ABSTRACT
Quantitative correlations between the contents of the flavonolignans silychristin A and silybins A/B provide biosynthetic clues that support a pathway in which one mesomeric form of a taxifolin radical is undergoing an oxidative coupling with a coniferyl alcohol radical. The flavonolignan content and patterns reported in the literature for 53 samples, representing populations of the Silybum marianum plant growing in different parts of the world, were subject to a meta-analysis. Linear regression analyses were carried out on these data sets, and a mathematical model was derived that predicts the content of silychristin A relative to the metabolomic pattern of its congeners. The validity of the model was verified by applying it to test samples. This approach could potentially become a tool to enhance the understanding of both the relative composition of the silymarin complex and the biosynthetic pathways that underlie its formation