Supplementary Material (ESI) for *PCCP*

Probing the specific interactions and structures of gas-phase vancomycin antibiotics with cell-wall precursors through IRMPD spectroscopy

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Supplementary Information :

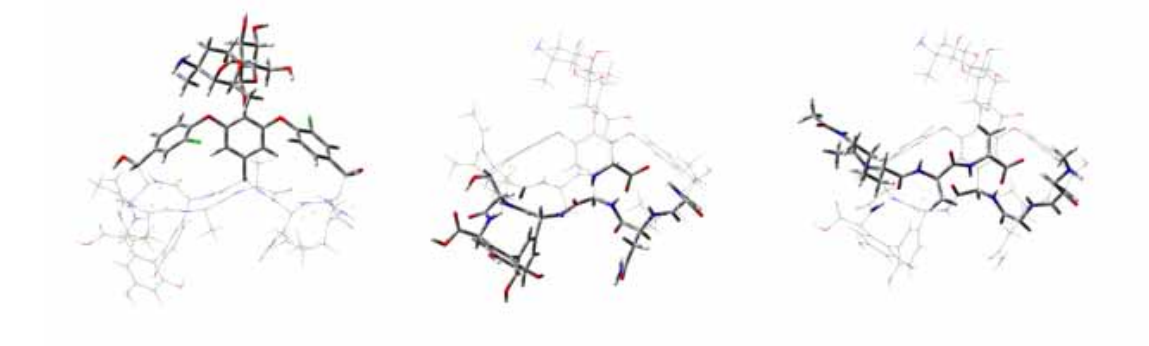

Fig. S1 the three partitions of $[V+ Ac_2{}^{L}K^{D}A^{D}A –H]^-$ for the ONIOM DFT/B3LYP/6-31+G*/AM1 calculation. high layer in tube, low layer in wireframe.

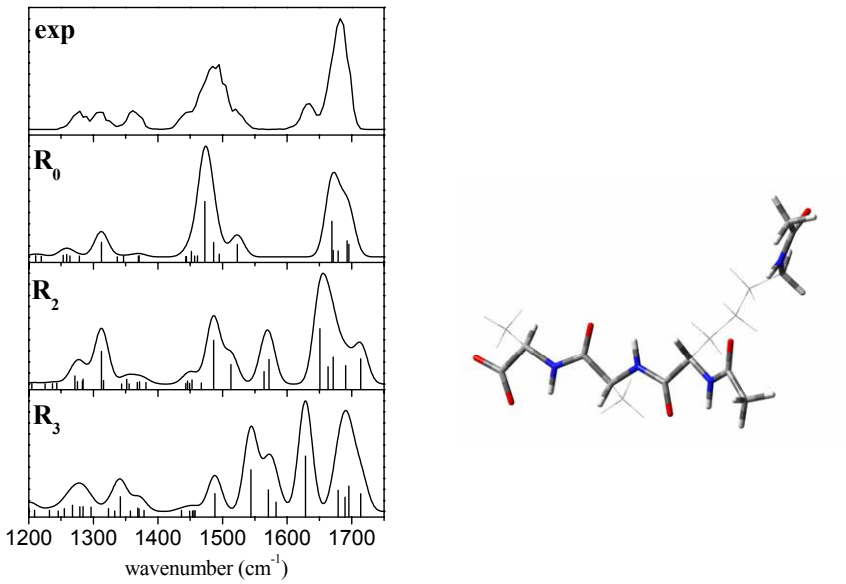

Fig. S2 ONIOM DFT/B3LYP/6-31+G*/AM1 simulated spectra of the selected conformers of $[Ac_2{}^{L}K^{D}A^{D}A –H]^-$. Conformer R_1 has been omitted because of the change in its optimized geometry at this level of theory as compared to the pure DFT calculations. The partitioning of

the tripeptide (R_0 conformer) is shown on the right side: high layer in tube, low layer in wireframe.

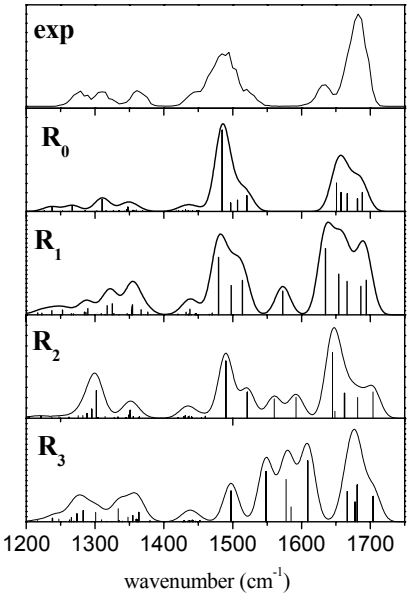

Fig. S3 DFT/B3LYP/aug-cc-pVDZ simulated spectra of the selected conformers of $[Ac_2{}^{L}K{}^{D}A{}^{D}A\ –H]^-$

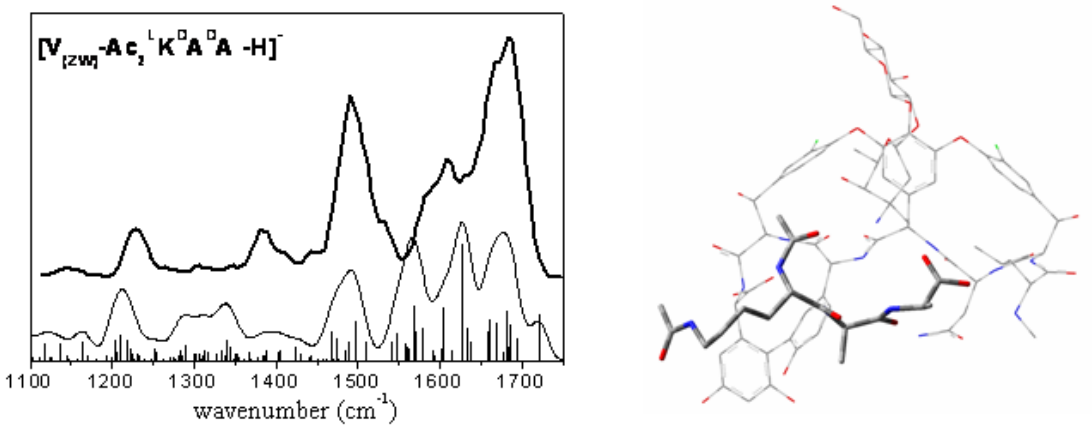

Fig. S4 ONIOM DFT:B3LYP/6-31+G*/AM1 simulated spectrum of $[V_{ZW}+ Ac_2{}^{L}K{}^{D}A{}^{D}A\ –H]^-$ where vancomycin (wireframe) is in zwitterionic form and the tripeptide (tube) is deprotonated. This structure is taken from ref. 30.