

Technical Note

The Characterization of Three FLY Compounds (2C-B-FLY, 3C-B-FLY, and Bromo-DragonFLY)

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ABSTRACT: The analysis and characterization of 1-(8-bromo-2,3,6,7-tetrahydrobenzo[1,2-*b*;4,5-*b'*]-difuran-4-yl)-2-aminoethane hydrochloride (2C-B-FLY), 1-(8-bromo-2,3,6,7-tetrahydrobenzo[1,2-*b*;4,5-*b'*]-difuran-4-yl)-2-aminopropane hydrochloride (3C-B-FLY), and 1-(8-bromobenzo[1,2-*b*;4,5-*b'*]-difuran-4-yl)-2-aminopropane hydrochloride (Bromo-DragonFLY) are presented. Gas chromatography/mass spectra (GC/MS), gas chromatography/infrared spectra (GC/IRD), and solid phase Fourier transform infrared (FTIR) spectra are presented.

KEYWORDS: 2C-B-FLY, 3C-B-FLY, Bromo-DragonFLY, Phenethylamines, GC/MS, GC/IRD, FTIR, Forensic Chemistry

Introduction

A large number of phenethylamine derivatives are abused for their hallucinogenic properties [1,2]. Recent submissions to various crime laboratories [e.g., 3,4], as well as commentary on various Internet websites and similar venues that are dedicated to drug abuse, indicate an increasing interest in a specific group of phenethylamine analogs referred to as the FLY compounds. Three of the better known FLY compounds are: 1-(8-Bromo-2,3,6,7-tetrahydrobenzo[1,2-*b*;4,5-*b'*]-difuran-4-yl)-2-aminoethane hydrochloride (2C-B-FLY), 1-(8-bromo-2,3,6,7-tetrahydrobenzo[1,2-*b*;4,5-*b'*]-difuran-4-yl)-2-aminopropane hydrochloride (3C-B-FLY, sometimes referred to as Bromo-FLY), and 1-(8-bromobenzo[1,2-*b*;4,5-*b'*]-difuran-4-yl)-2-aminopropane hydrochloride (Bromo-DragonFLY) (see Figure 1, next page). Several other FLY compounds are known but are more obscure. The “FLY” designation allegedly derives from the two “wing-like” furan or dihydrofuran rings that are fused on the opposite sides of the central benzene ring, giving an insect-like appearance with the bromo substituent as the head and the ethylamine or isopropylamine substituent as the tail.

At present (early 2008), none of the above FLY compounds are formally controlled in the United States. However, their core structures are highly similar to the Schedule I hallucinogens 4-bromo-2,5-dimethoxyphenethylamine (2C-B) and 4-bromo-2,5-dimethoxyamphetamine (DOB). For this reason, they could potentially be prosecuted under the tenets of the Controlled Substances Analogue Enforcement Act.

Due to the scarcity of known standards and consequent lack of instrumental data, the identification of these compounds has been hindered. In order to address this issue, mass spectra, gas phase FTIR spectra, and solid phase FTIR spectra are presented for 2C-B-FLY, 3C-B-FLY, and Bromo-DragonFLY.

