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Finding shifts in the evolution of mitochondrial metabolism

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Motivation and Aim: It is well known that metabolic rates change significantly during Vertebrata evolution. However, the evolutionary time points and the molecular basis of these metabolic shifts are unknown.
Methods and Algorithms: Because mitochondria is strongly involved in the maintenance of basal metabolism, we focused on the molecular co-evolution of mitochondrial proteins with more than 500 nuclear proteins tightly associated with mitochondria (from MitoMiner4.0 database). In order to find the inner branches of Vertebrata tree with such changes, the evolution of protein structure was analyzed based on about 3000 species with completely sequenced mtDNAs and based on more than 100 species with completely sequenced nuclear genomes. Taking into account various known drawbacks in the evolutionary analyze of protein structures (the technical impossibility to reconstruct ancestral protein structures in all inner nodes of tree; heterotachy; inequality in various taxa sampling, etc.) we invented and implemented our software pipeline. It is based on the comparative analysis of 3 sets of heterotachy-aware and species-tree informed phylogenetic trees that were reconstructed using 50 % jackknife of multiple alignments of (1) protein sequences, (2) residue solvent accessibilities and (3) residue secondary structures. For the reconstruction of trees (2) and (3) 3D protein structure properties were predicted using SCRATCH-1D v.1.1.
Results: We observed highly significant accelerations in protein structure evolution at several inner tree branches of mitochondrial and nuclear proteins that tightly linked with well-known evolutionary innovations in maintenance of basal metabolism. The tree branches with accelerations in nuclear proteins evolution concentrated on Mammalia clade at either relatively recent divergences, e.g. Primates, Rodentia, Chiroptera, Carnivora, or evolutionary old divergences such as Mammalia or Monotremata. At the same time, mitochondrial proteins also have evolutionary accelerations at relatively recent Primates and Carnivora divergences, while the spectra of evolutionary old divergences is much more extensive. Among the nuclear proteins that enriched with accelerated structure evolution events, we found the Succinate Dehydrogenase Complex Assembly Factors, mitochondrion morphogenesis proteins, ADP/ATP translocases. It is also interesting that nuclear proteins enriched with accelerated structure evolution on Primate divergence related with mitochondrial nucleoid while the other divergences demonstrated acceleration of nuclear proteins of mitochondrial matrix and/or membrane.
Conclusion: Thus, the vast majority of observed accelerations in structure evolution of mitochondrial and mitochondria-related nuclear proteins are most likely driven by adaptive functional changes because they are tightly associated with changes in environment and physiology at the course of evolution.
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