

We Need More Information on Proteins, Regulation and Catalysis

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Although 'genetics' is now mainstream evolution, we need to know much more about proteins in order to tell/predict much more about protein evolution, and its organizing principles. This involves understanding regulation, levels of gene expression, and catalysis. The sequence of events that DNA makes mRNA makes protein is well understood, but there are remaining questions. Tertiary (and quaternary) structure of proteins is now an important question, and similarly, the tertiary structure of RNA molecules is very important to the cell. Still, this has not led to any further understanding of the methods that limit protein expression. Possibly a next question is understanding/predicting the reason why catalysis is so important, and is mostly carried now out by proteins. Catalysis (mainly by proteins, but also by cofactors - often RNA-derived [1] is essential to living systems. The RNA-world is the best acceptor hypothesis about the origin of life, but even here there is considerable uncertainty [2]. Epigenetics is now normal science, and has been at least since Waddington [3], so that part is 'out of the way', and is helping gene regulation by modifying proteins and RNA.

Certainly, the prediction of tertiary structure of proteins is currently well advanced. I-TASSER is perhaps currently the best at predicting the tertiary structure of proteins [4]. There is a biennial competition of programs for predicting protein structure - CASP (Critical Assessment of techniques for protein Structure Prediction). Some coordinates of new proteins are withheld for a few weeks, and various programs are then predicting their structures. I-TASSER has won the award for the last couple of times. Thus we have to determine tertiary (and quaternary-dynamic) structure of proteins [5]. Some will be determined by X-ray (and increasingly at very low temperature too), others by calculation. This is a start, but we really need to go beyond to predicting tertiary structure.

As a first step, we will need to know just how the tertiary structures themselves evolve in order to get proper alignments. But ultimately, we will need to know how the molecules really function. For example, why do some proteins catalyze reaction A, and others catalyze reaction B? There is much to learn here, and it is critical to our understanding. We have to determine tertiary (and quaternary-dynamic) structure of proteins. As a first step we will need to know just how the tertiary structures themselves evolve in order to get proper alignments. But ultimately, we will need to know how the molecules really function.

There are alternative problems that now must be solved; probably one that is important is why proteins are expressed differently in different cells of multicellular plants and animals. For example, why (in root cells) are chloroplast genes not generally expressed. They are still there; because it is known that often root cells can regenerate stem (and leaf) cells and the genes are then expressed. There is no reason to suspect that plants and animal regulate gene expression by the same mechanisms—they could have developed independently. Thus it could be that they have independently learned how to control genes. But perhaps they use the same method? But the main thing is that we need a method for understanding/describing this process—it is a major gap in our present-day understanding.

A problem is that proteins evolve new catalytic functions, and this must be understood. We need to know much more about the principles of protein catalysis, it is not enough to say that 'proteins catalyze'. Why do they? As we have seen, a given 'gene' might carry out function 'A', and then a copy (or duplicate) might evolve function 'B'. Does any individual protein catalyze several reactions, and it is relatively easy to swap the main one? It is necessary to find out/work out much more about the reasons why protein evolution is so essential. There is recent work by Levin and Mishmar [6] that attempts just that.

The main point about this note/letter is that we need to go beyond just the structure of proteins, and work on catalysis and regulation of gene levels. These are important principles here. There is no reason to suppose that we have a full understanding at present of gene function and regulation and catalysis—we must expect to understand more fully on the future about a number of things, this is an essential part of protein evolution.

Overall, this is a very optimistic view, because there is so much to learn. I grew up, and did my undergraduate degree, at a university where the philosopher of science Karl Popper had taught for a number of years [7]. Although he had taught philosophy, had had a profound effect on the scientists there, so this very Popperian view is optimistic for the future—we have very much more still to learn. This is good news for future work—there is much more to learn.

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