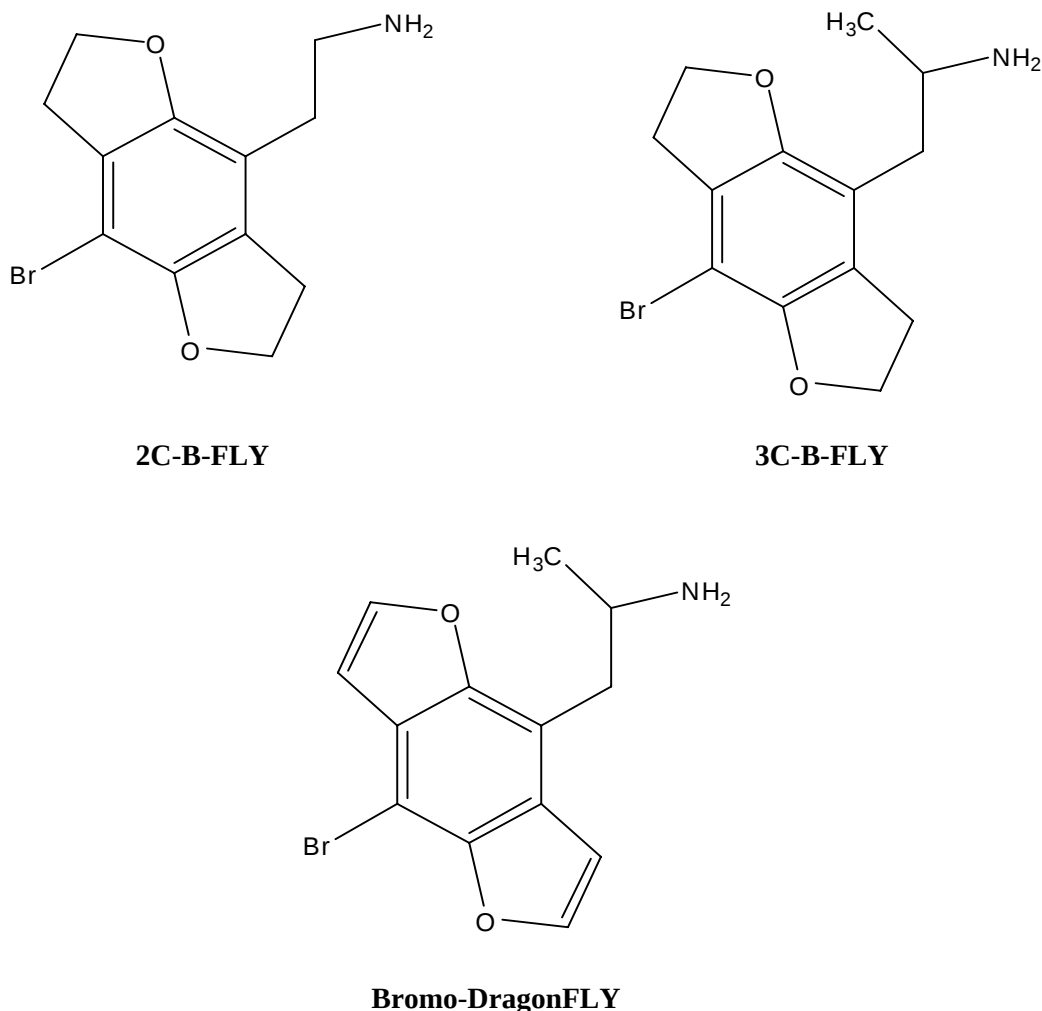


Figure 1. Structures of 2C-B-FLY, 3C-B-FLY, and Bromo-DragonFLY

Experimental

Standards: 2C-B-FLY, 3C-B-FLY, and Bromo-DragonFLY standards were synthesized and provided by the Department of Medicinal Chemistry and Molecular Pharmacology, School of Pharmacy and Pharmacal Sciences at Purdue University [5,6].

Gas Chromatography/Mass Spectrometry (GC/MS): Spectra were acquired using an Agilent Model 6890N GC equipped with an Agilent Model 5973 quadrupole mass-selective detector (MSD). The MSD was operated using 70 eV E.I. ionization. The GC was fitted with a 30 m x 0.25 mm I.D. fused silica capillary column coated with 0.52 μ m 5% phenylmethyl siloxane (HP-5MS), and was operated using a 50:1 split ratio. The injector port was maintained at 250°C. The oven temperature program was as follows: Initial temperature 200°C (2 minutes), ramped to 280°C at 20°C per minute (final hold 14 minutes). Helium was used as a purge gas at a rate of 39 cm/second.

Gas Chromatography/Infrared Spectroscopy (GC/IRD): Spectra were acquired using an Agilent Model 6890N GC interfaced with a BioRad Infrared Detector II. The GC was fitted with a 30 m x 0.32 mm I.D. fused silica capillary column coated with 0.52 μm 5% phenylmethyl siloxane (HP-5), and was operated in splitless mode. The injector port temperature was maintained at 250°C. The oven temperature program was as follows: Initial temperature 55°C (1 minute), ramped to 275°C at 25°C per minute (final hold 6 minutes). The flow cell and transfer line were maintained at 300°C. Helium was used as a carrier gas at a flow rate of 2 mL/minute.

Fourier Transform Infrared Spectroscopy (FTIR-ATR): Spectra were acquired using a Perkin Elmer Spectrum One Spectrophotometer with a universal attenuated total reflectance (UATR) accessory. Spectra were collected using 4 scans between 4000 cm^{-1} and 500 cm^{-1} .

Results and Discussion

The FLY compounds are alleged to be potent hallucinogens, and they and various other hallucinogenic phenethylamines and tryptamines are often represented to be LSD. The FLY compounds have been submitted to forensic laboratories both in liquid form and on blotter paper. The mass spectra of 2C-B-FLY, 3C-B-FLY, and Bromo-DragonFLY are presented in Figures 2-4. Unlike many simpler phenethylamines, the mass spectrum of each compound displayed a molecular ion peak. Also present are the fragmentation patterns which are characteristic of naturally occurring bromine isotopes. For each compound, *alpha* cleavage is responsible for the base peak. For this reason it is important to ensure that data is collected at a mass range with a minimum below $m/z = 30$. The gas and solid phase FTIR spectra of 2C-B-FLY, 3C-B-FLY, and Bromo-DragonFLY are presented in Figures 5-7 and 7-10, respectively. [Note: References are listed on page 33.]

