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