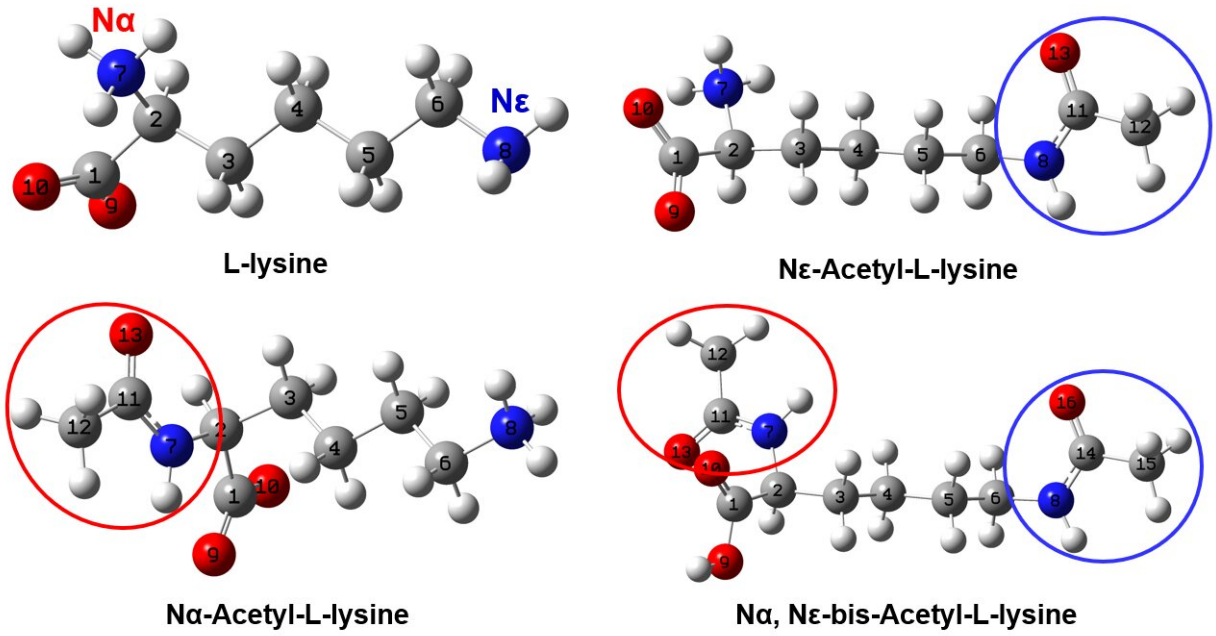
Raman and infrared spectroscopy help identify different acetylated lysines

