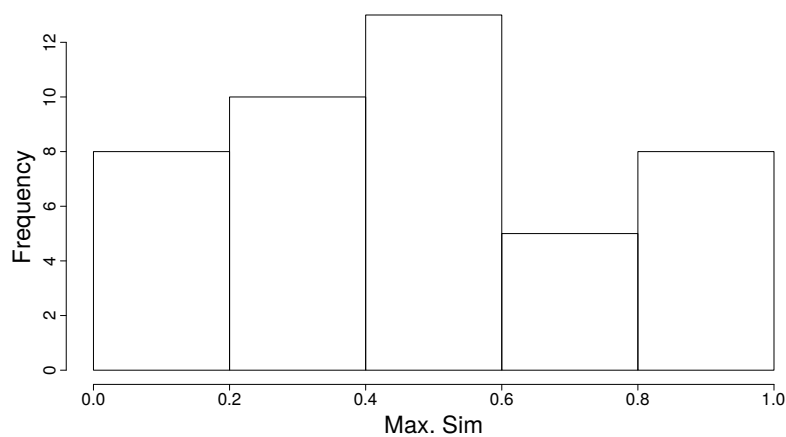


Figure S2: **Maximum spectral similarities.** Maximum spectral similarities found in the training spectra set (excluding CASMI 2016 training spectra) for each challenge (test) spectrum. Top: 44 challenge spectra in positive mode. Bottom: 43 challenge spectra in negative mode. The figures indicate the similarity of training and test spectra used.

(a) Positive mode



(b) Negative mode

