

Structure of a three-domain sesquiterpene synthase: a prospective target for advanced biofuels production

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Project Goal:

The high similarity of AgBIS to diterpene synthases makes it an important link in understanding terpene synthase evolution. More practically, the AgBIS crystal structure is important in future protein engineering efforts. Through structural analysis, we can begin to engineer more stable enzymes for increased biofuel production.

The sesquiterpene bisabolene was recently identified as a biosynthetic precursor to bisabolane, an advanced biofuel with physico-chemical properties similar to D2 diesel. Here, we report the structure of AgBIS, a three-domain plant sesquiterpene synthase, crystallized in its apo form and bound to five different inhibitors. Structural and biochemical characterization of the AgBIS terpene synthase Class I active site leads us to propose a catalytic mechanism for the cyclization of farnesyl diphosphate into bisabolene via a bisabolylyl cation intermediate.