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标题: Far-infrared spectroscopy analysis of linear and cyclic peptides, and lysozyme
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来源出版物: VIBRATIONAL SPECTROSCOPY 卷: 61 页: 144-150 DOI: 10.1016/j.vibspec.2012.02.020 出版年: JUL 2012

引用的参考文献数: 35
摘要: The far-infrared spectra of lysozyme, alanine-rich peptides and small cyclic helical peptides were studied. Both lysozyme and the alanine-rich peptides had a dome in the spectral background centred on 180-220 cm(-1) consistent with either structural collective modes or an ensemble of hydrogen bond vibrational modes associated with the peptide backbone. Molecular dynamics simulation of the alanine-rich peptide's infrared spectrum produced bands with similar positions to the experimental data and vibrational density of states simulation was able to attribute several of these bands to backbone and side chain vibrational modes. Evidence is presented that peaks at 333 and 375 cm(-1) are associated with alpha-helices in lysozyme and the alanine-rich peptides, and the peak at 445 cm(-1) is associated with beta-pleated sheet. Also, results suggest that peaks at 385, 402 and 470 cm(-1) are associated with the secondary structure of the cyclic helical peptide KARAD. This supports the hypothesis the low energy vibrational modes between 300 and 500 cm(-1) are diagnostic of the presence of secondary structures in (poly)peptides. (C) 2012 Elsevier B.V. All rights reserved.
入藏号: WOS:000304686400020
语种: English
文献类型: Article
作者关键词: Terahertz; Far-infrared; Synchrotron; Molecular dynamics; VDOS
KeyWords Plus: PROTEIN SECONDARY STRUCTURE; MOLECULAR-DYNAMICS; TERAHERTZ; SPECTRA; MODES; POLYPEPTIDES; CONFORMATION; PHASE; WATER; THZ
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出版商: ELSEVIER SCIENCE BV
出版商地址: PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS
Web of Science 分类: Chemistry, Analytical; Chemistry, Physical; Spectroscopy
学科类别: Chemistry; Spectroscopy
IDS 号: 950XY
ISSN: 0924-2031
29 字符的来源出版物名称缩写: VIB SPECTROSC

ISO 来源出版物缩写: Vib. Spectrosc.
来源出版物页码计数: 7