June 24 2022, by Zhang Nannan



Molecular structures of lysine and three acetylated lysines. Credit: Yao Guohua

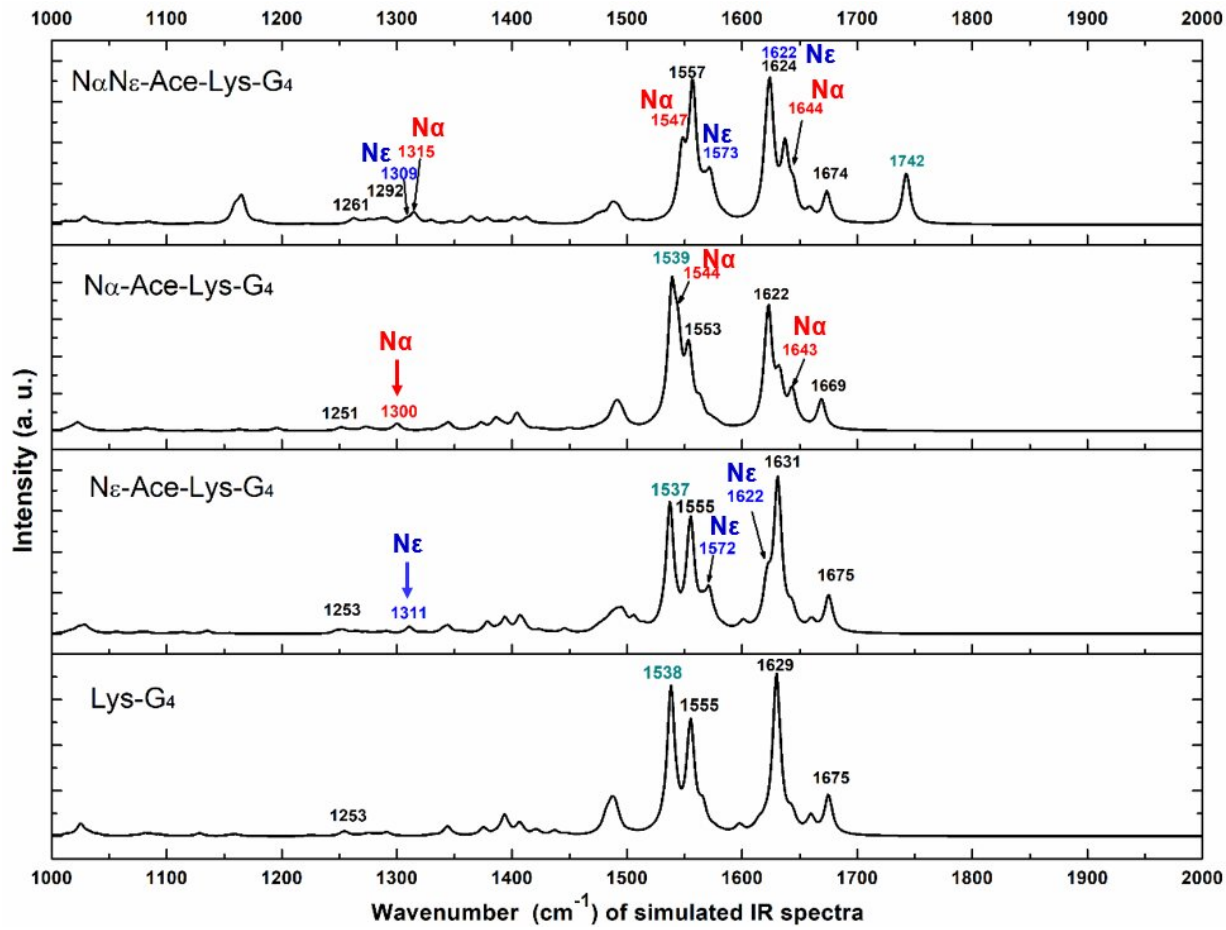
A research team led by Prof. Huang Qing from the Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences has used infrared and Raman spectroscopy to identify lysine acetylation features, providing a theoretical and experimental basis for the analysis of protein acetylation structures in biological systems.

Their results were published in *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*.

Acetylation is a common and important protein modification in biology and plays a key regulatory role in cellular metabolism. There are two ways of protein acetylation, one is Nε-acetylation specific to lysine residues, and the other is N-terminal acetylation that can occur on various amino acid residues.

At present, N-terminal acetyltransferase is generally used to label to determine whether lysine residues are acetylated, but the accuracy of this method is still controversial. Identifying protein acetylation at molecular level is one of the current research challenges, and the key is to accurately localize and characterize the acetylation of lysine to gain a clear and systematic understanding.

To solve this problem, the research team systematically studied the structural changes and corresponding vibrational spectral characteristics of the three acetylation types (Nε-Ace-Lys, Nα-Ace-Lys and NαNε-Ace-Lys) of L-lysine through infrared and Raman spectroscopy experiments and density function theory calculations. They found that the infrared and Raman characteristic bands of amide group, carboxyl group and other groups can be used to effectively identify different acetylation types.



Bottom: theoretically calculated infrared spectra of Lys-G4 polypeptide and its three acetylated molecules. Red is Nα-acetyl, blue is Nε-acetyl. Credit: Yao Guohua

In other words, whether lysine was acetylated can be told from the characteristics of infrared and Raman spectra, as well as the type of lysine.

At the same time, the team's vibrational spectroscopy identification strategy for acetylation was also verified in the peptide model.

This research provides the vibrational mode analysis of acetylated lysine

and proposes a spectral identification and a new characterization method for lysine acetylation.

More information: Guohua Yao et al, Theoretical and experimental study of the infrared and Raman spectra of L-lysine acetylation, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2022). DOI: 10.1016/j.saa.2022.121371

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