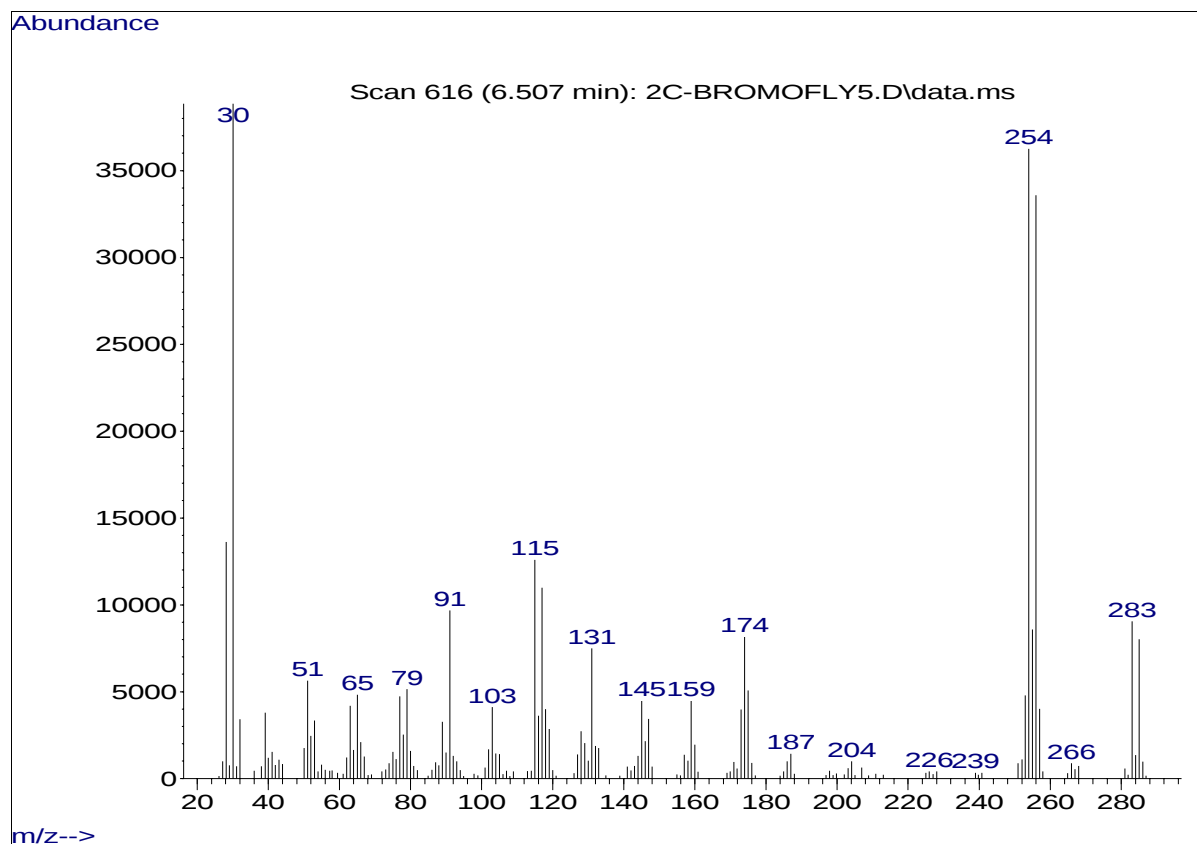


Figure 2. Mass Spectrum of 2C-B-FLY.

