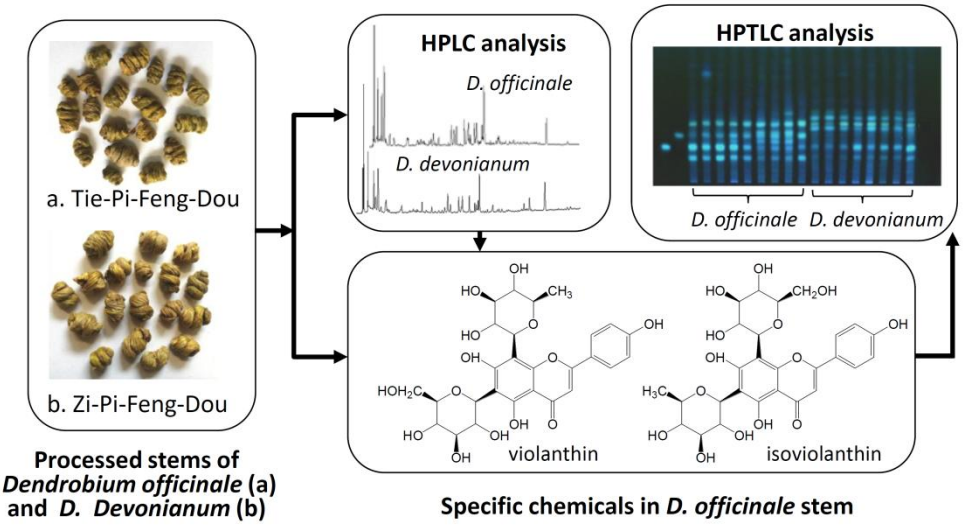
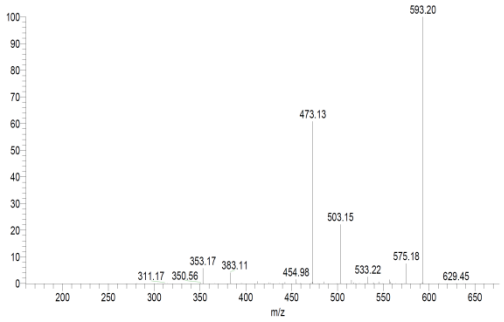
Supporting figures

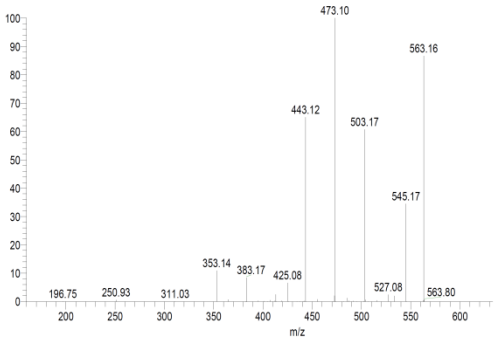


Supporting Fig. 1 Graphical abstract

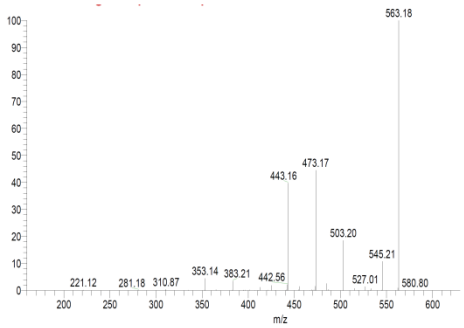
Compound9： Vicenin-2



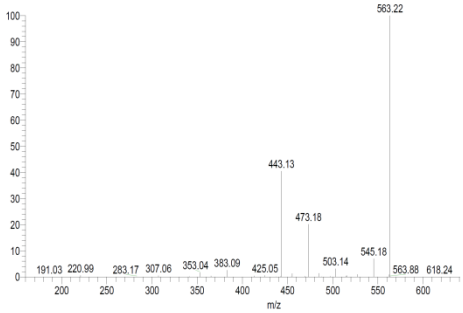
Compound10： Apigenin-6-*C*-β-*D*-xyloside-8-*C*-β-*D*-glucoside



