to it.

The driving force behind these changes is the evolution the field itself is going through. For example, many structural biologists, like researchers in other fields, are increasingly studying biological systems, rather than individual molecules. So it follows that we will increasingly publish the results of molecular studies on those systems, including: DNA replication and repair, transcription, splicing, translation, protein degradation, signal transduction, membrane trafficking, nuclear transport and, indeed, all the processes that underpin life.

The analysis of these complex spatial and temporal array of macromolecules will present many questions to be answered — the order of additional of components to a complex, their sub-cellular or extracellular locations, the nature of transient macromolecular interactions, non-specific interactions, and so on — which are not easily or directly accessible to the traditional tools of the structural

biologist. Rather, to be successful in studying such biological system, structural biologists will have to adopt a battery of techniques culled from diverse scientific disciplines to tackle these problems: structure then becomes merely *part* of the armory scientists use to inform their biological research effort. Indeed, the future will see an increased blurring of the definition of ‘structural biologist’ with those of ‘molecular biologist’, ‘cell biologist’, ‘biophysicist’ and ‘biochemist’. Again, it follows that the results that appear in our pages will increasingly be derived using methods ranging from cell biology to biophysics.

What is driving this change in structural biology? First, structural

Table 1 Impact factors for a selection of journals¹

		ISI Impact factor ²		
		1997	1996	1995
FASEB J	↑↑ ³	14.629	13.771	13.404
EMBO J	↓	12.643	13.255	13.505
Nature Structural Biology	↑	10.782	9.430	8.738
Pro. Natl. Acad. Sci. USA	↓	9.040	10.244	10.520
Structure	↓	7.633	7.792	8.082
Journal of Biological Chemistry	↓	6.963	7.452	7.385
RNA	↓	5.970	6.304	na
Journal of Molecular Biology	↑	5.673	5.195	5.346
Journal of Biomolecular NMR	↓	5.154	4.361	6.047
Biochemistry	↓	4.572	4.818	5.144

¹Institute for Scientific Information (ISI) impact factors for a selection of molecular biological, biochemical and structural biology journals reported by the ISI over the last three years.

²1997 (most recent report), 1996, 1995 ISI Journal Citation Reports.

³Arrows indicate whether the impact factors have increased or decreased between 1995 and 1997.

editorial

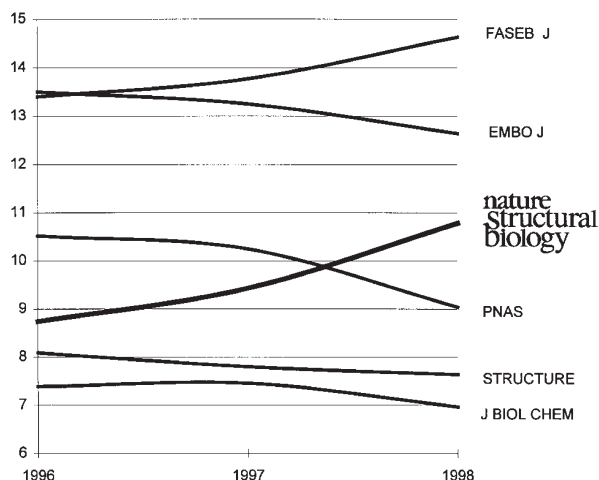


Fig. 1 Graph showing the change in ISI impact factor over a three year period for a selection of the journals listed in Table 1.

biology, in part through its own success, is much less insulated from the rest of the biological scientific community than it used to be. The results of structural studies are now generally appreciated for their (often considerable) utility and therefore are in great demand; one need only consider the pharmaceutical/biotechnology industry to see the importance that structural biology can play in a broad ranging research effort. Second, although molecular and cellular biology continue to provide a rich vein of biologically important proteins ripe for structural analysis, this vein is not inexhaustible (especially in the face of the organized and systematized proteomics projects being planned). Thus, structural biologists as a group are, of necessity, focusing in much more detail on the function of the biomolecules whose structures they have already determined. Third, structural biology is easier to do than it was: the processes of structure determination — X-ray crystallography, nuclear magnetic resonance, electron microscopy, electron crystallography and so on — are becoming increasingly well established (and, for X-ray crystallography at least, almost automatic in some cases, once the protein has crystallized and derivatives obtained), fuelling an explosion in the numbers of structures being determined.

There is no question that the study of the atomic structures of biological macromolecules in their own right remains an important endeavor and will remain at the core of the journal. There are many basic principals of biomolecular structure that are still poorly understood, principals that, once elucidated, will have a profound implications for our ability to manipulate macromolecular systems. There will also be many important technical developments that extend the range and scope of structural biology. And there will also be structures that, in and of themselves, provide significant biological insight. *Nature Structural Biology* will continue to cover all of these aspects of structural biology.

Nevertheless, over the next year we will be actively encouraging submission of, and publishing this heady mix of science. There are some who may regret this change; they should not. It merely reflects the growing relevance of structural biology to a broader biological audience: perusal of our ISI impact factors over the last three years (Table 1, Fig. 1) provides a striking demonstration of this trend.

Six-month hold

A pressing issue for those who generate the many high resolution three-dimensional structures published in our pages is that of release of the primary data and coordinate files for the structures. Since the beginning of the year we have debated the matter in a series of editorials²⁻⁴, hosted a web-based straw poll on a petition put forward by Alex Wlodawer⁵ and catalogued and presented a large volume of correspondence on the matter⁵. Since that time we have been debating the issue among ourselves, as well as continuing to consult informally with those in the field.

In the light of these events and discussions, we have decided, as of January 1999, to allow no more than a six-month hold period for coordinates deposited in the Protein Data Bank (PDB), rather than our present policy of allowing a one-year hold. Nevertheless, we will continue to strongly encourage that all coordinates be released immediately on publication. We will also require that structure factors for X-ray structures, and equivalent data for NMR structures, be deposited in either the PDB or the BMRB, with an optional hold period of no more than one year.

Unlike a number of other journals (including *Nature*, *Science*, *Proceedings of the National Academy of Sciences of the USA* and the *Journal of Biological Chemistry*), which have adopted a policy of immediate release for all structure coordinates deposited in the PDB, we will not be moving to a policy of obligatory immediate release, at least for the time being. This does not mean that we intend to encourage the use of the six month hold — far from it. The ideal condition is that all data be available immediately. But until such time as all journals agree to require and (just as importantly) enforce the immediate release of coordinates, we do not feel that we can demand immediate release by our authors.

Even so, we will continue to support the principal of immediate release and would hope to be able to instigate such a policy in the near future. It is here that the International Union of Crystallographers (IUCr) can play a vital role in moving the debate even further forward. Their recommendations for the release of structure related data (one year hold for coordinates and a four year hold for structure factors) formulated over 10 years ago have been very effective in encouraging deposition of data. The views of the crystallographers, as voiced through the IUCr, could play an equally critical role in setting new standards not just for the release of coordinates, but of all published scientific data.

1. Editorial, *Nature Struct. Biol.* **5**, 1–2 (1998)
2. Editorial, *Nature Struct. Biol.* **5**, 83–84 (1998)
3. Editorial, *Nature Struct. Biol.* **5**, 165–166 (1998)
4. Editorial, *Nature Struct. Biol.* **5**, 245–246 (1998)
5. Editorial, *Nature Struct. Biol.* **5**, 407–408 (1998)