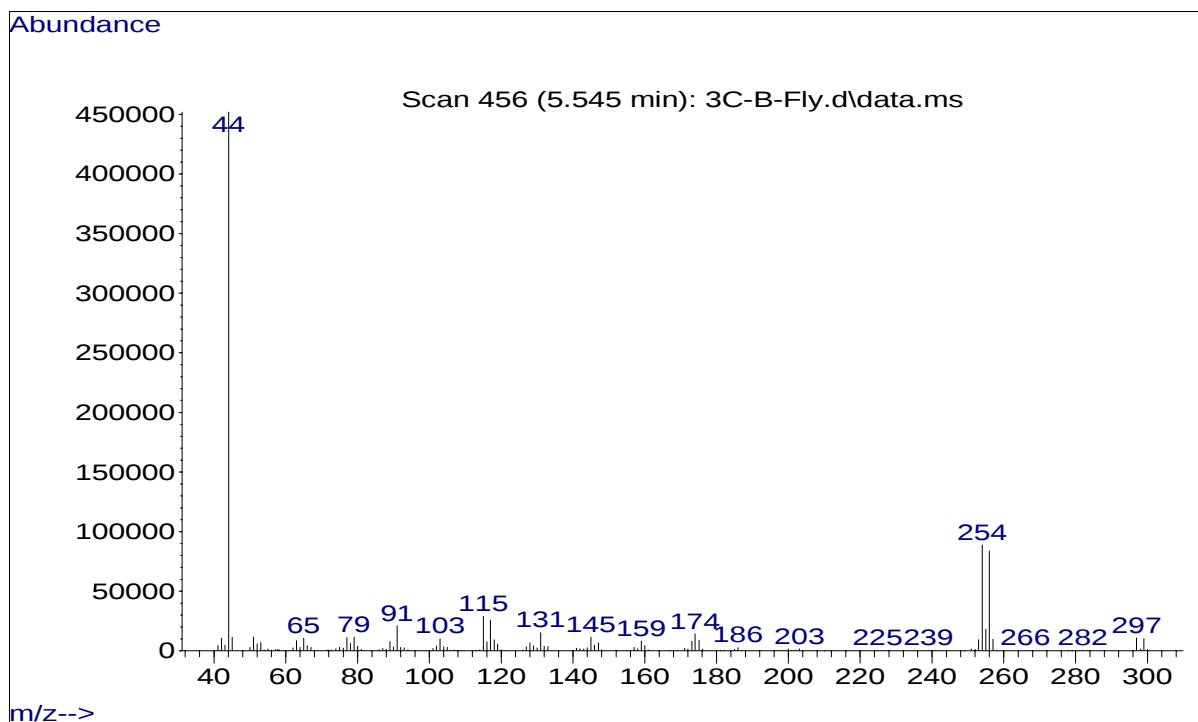


Figure 3a. Mass Spectrum of 3C-B-Fly (Bromo-Fly).

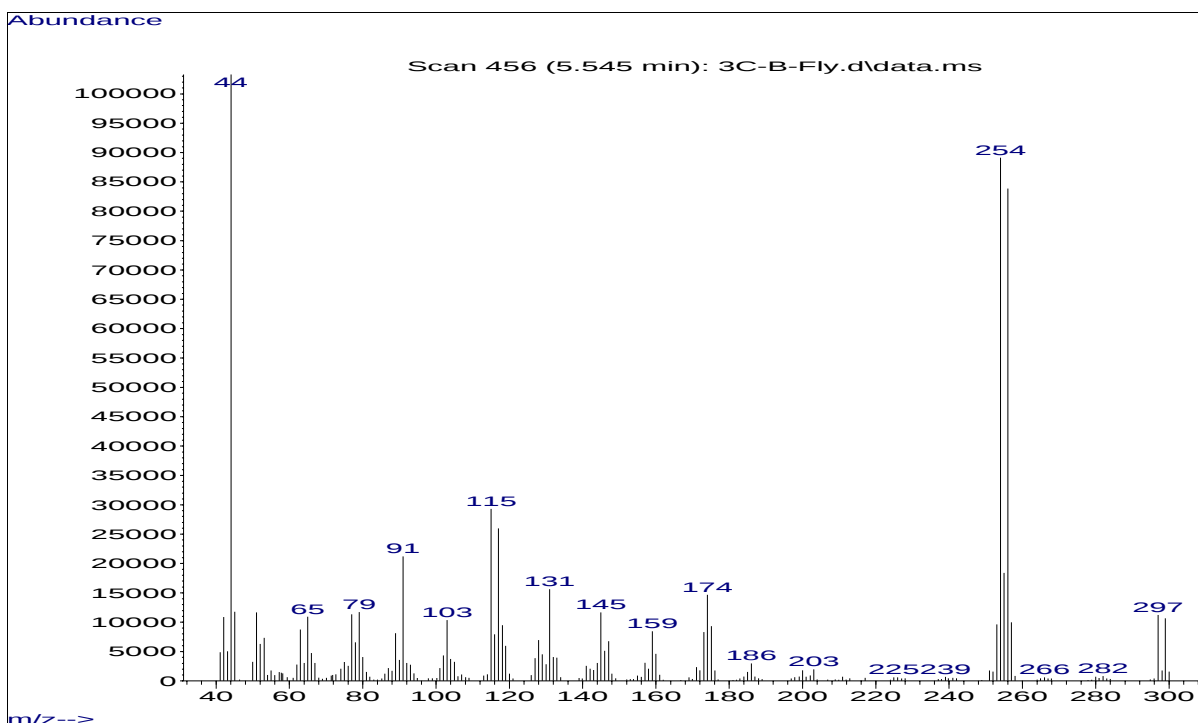


Figure 3b. Mass Spectrum of 3C-B-FLY (Bromo-FLY), Normalized to the 254 ion.