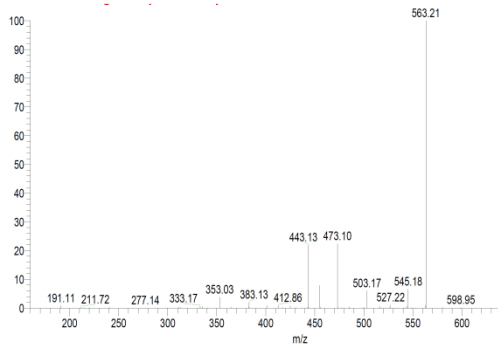
Compound12：Isoshafotoside



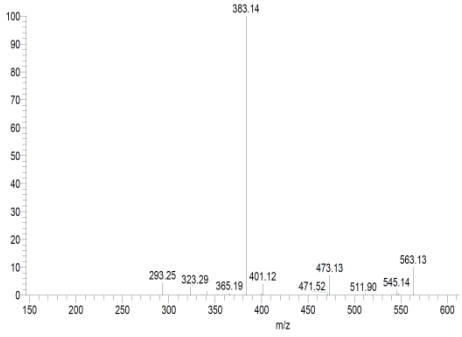
Compound13: Shafotoside



Compound16： Apigenin-6-*C*-β-*D*-glucoside-8-*C*-β-*D*–xyloside

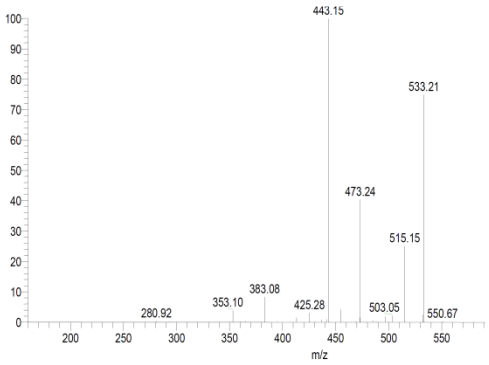


Compound24： Apigenin-6-C-(2''-*O*-β-*D*-glucopyranoside)-α-*L*-arabinoside

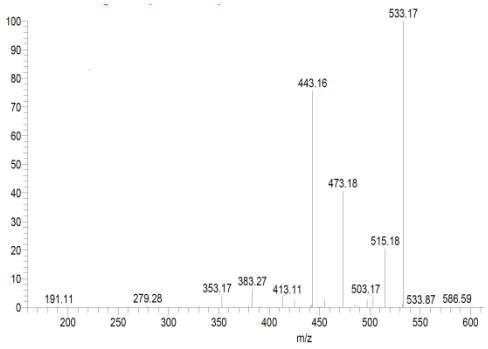


Supporting Fig. 2 LC-MS/MS spectrums of vicenin-2, apigenin-6-*C*-β-*D*-xyloside-8-*C*-β-*D*-glucoside, isoshafotoside, shafotoside, apigenin-6-*C*-β-*D*-glucoside-8-*C*-β-*D*–xyloside and apigenin-6-*C*-(2''-*O*-β-*D*-glucopyranoside)-α-*L*-arabinoside from the stem of *D. officinale* （negative ion mode）.

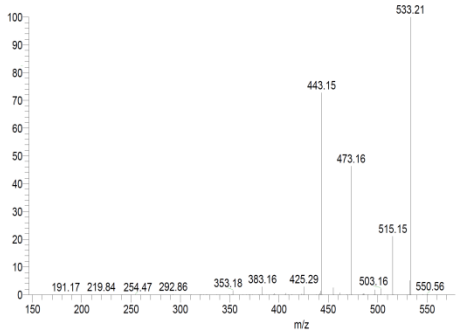
Compound 17: Apigenin-6-*C*-β-*D*-xyloside-8-*C*-β-*D*-arabinoside



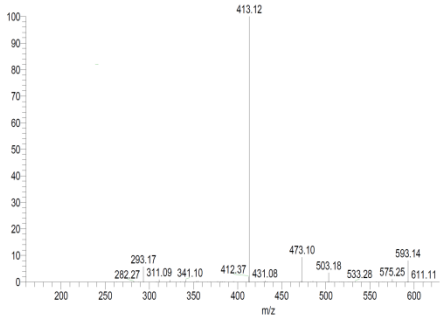
Compound 18: Apigenin-6,8-*di*-*C*-α-*L*-arabinoside



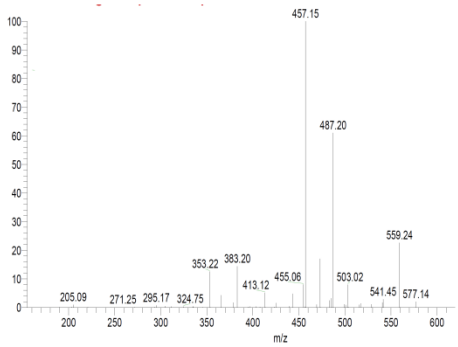
Compound 23: Apigenin-6-*C*-α-*L*-arabinoside-8-*C*-β-*D*-xyloside



