



# Positive selection sites in tertiary structure of Leguminosae *Chalcone isomerase 1*

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**ABSTRACT.** Isoflavonoids and the related synthesis enzyme, chalcone isomerase 1 (CHI1), are unique in the Leguminosae, with diverse biological functions. Among the Leguminosae, the soybean is an important oil, protein crop, and model plant. In this study, we aimed to detect the generation pattern of Leguminosae *CHI1*. Genome-wide sequence analysis of *CHI* in 3 Leguminosae and 3 other closely related model plants was performed; the expression levels of soybean chalcone isomerases were also analyzed. By comparing positively selected sites and their protein structures, we retrieved the evolution patterns for Leguminosae *CHI1*. A total of 28 *CHI* and 7 *FAP3* (*CHI4*) genes were identified and separated into 4 clades: *CHI1*, *CHI2*, *CHI3*, and *FAP3*. Soybean genes belonging to the same chalcone isomerase subfamily had similar expression patterns. *CHI1*, the unique chalcone isomerase subfamily in Leguminosae, showed signs of significant positive selection as well as special expression characteristics, indicating an accelerated evolution throughout its divergence. Eight sites were identified as

undergoing positive selection with high confidence. When mapped onto the tertiary structure of CHI1, these 8 sites were observed surrounding the enzyme substrate only; some of them connected to the catalytic core of CHI. Thus, we inferred that the generation of Leguminosae CHI1 is dependent on the positively selected amino acids surrounding its catalytic substrate. In other words, the evolution of CHI1 was driven by specific selection or processing conditions within the substrate.

**Key words:** Leguminosae; Soybean; Chalcone isomerase; Positive selection; Protein structure