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Synthesis, Crystal Structure and Prodrug Studies of Daidzein Sulfonate

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SUMMARY. 7-Enthyl-4'-phenylsulfonyldaidzein (EPD 3), a potential prodrug for daidzein 1, was synthesized in high yield and its crystal structure was reported firstly. It possesses better physical and chemical properties such as solubility, lipid/water partition coefficient LogP, and hydrolysis kinetics than its original form. The LogP value (3.07) and the half-life of the hydrolysis value (24.06 h) show that its oral bioavailability is possibly improved evidently compared with that of daidzein. These results indicate that EPD can be considered a potential prodrug for daidzein.

KEY WORDS: Daidzein sulfonate, Crystal structure, Prodrug; Hydrolysis, Partition coefficient.

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