

Electronic Supplementary Information for

Identification of the smallest peptide with a zwitterion as the global minimum: a first-principles study on arginine-containing peptides

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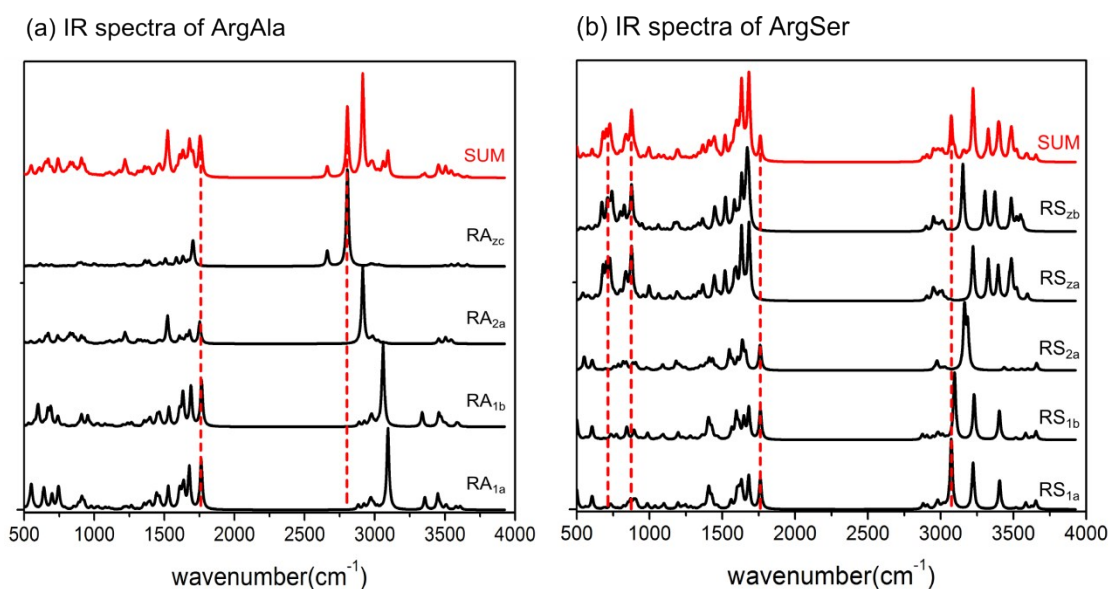


Fig. S1 Simulated IR spectra of the most abundant conformers of the two arginine-containing peptides (a) ArgAla and (b) ArgSer at 298 K. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.