Fig. S1 PC1 *vs.* PC2 plot showing distinct discrimination among *R. hookeri, R. micrantha, R. serpentina, R. tetraphylla, R. verticillata* and *R. vomitoria* on the basis of total peaks: (A) roots; (B) leaves. Blue and red spots represent training sets and validated respectively.
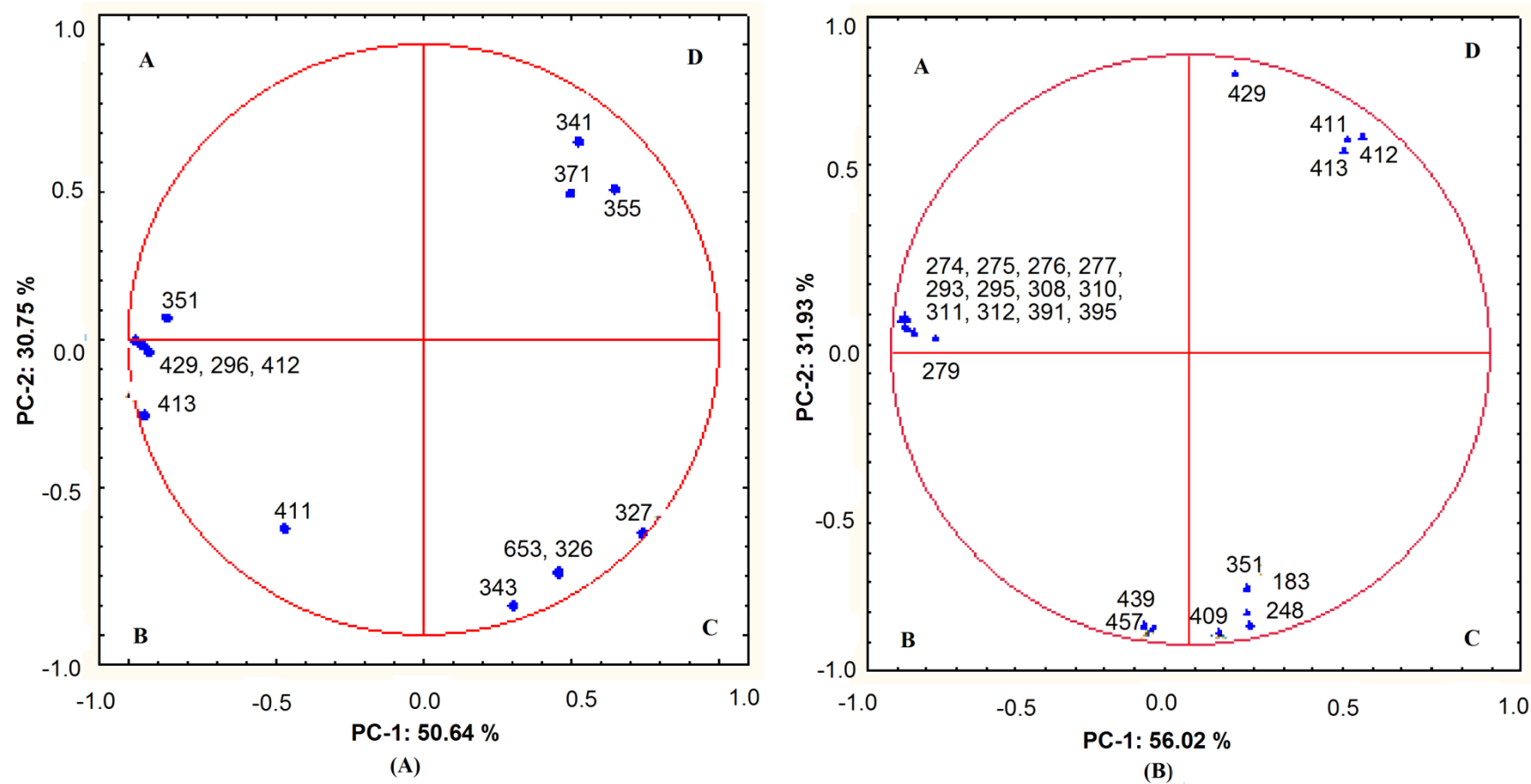
Fig. S2 PC1 *vs*. PC2 loading plot showing distribution of variables: (A) roots and (B) leaves.

