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Genome-scale modeling of the evolutionary path to C4 photosynthesis CHRISTOPHER R. MYERS, Cornell University, ELI BOGART, Cornell University Brigham and Women's Hospital — In C4 photosynthesis, plants maintain a high carbon dioxide level in specialized bundle sheath cells surrounding leaf veins and restrict CO₂ assimilation to those cells, favoring CO₂ over O₂ in competition for Rubisco active sites. In C3 plants, which do not possess such a carbon concentrating mechanism, CO₂ fixation is reduced due to this competition. Despite the complexity of the C4 system, it has evolved convergently from more than 60 independent origins in diverse families of plants around the world over the last 30 million years. We study the evolution of the C4 system in a genome-scale model of plant metabolism that describes interacting mesophyll and bundle sheath cells and enforces key nonlinear kinetic relationships. Adapting the zero-temperature string method for simulating transition paths in physics and chemistry, we find the highest-fitness paths connecting C3 and C4 positions in the model's high-dimensional parameter space, and show that they reproduce known aspects of the C3-C4 transition while making additional predictions about metabolic changes along the path. We explore the relationship between evolutionary history and C4 biochemical subtype, and the effects of atmospheric carbon dioxide levels.

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