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Protein structures: the evolutionary time capsules

If you wanted to probe life's origins, billions of years back, how could you do it? You'd need a preserved message from different points in history, time capsules left by evolution. Amazingly, evolution has left such time capsules in the chemical makeup of every living being.

The biological machinery of living cells is heavily composed of proteins. Like a lock that only accepts certain keys, the machine's three-dimensional structure determines the machine's function. Since protein molecular structure determines function, and structural deviation can result in death, structure is also more likely to be conserved. Thus, if we understand the evolutionary history of protein structure, we can reconstruct some of the evolutionary history of life itself. This is the inspiration for this research.

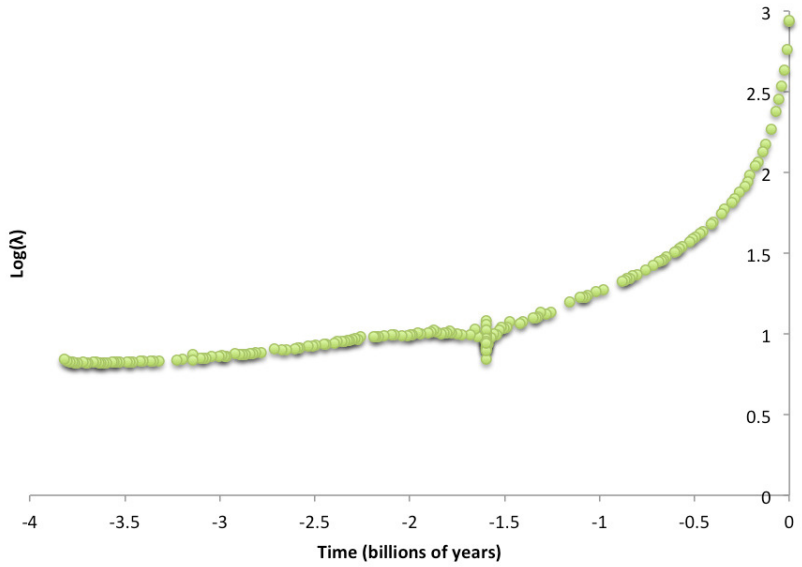

Fig. 1. (log of the) rate at which structure variations accumulate over time. 0 is the present.

Our research begins by building on previous work in the lab that builds evolutionary trees of protein structures in all organisms by assuming first that all structures are related by a common ancestor, and second that if a structure is present in many different kinds of organisms it's likely to be older than one present in only a few organisms. These evolutionary trees are similar to family trees and they show which of today's structures are more closely related.

Our study paints a dynamic story on the evolutionary tree of structures by modeling the evolution of protein structures as a succession of small mutations that create variations on a theme and eventually lead to transitions to new structures. With the assumption that only transitions that actually occur on the tree, which we take to approximate reality, are allowed to occur in the model, we calculated change in two global variables over time: the rate at which structure variations accumulate (λ), and the rate at which transitions to new structures occur (a). Figures 1 and 2 summarize our results.

There is a remarkable behavioral change in both rates occurring approximately 1.5 billion years ago. The rate at which structure variations accumulate increases drastically, while the rate at which transitions to new structures occur begins a course of permanent, steep decline. All organisms on the planet fall into one of three superkingdom groups, Eukarya, Bacteria, and Archaea. The spikes in the Figures roughly correspond to the end of the specification of superkingdoms and the beginning of organismal diversification within each superkingdom.

Once combinations of different structures in proteins started to materialize in evolution, the rate of structural variants visibly increased (Fig. 1). This enabled access to new evolutionary niches occurring faster through combinations rather than through novel structural discoveries. Hence a decline in Figure 2. An analogy to this time course is that of a developing field of knowledge. The first researchers of the field cannot help but make many fresh discoveries. The next wave of researchers, however, fail to make as many fundamental discoveries, partly due to the scarcity of results, but also because it is easy to combine many of the basic results into innovative combinations.

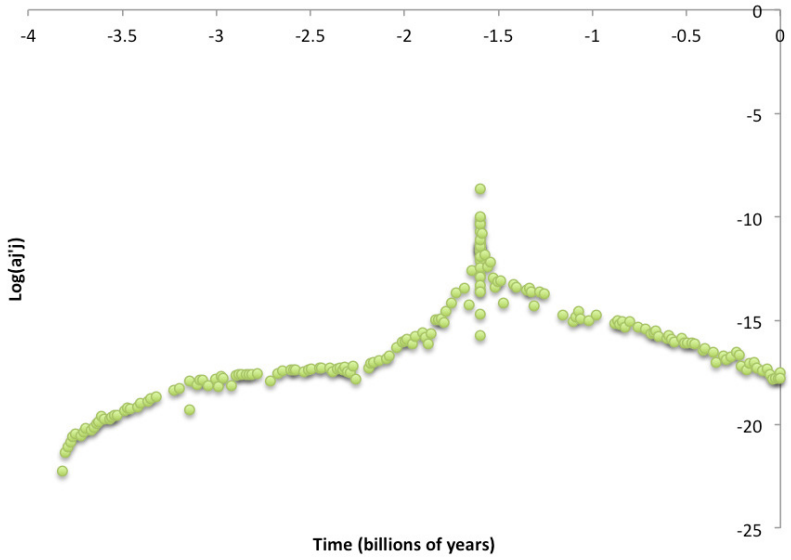

Fig. 2. (log of the) rate at which transitions to new structures occur. 0 is the present.

Our research contributes another layer to the developing story of life's origins and evolution. It provides a powerful new technique of peering deeper into the past. Also, there is an analogy to be made with language. Written words are to protein sequences, as spoken words are to protein structures, as meaning is to function. Is this analogy precise? Do similar evolutionary conclusions follow? Are our results only one instance in a deeper truth describing the emergence of modules? Only future research will decide.

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Publication

A Dynamic Model for the Evolution of Protein Structure.
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