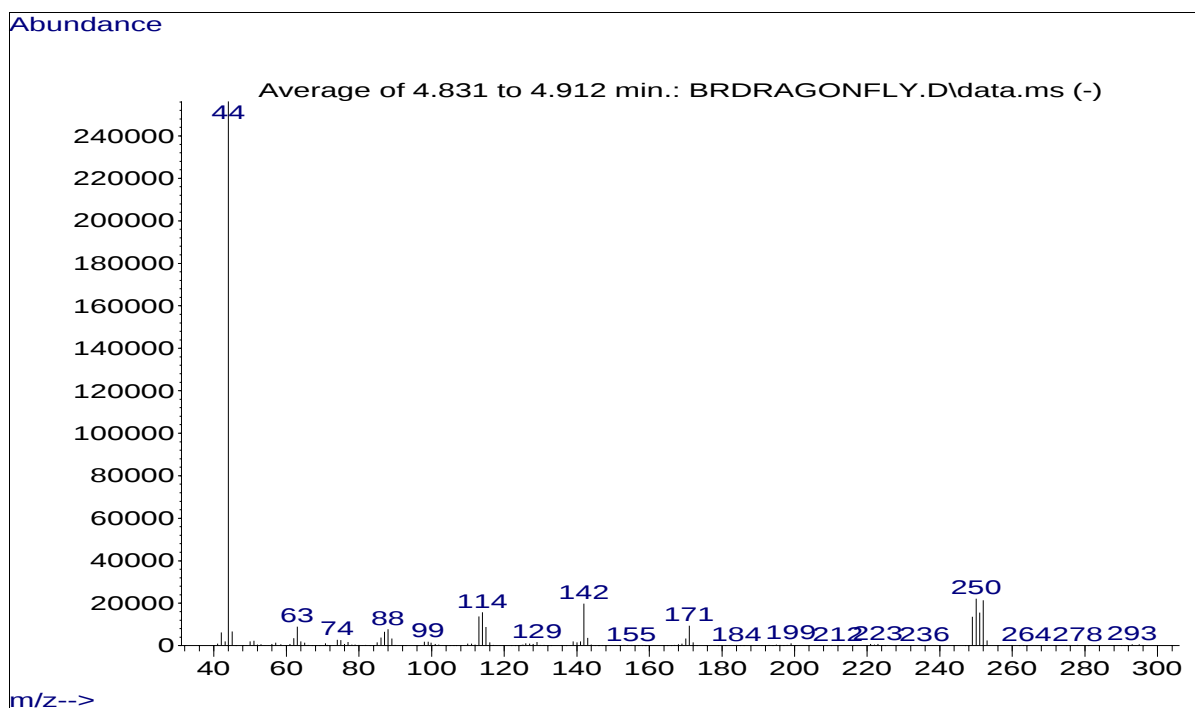


Figure 4a. Mass Spectrum of Bromo-DragonFLY.

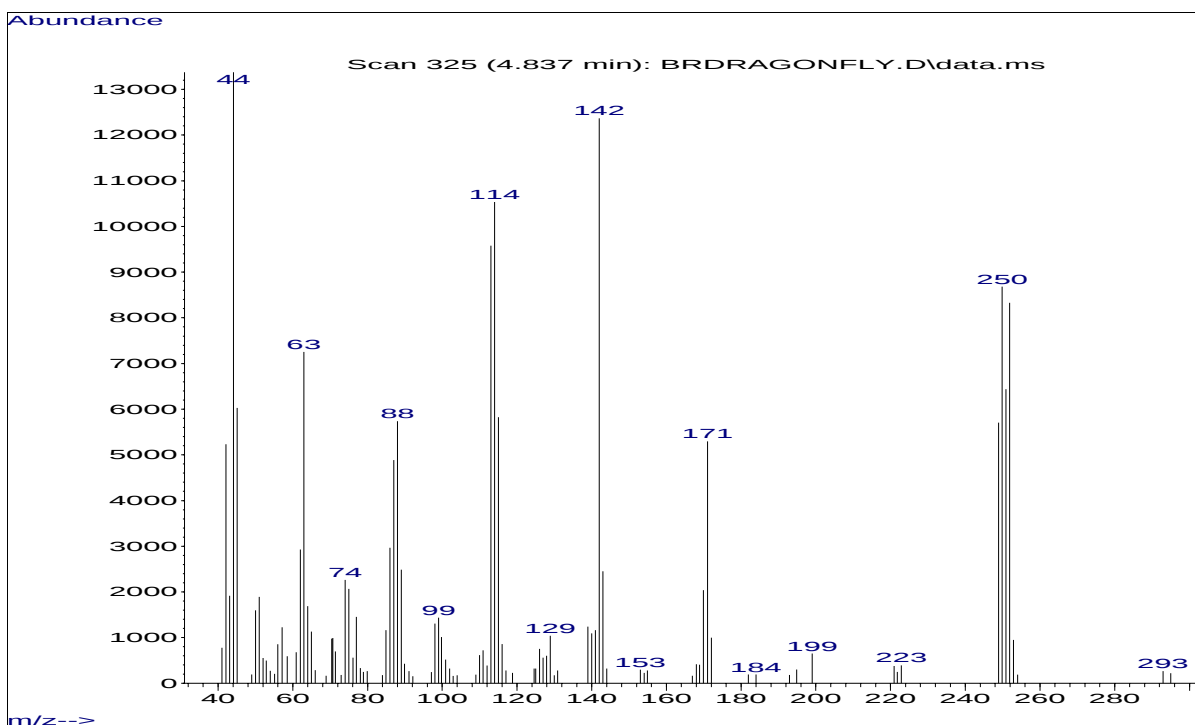


Figure 4b. Mass Spectrum of Bromo-DragonFLY, Normalized to the 142 Ion.

