2.6. *Chemometrics*

Chemometrics of hierarchical cluster analysis (HCA) and principal component analysis (PCA) was applied to the FTIR and Raman data of *R. damascena* essential oils and commercial samples using the OPUS software version 7.2 (Bruker, Germany). Dissimilarities and similarities were clearly observed by HCA dendrogram. The HCA dendrogram was built using second derivative spectra (9 smoothing points), Euclidian distance and Ward's algorithm. Three dimensional PCA plots were obtained for displaying the scattering pattern of authentic and commercial samples. Second derivative spectra were used through the factorization algorithm for the PCA analyses. The spectral range of 1800-500 cm^{-1} and 2000-200 cm^{-1} was used in the FTIR and Raman analyses, respectively.

SIMCA 15 (Umetrics, Umea, Sweden), as a supervised chemometrics technique, was used to perform HCA and PCA analyses of GC-MS data, which were obtained from *R. damascena* essential oil samples (n=12) and commercial (n=20) samples.

3. Results

3.1. *Analysis of FTIR spectra of R. damascena essential oil*

The typical FTIR spectrum of *R. damascena* essential oil and overlaid FTIR spectra of *R. damascene* essential oil samples and commercial samples are presented in **Figure 1(A)** and **Figure 1(B)**, respectively. The FTIR spectrum of *R. damascene* essential oil had significant vibrational bands at 3345, 2960, 2922, 2853, 1668, 1515, 1451, 1377, 1260, 1235, 1053, 1004 and 829 cm^{-1}. The spectral band at 3345 cm^{-1} could be assigned to the stretching vibrations of the OH functional group of alcohols (Sandasi et., 2011; Tankeu., 2014). The band with a peak point at 2960 cm^{-1} may be attributed to the C=C-C ring vibrations of volatile compounds (Tankeu et al., 2014). Two bands at 2922 and 2853 cm^{-1} were assigned to the methylene C-H asymmetric and symmetric stretching vibrations, respectively (Berechet et al., 2015).

> **Commented [HSB1]:** I looked this up and my search suggested that the correct spelling is R.damascena, but you've used damascene quite a few times. I'm not sure which is correct, so I suggest you go a find/replace to make it consistent. I'm not a subject specialist, so I'm not sure if this is some sort of derivative. Sorry. The correct spelling needs mapping across the work.