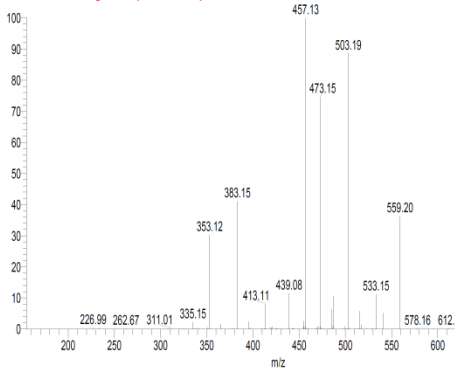
Compound 14: Vitexin 2''-*O*-β-*D*-glucopyranoside



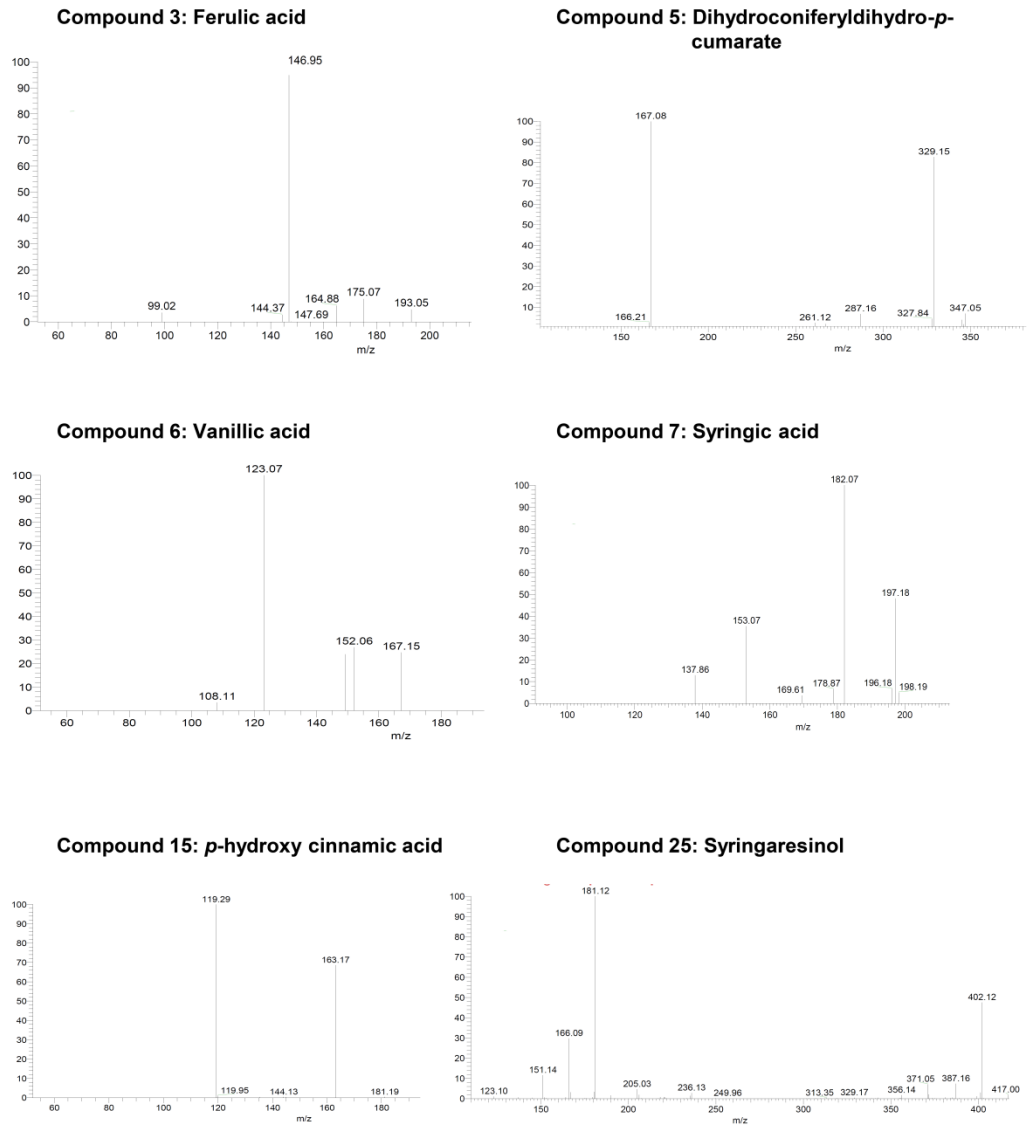
Compound 19: Violanthin



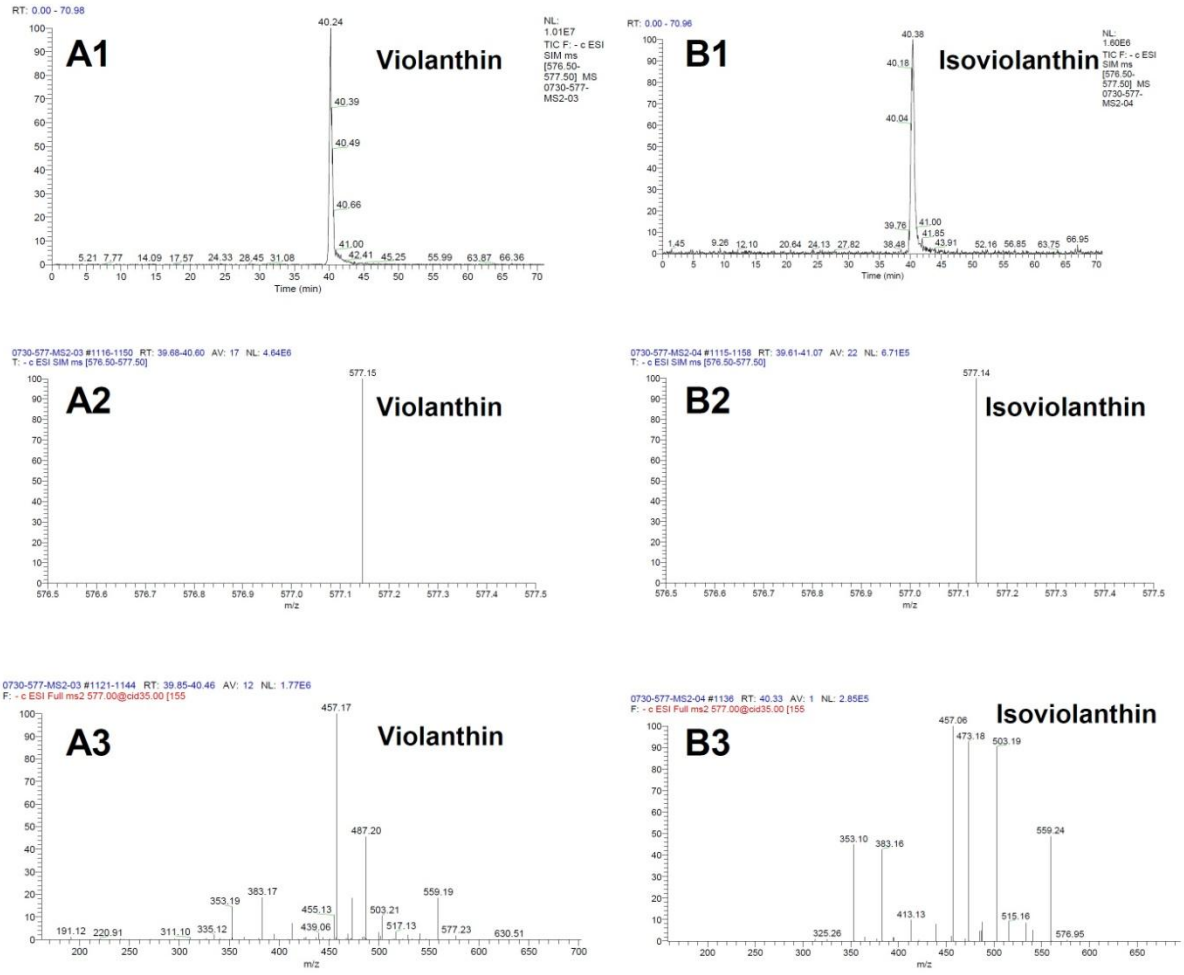
Compound 20: Isoviolanthin



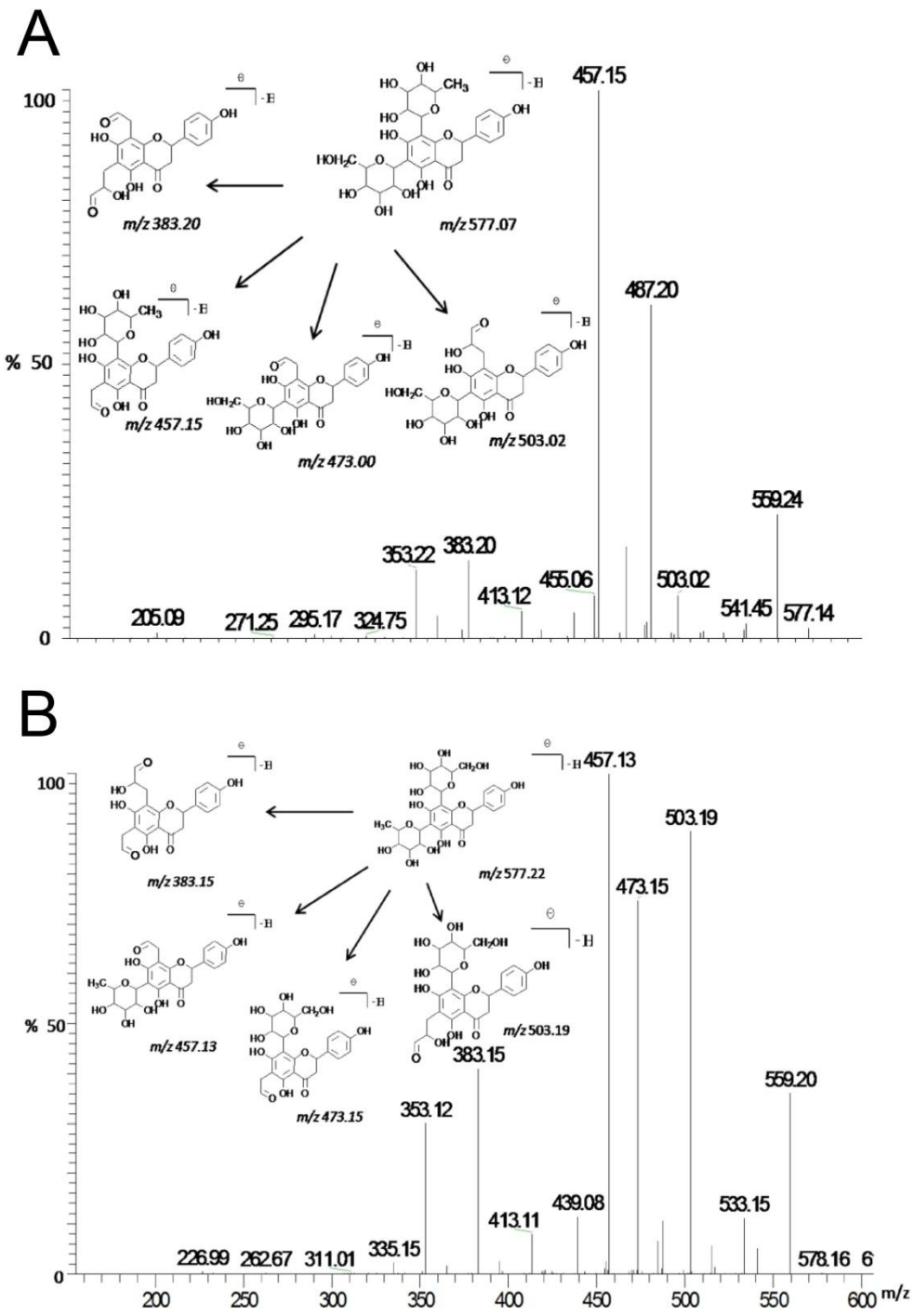
Supporting Fig.3 LC-MS/MS spectrums of apigenin-6-*C*-β-*D*-xyloside-8-*C*-β-*D*-arabinoside, apigenin-6,8-*di*-*C*-α-*L*- arabinoside, apigenin-6-*C*-α-*L*-arabinoside-8-*C*-β-*D*-xyloside, vitexin 2''-*O*-β-*D*-glucopyranoside, violanthin and isoviolanthin from the stem of *D. officinale*（negative ion mode）**.**



Supporting Fig. 4 LC-MS/MS spectrums of ferulic acid, dihydroconiferyldihydro-*p*-cumarate, vanillic acid, syringic acid, *p*-hydroxycinnamic acid and syringaresinol from the stem of *D. officinale*（negative ion mode）.



Supporting Fig.5 LC-MS chromatograms (1) LC-MS spectrums (2) and LC-MS^2 spectrums (3) of violanthin (A) and isoviolanthin(B) from the stem of *D. officinale*（negative ion mode）



Supporting Fig.6 The MS spectra and the characteristic fragmentation pathway of violanthin and isoviolanthin. Violanthin (**A**; compound 19) and isoviolanthin (**B**; compound 20) were shown here.