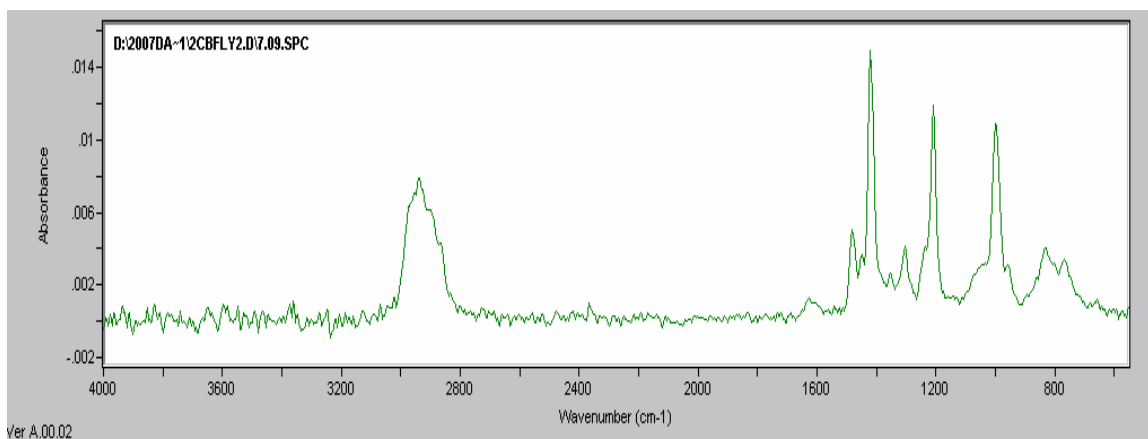


Figure 5. GC/IRD of 2C-B-FLY.

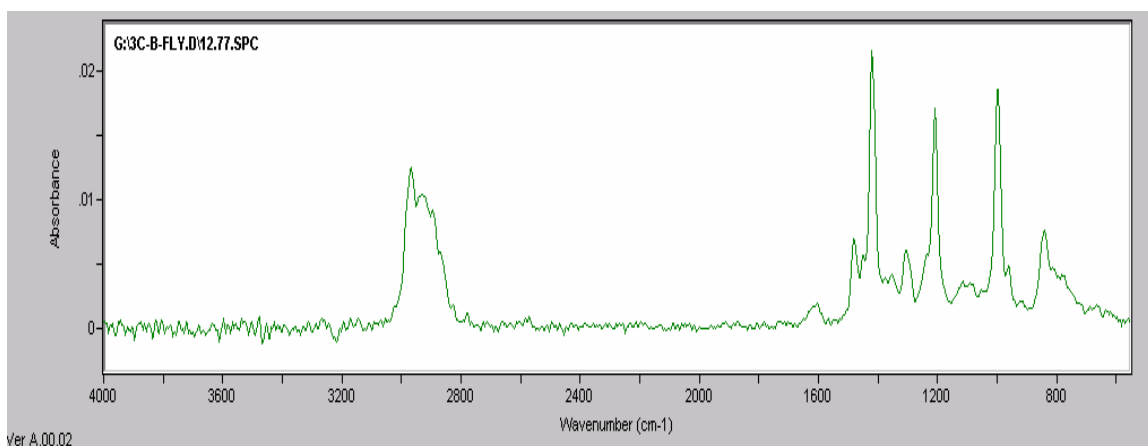


Figure 6. GC/IRD of 3C-B-FLY (Bromo-FLY).

