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Stereochemical determination of O-desmethylangolensin produced from daidzein

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We had isolated an O-desmethylangolensin (O-DMA)-producing bacterium, Clostridium rRNA cluster XIVa strain SY8519. According to chiral separation using HPLC, the SY8519-produced O-DMA exhibited high optical purity. To determine the absolute stereochemistry of O-DMA, we prepared 2-(4-hydroxyphenyl) propionic acid (2-HPPA) from the O-DMA using the Baeyer-Villiger reaction. From chiral analysis of the product, the major peak had the same stereochemistry to that of 2-HPPA produced from genistein by the same bacteria. As we have determined the stereochemistry of SY8519-produced 2-HPPA to have an R configuration, by the chemical synthesis of (S)-2-HPPA, the SY8519-produced O-DMA must also possess R stereochemistry at the 2-position. To study the stereoselective metabolism, we applied racemic dihydrodaidzein to SY8519. The O-DMA was isolated from the culture media and starting material was also recovered. The O-DMA produced was optically active in a similar manner to that produced from daidzein. However, the remaining dihydrodaidzein exhibited no difference between the enantiomers. These results suggested that SY8519 produces (R)-O-DMA from both enantiomers of dihydrodaidzein.