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基础研究和新技术

ESI-MS/MS法鉴别环肽非对映异构体和碎裂机理的研究

袁谷[1];郑波[1];刘逸佺[1];李卉卉[1,2];叶蕴华[1];周 江[1]

1. 北京大学化学学院化学生物学系，北京分子科学国家实验室，生物有机与分子工程教育部重点实验室，北京 100871
2. 南京师范大学化学与环境科学学院，江苏 南京 210097

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摘要

关键词

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Discrimination of Cyclic Peptide Diastereomer and Fragmentation Mechanisms by ESI Mass Spectrometry

YUAN Gu[1], ZHENG Bo[1], LIU Yi-quan[1], LI Hui-hui[1,2], YE Yun-hua[1], ZHOU Jiang[1]

1. Beijing National Laboratory for Molecular Sciences, Key Laboratory of Bioorganic Chemistry and Molecular Engineering, Department of Chemical Biology, College of Chemistry, Peking University, Beijing 100871, China;
2. School of Chemistry and Environmental Science, Nanjing Normal University, Nanjing 210097, China

Abstract The discrimination of four pairs of cyclic peptide diastereomers were successfully achieved by ESI-MS. The ratio of ions' abundance ratios between A and B isomers in MS/MS spectra was defined as a parameter(rA, B) for discriminating diastereomers. All the four rA, B values deviates far from 1, which demonstrates excellent discrimination of the four pairs of diastereomers. The diverse spectral behaviors of CP1-CP6 was found attributing to 'mobile proton' transfer diversities and steric hindrance at fragmentation sub-surrounding due to chiral differences. MSn spectra illustrate that both CP7 and CP8 fragment through bx-yz and a1-yx ring-opening mechanisms and their chiral differences result in the predilection of the two ring-opening modes.

Key words ESI mass spectrometry _ cyclic peptides diastereomer _ distinguishing diastereomer

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