

Infrared Detector

ISOMERS RELATED TO DRUGS OF ABUSE

Introduction

The value of gas chromatography with vapor phase infrared spectrophotometric detection is described for a series of isomeric phenethylamines. The major mass spectral fragments for these unique isomers occur at equivalent mass and members of each series have equal molecular weights. The infrared spectra for these compounds allow for identification of any one of these amines to the exclusion of all other isomers of the series. This differentiation is accomplished without the need for chemical derivatization. All the studied regioisomers could be differentiated from the controlled drug substance via their vapor phase IR spectra. Capillary gas chromatography successfully resolved the side chain and ring regioisomers for those isomers included in this study.

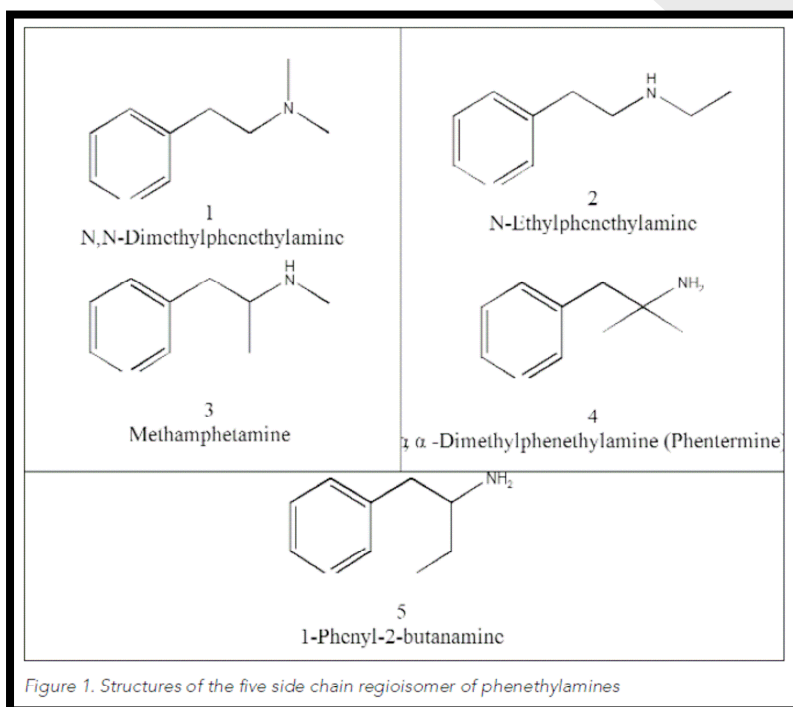
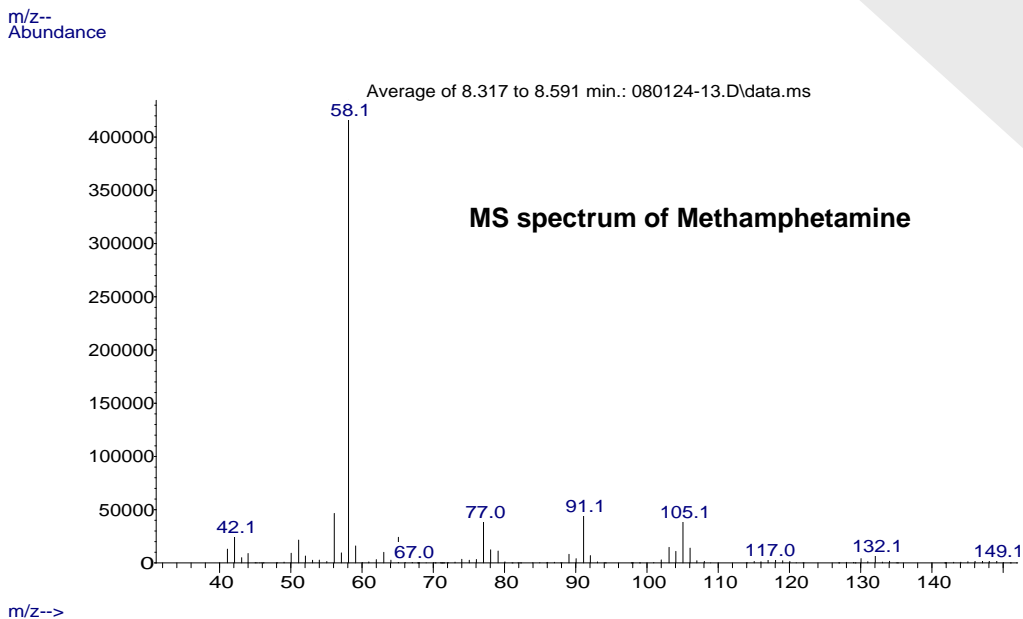
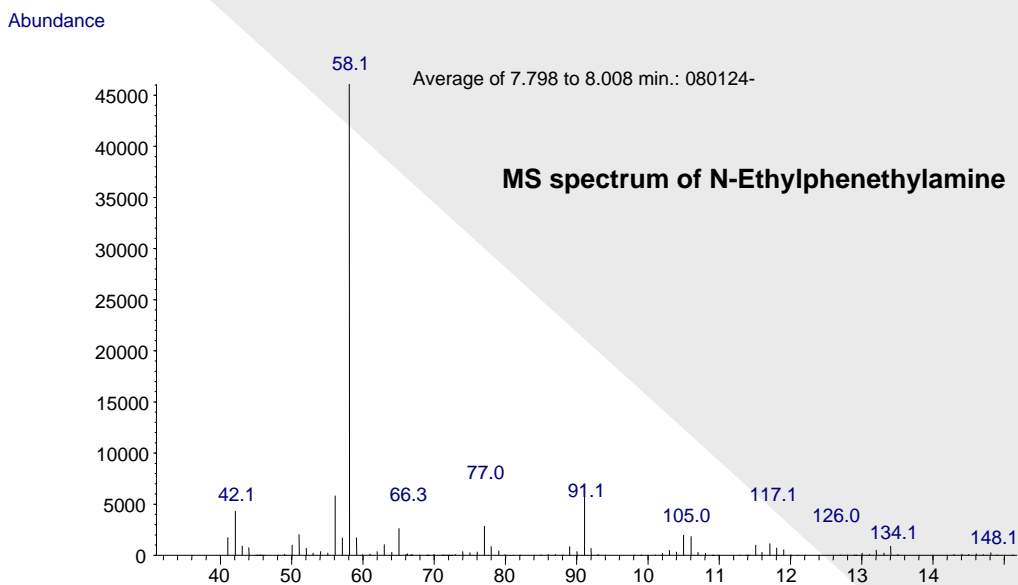


