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## 溴苯腈辛酸酯原药中主要杂质的GC/MS定性研究

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**摘要** 利用气相色谱-质谱联用仪对除草剂溴苯腈辛酸酯原药中所含主要杂质进行了定性研究,通过质谱图推断出主要杂质及其结构,合成杂质标样,由保留时间及质谱图确认了所推断的杂质组成和结构。

**关键词** [质谱学](#) [溴苯腈辛酸酯原药杂质定性鉴定](#) [气相色谱-质谱联用\(GC/MS\)](#) [除草剂](#) [特征离子](#) [裂解途径](#)

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## Research on the Identification for Main Impurities in Bromoxynil Octanoate by GC/MS

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**Abstract** The original bromoxynil octanoate and its main impurities are identified by GC/MS. Original bromoxynil octanoate sample are dissolved in acetone, injecting the solution and separates on HP-5MS 30 m×0.25 μm×0.25 mm column coupled with GC. The peak information of significant impurities is captured by mass detector. The compounds are qualitatively confirmed by comparing with retention time and MS spectrum of the standards. Under above GC/MS conditions, all components are fully separated, impurity I is measured to be m/z 158; impurity II is m/z 317; impurity III is m/z 434. The result indicates that impurity I, II and III is methyl caprylate, 2,6-dibromo-4-cyanophenyl acetate, 2,6-dibromo-4-methoxycarbonylphenyl octanoate, respectively.

**Key words** [mass spectrometry](#) [identification of main impurities in bromoxynil octanoate](#) [GC/MS](#) [weedicide](#) [characteristic ion](#) [fragment pathway](#)

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