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西地那非哌啶衍生物的负离子电喷雾多级质谱研究

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摘要 采用负离子检测方式对 4种西地那非哌啶衍生物进行了电喷雾离子阱质谱研究。这 4种化合物在结构上的差异仅在于烷基取代基不同,通过比较它们之间碎片离子的异同,对其质谱裂解图解进行分析,获得了它们的结构碎片信息。在阐明化合物结构信息方面,这一方法与通常所用的同位素标记的方法类似。实验结果表明,这 4种西地那非哌啶衍生物的 (-)ESI-MS² 质谱均产生磺酰基 S-N键断裂的碎片;其 (-)ESI-MS³质谱均产生 S-C键断裂的碎片;其 (-)ESI-MS⁴质谱均产生脱去苯环上烷氧基的烷基自由基碎片。这些特征可用于阐明西地那非衍生物及其结构类似物的结构

关键词 [西地那非哌啶衍生物](#) [电喷雾离子阱质谱](#) [裂解图解](#)

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A Study of the Electrospray Ionization Mass Spectrometry of Sildenafil Piperidine Derivatives

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Abstract To investigate the characteristics of mass spectra of four sildenafil piperidine derivatives, their fragments were analyzed by electrospray ion trap mass spectrometry in a multi-stage tandem MS full scan mode performed on a Finnigan LCQ instrument. The mass spectrometry was operated in the negative mode. The mass spectra were obtained mainly by analyzing the fragments of the four compounds, the structures of which resemble with each other except the substituted alkyl group. The full scan MS² spectra of each compound gave characteristic fragment ions formed through cleavage of the sulfonyl amide S-N bond; The full scan MS³ spectra gave characteristic fragment ions obtained through the sulfonyl C-O cleavage after elimination of sulfur dioxide; The full scan MS⁴ spectra gave characteristic fragment ions formed by loss of the alkyl group on the alkoxy substituent on the phenyl ring as alkyl radical. These characteristics can be used for future structure elucidation in studies of analogues of sildenafil.

Key words [sildenafil piperidine derivative](#) [electrospray ion trap mass spectrometry](#) [fragmentation](#)

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