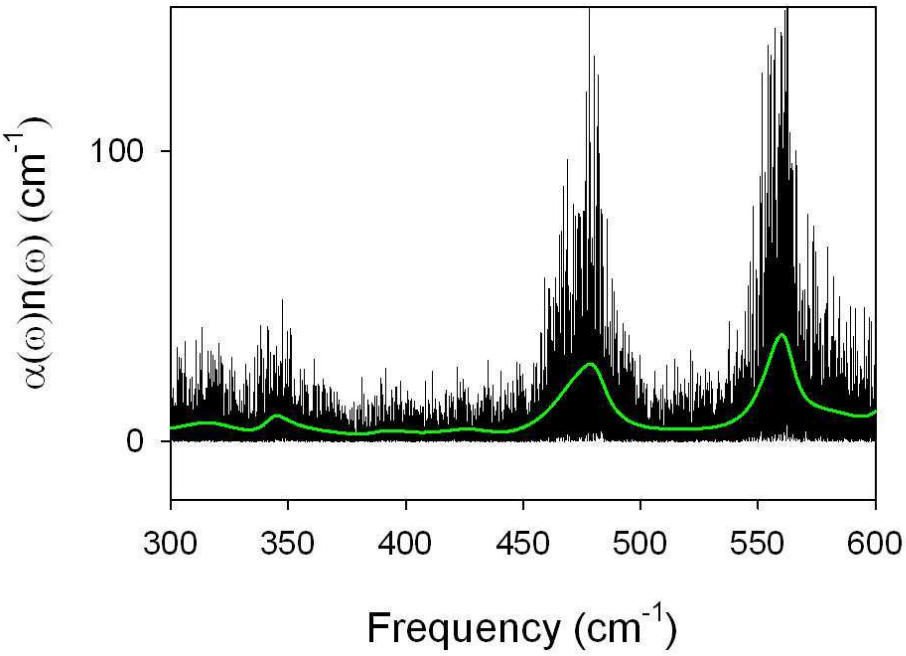
Supplementary Figure 1. The IR spectrum was calculated from time-dependent dipole moment generated from 1ns of MD simulation for AK17 (A), AK10G (B) and AK9P (C). For AK10G and AK9P, higher noise level and broader bands were observed in the raw data. This observation reflected the fact that these two peptides possess higher degree of freedom compared to the ordered helical structure in AK17, therefore more conformations were sampled during the simulation period. Despite that, after simple signal processing procedure, the IR active modes were still observable around 470 and 560 cm^{-1}; simulation bands 3 and 4 respectively (Figure 5). Note in the far-infrared spectroscopy data experimental band I (simulation band 1) and experimental band II (simulation band 2) are reduced in the aqueous samples of AK9P (Figure 2) and disappear in lyophilised AK9P (Figure 3) while experimental band III (simulation band 4) remains, which is consistent with the trend in the simulations.



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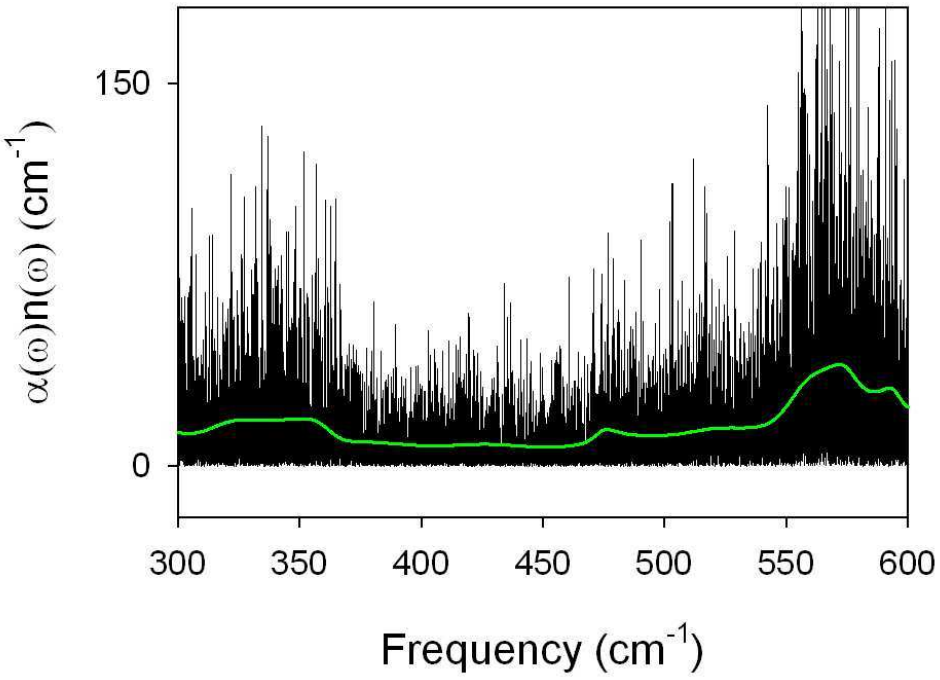

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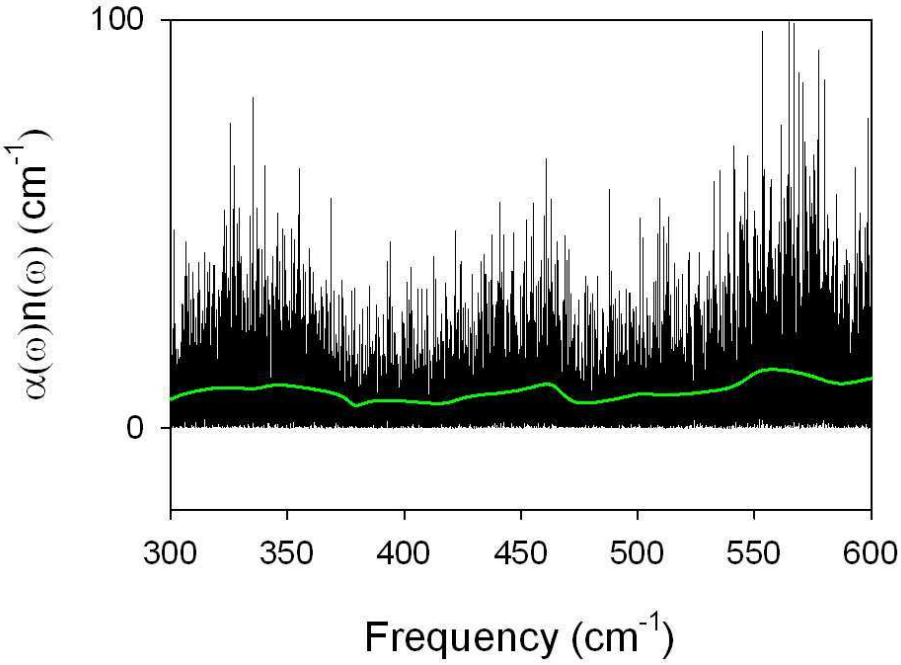

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