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# Structure- and stereospecific transport of strigolactones from roots to shoots

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*Supplementary data for Xie et al.,*

*LC-MS/MS analytical conditions for detection and identification of deuterated strigolactones from extracts of shoots harvested 20 hr after treatment.*

Identification of strigolactones were performed using a triple quadrapole/linear ion trap instrument (LIT) (QTRAP5500; AB Sciex) with an electrospray ionization (ESI) source and coupled to a UHPLC system (Nexera X2; Shimadzu). Chromatographic separation was achieved on isocratic (65% MeCN–$H_2O$ containing 0.1% acetic acid) UHPLC on a chiral column (CHIRAL-PACK AD-3R, ϕ 2.1 × 150 mm, 3.0 μm; DAICEL Corp., Japan). The column was operated at 20°C with a flow-rate of 0.2 mL/min. MS/MS spectra were recorded in product ion scan mode using LIT. Ion source was maintained at 400°C with curtain gas at 20 psi, collisional activated dissociation (CAD) gas at 7 psi (12 psi for LIT), ion source gas at 80 psi, and ion source gas2 at 70 psi. Ionspray voltage was set at 5,500 V in positive ion mode and −4,500 V in negative ion mode. Declustering, entrance, and collision cell exit potentials were maintained at 60, 10, and 15 V, respectively.

One-fifth of the samples dissolved in 5 μL MeCN were injected to the LC–MS/MS. The transitions of *m/z* 348–234, 348–206 and 348–97 were monitored for $d_1$-orobanchol and its isomers; *m/z* 337–240, 337–222, and 337–97 for $d_6$-4-deoxyorobanchol and its isomers in the ESI positive mode.