Computing the various pathways of penicillin synthesis and their molar yields.

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Details

Abstract

More than 80 years after its discovery, penicillin is still a widely used and commercially highly important antibiotic. Here, we analyse the metabolic network of penicillin synthesis in *Penicillium chrysogenum* based on the concept of elementary flux modes. In particular, we consider the synthesis of the invariant molecular core of the various subtypes of penicillin and the two major ways of incorporating sulfur: transsulfuration and direct sulfhydrylation. 66 elementary modes producing this invariant core are obtained. These show four different yields with respect to glucose, notably ½, 2/5, 1/3 and 2/7, with the highest yield of ½ occurring only when direct sulfhydrylation is used and α-aminoadipate is completely recycled. In the case of no recycling of this intermediate, we find the maximum yield to be 2/7. We compare these values with earlier literature values. Our analysis provides a systematic overview of the redundancy in penicillin synthesis and a detailed insight into the corresponding routes. Moreover, we derive suggestions for potential knockouts that could increase the average yield.

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