MS/MS spectra obtained from Agilent 6520 ESI-QTOF-MS/MS system was coupled with an Agilent 1200 HPLC (Agilent technologies, USA)
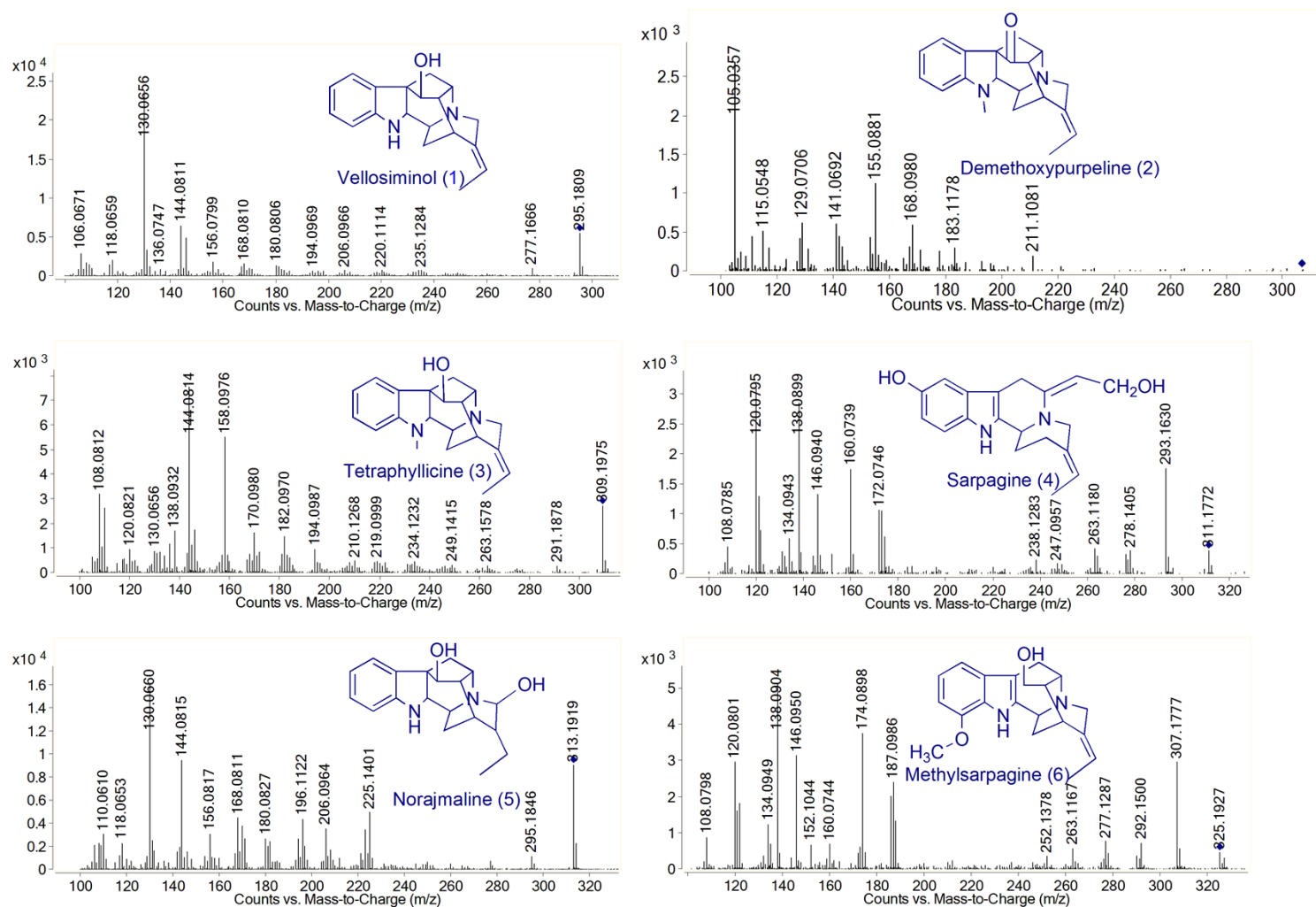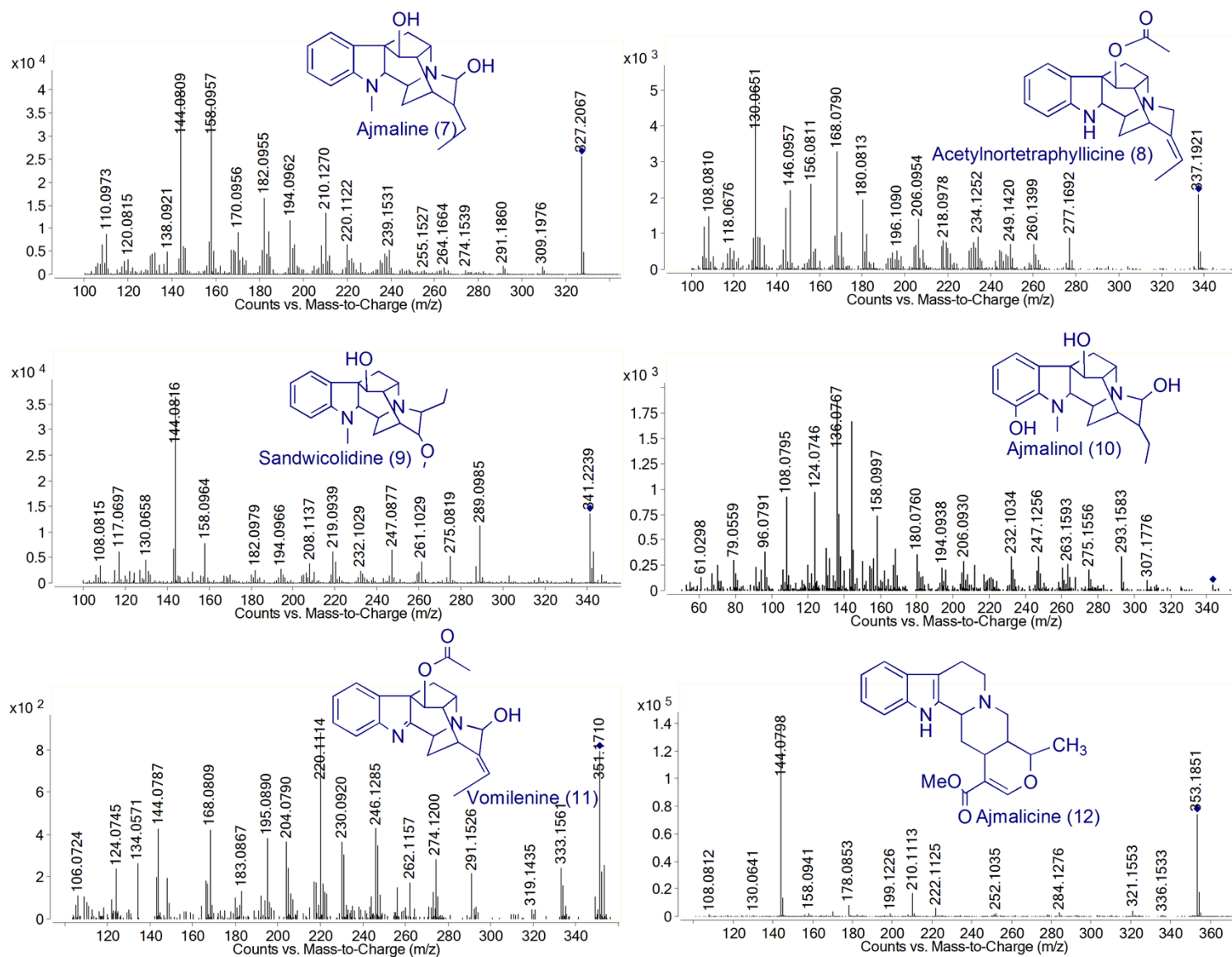

Fig. S3 HRMS/MS spectra of compounds **1-6**