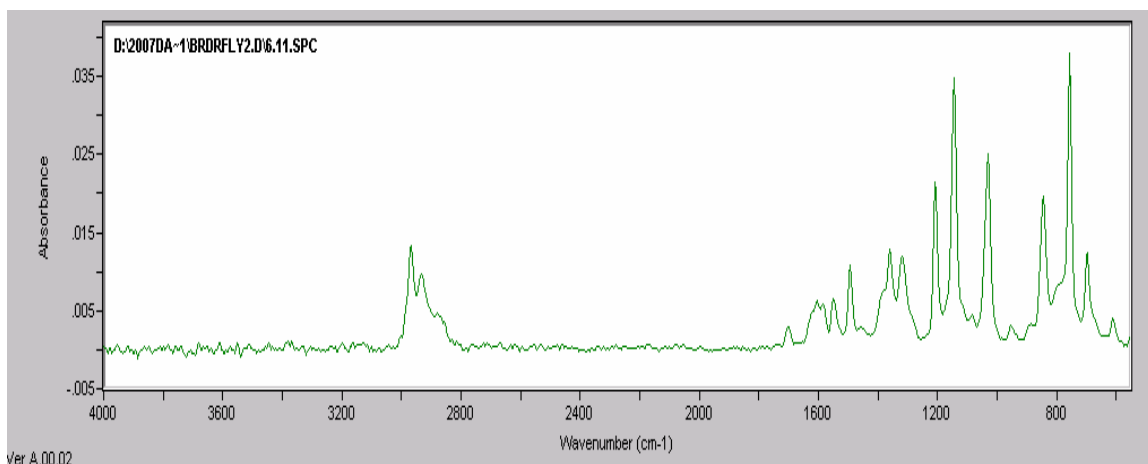


Figure 7. GC/IRD of Bromo-DragonFLY.

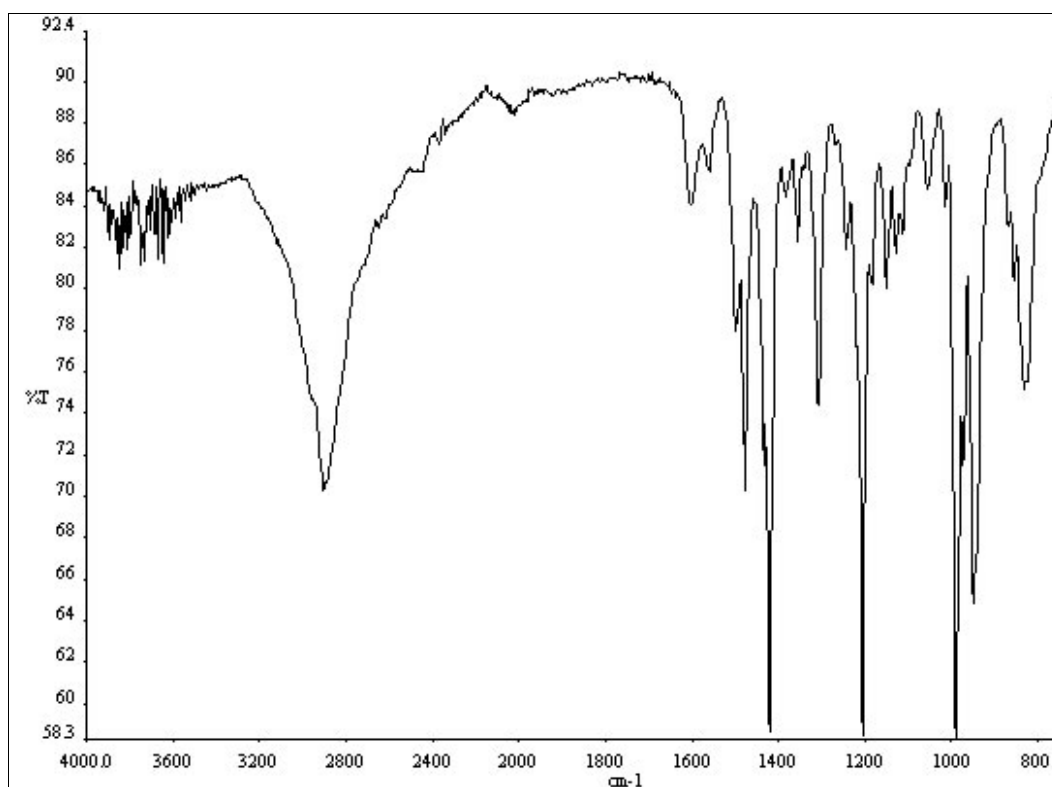


Figure 8. FTIR/ATR Spectrum of 2C-B-FLY.