Figure 1. Structures of the five side chain regioisomer of phenethylamines

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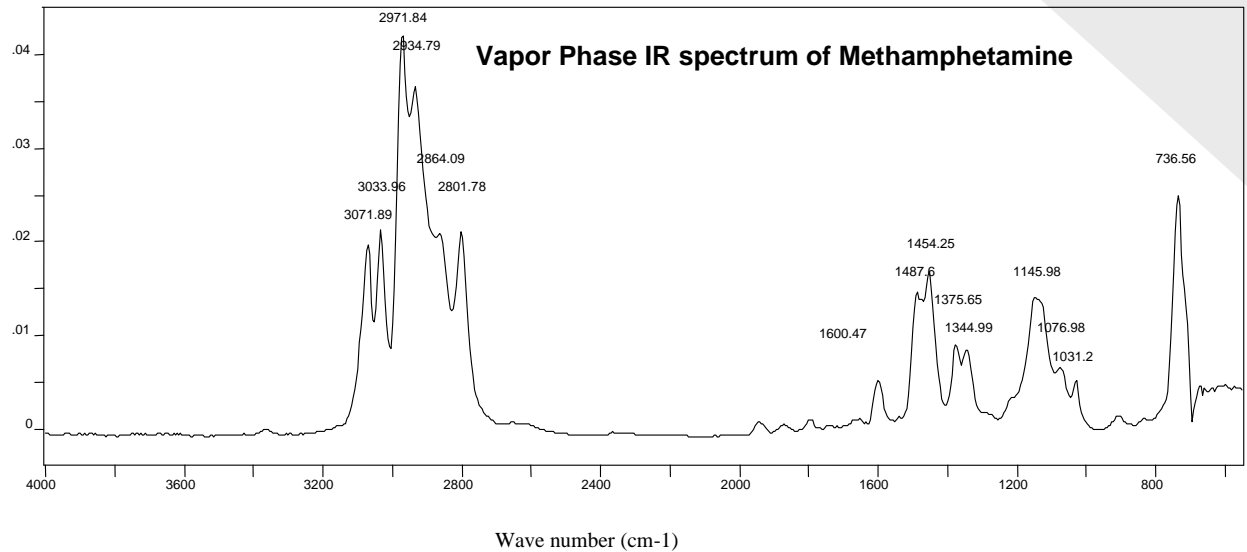
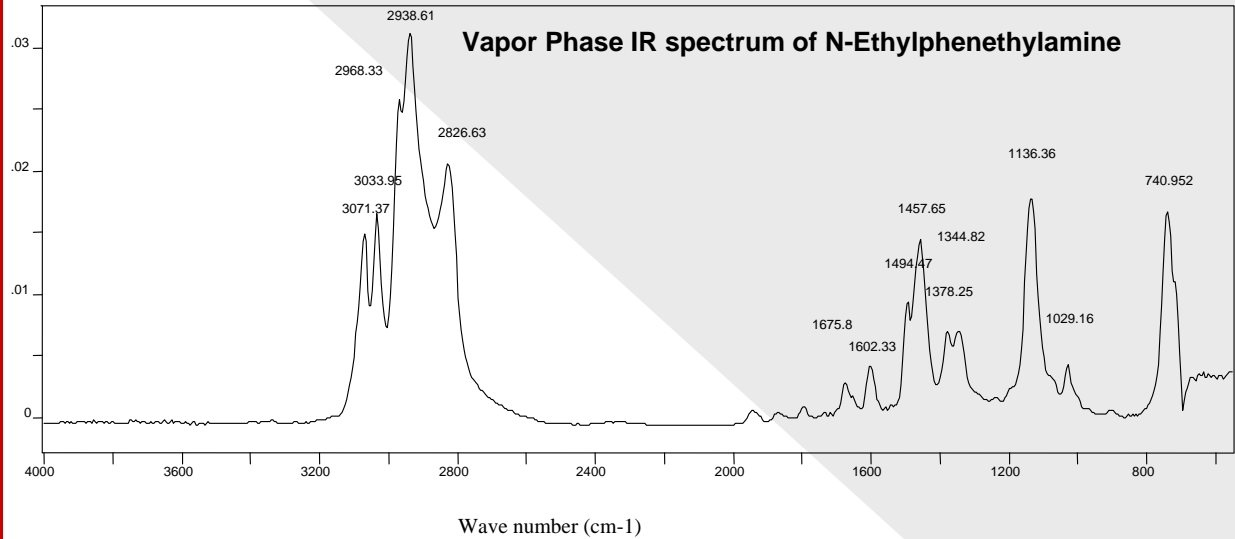
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Conditions:

Gas Chromatograph: 100°C for 1 min to 180°C at 9°/min, 180°C for 2 minutes to 200°C at 10°C/min

Injection: Splitless

Column: Rtx-50 30m x .25 x 0.5

IRD: scan from 4000 to 550 wavenumbers

Optical Resolution: 8 cm⁻¹ wavenumber

Transfer Line Temperature: 280°C

Summary

The vapor phase infrared spectra can provide unique information to assist in the differentiation of regioisomeric substances. The GC-IRD method provides complimentary data to that obtained by GC-MS. In the analysis of substances having the possibility of many regioisomeric equivalents it is necessary to apply multiple methods of structural confirmation. A searchable library of vapor phase generated infrared spectra could offer direct access to an additional level of structural confirmation having advantages of chromatographic purity as well as the elimination of possible polymorphism often observed in solid phase infrared analysis.

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