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甾体磷酸胺类缀合物在电喷雾质谱中的裂解特征

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摘要 一系列新型甾体与AZT和氨基酸酯的磷酸胺缀合物被合成, 其结构通过电喷雾正、负离子质谱得以确认。通过串联质谱, 对甾体磷酸胺类缀合物的质谱裂解特征进行了系统研究。结果表明, 在正离子质谱中, 有三种特征裂解碎片离子, 分别为从准分子离子中丢失甾体部分和氨基酸酯部分产生的钠加合离子, 以及磷酸胺经过 α 裂解产生的磷酸化氨基酸的钠加合离子。在负离子质谱中, 除(M-H)⁻外, 主要碎片离子为(M-HN₃)⁻

, (M-AZT-H)⁻, (M-steroidal moiety-H)⁻, 裂解途径与连接的氨基酸酯无关。

关键词 [steroidal conjugate](#) [phosphoramidate](#) [3'-azido-2',3'-deoxythymidine](#) [amino acid ester](#)

分类号

Characteristic Fragmentation Behavior of Steroidal Phosphor- amidate Conjugates in Electrospray Ionization Tandem Mass Spectrometry

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Abstract Novel steroidal phosphoramidate conjugates of 3'-azido-2',3'-dideoxythymidine (AZT) and amino acid esters were synthesized and determined by positive and negative ion electrospray ionization mass spectrometry. The MS fragmentation behaviors of the steroidal phosphoramidate conjugates have been investigated in conjunction with tandem mass spectrometry of ESI-MS/MS. There were three characteristic fragment ions in the positive ion ESI mass spectra, which were the Na adduct ions with loss of steroidal moiety, amino acid ester moiety from pseudo molecular ion (M+Na)⁺, and the phosphoamino acid methyl ester Na adduct ion by α -cleavage of the phosphoramidate respectively. The main fragment ions in negative ion ESI mass spectra were the ion (M-HN₃)⁻, the ion (M-AZT-H)⁻, and the ion (M-steroidal moiety-H)⁻ besides the pseudo molecular ion (M-H)⁻. The fragmentation patterns did not depend on the attached amino acid ester moiety.

Key words [steroidal conjugate](#) [phosphoramidate](#) [3'-azido-2'](#) [3'-deoxythymidine](#) [amino acid ester](#)

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