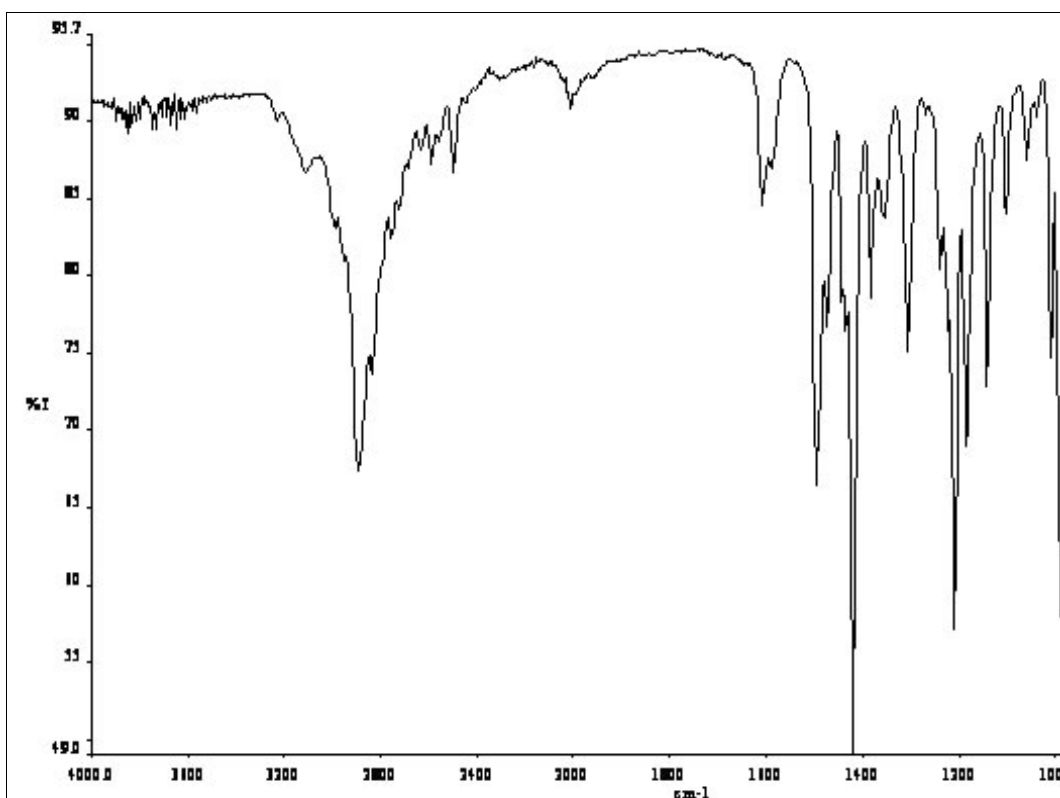


Figure 9. FTIR/ATR Spectrum of 3C-B-FLY (Bromo-FLY).

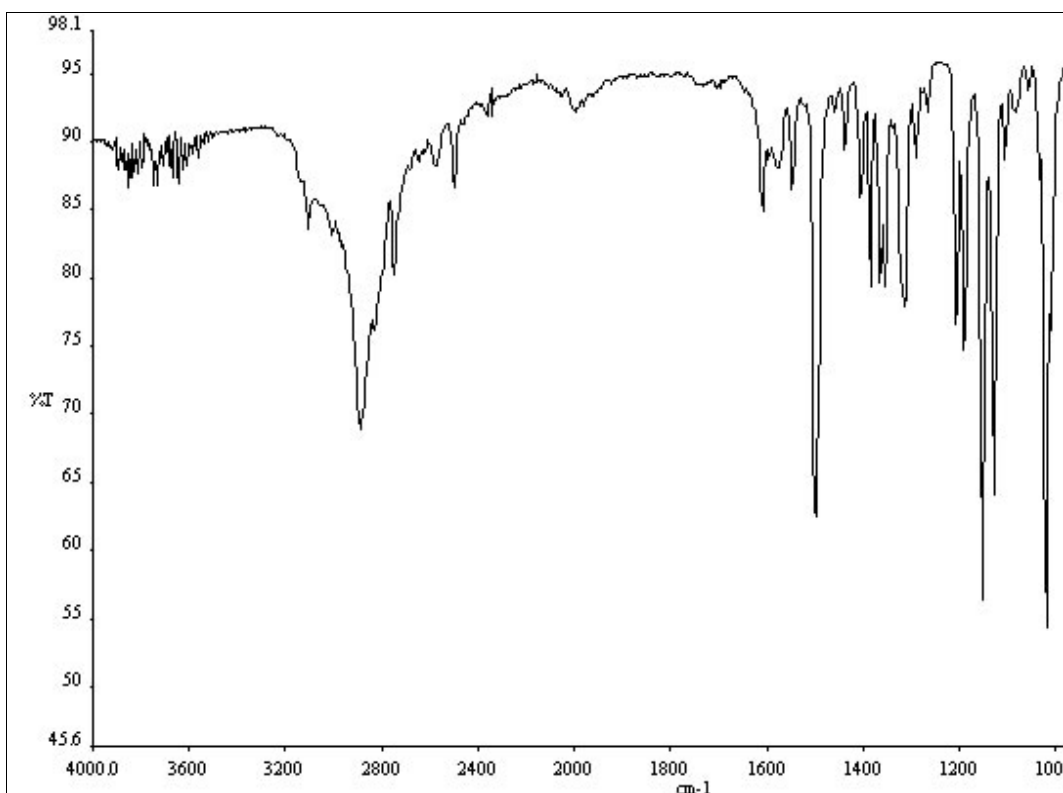


Figure 10. FTIR/ATR Spectrum of Bromo-DragonFLY.

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