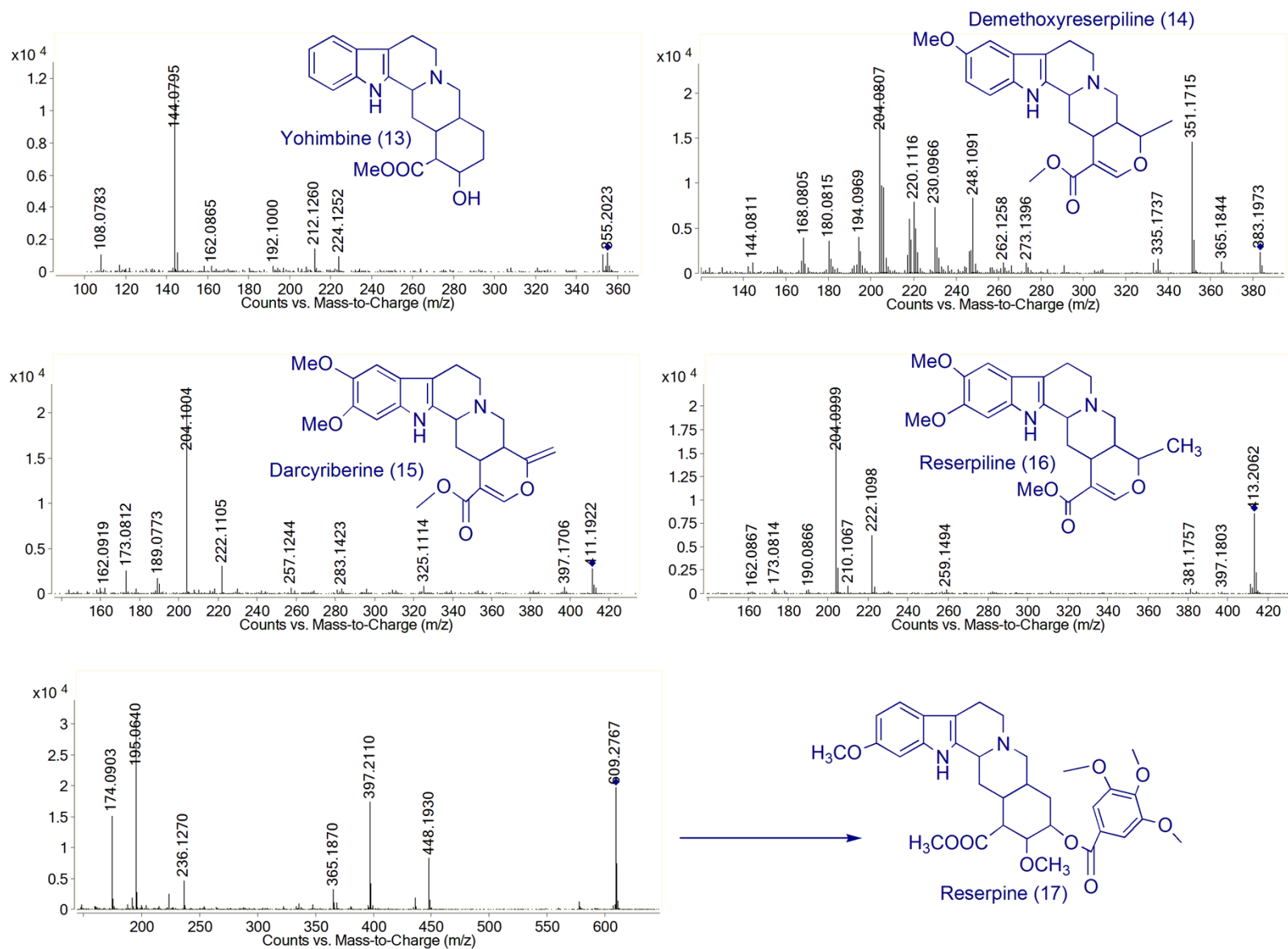**Fig. S4** HRMS/MS spectra of compounds **7-12**

Fig. S5 HRMS/MS spectra of compounds **13-17**