IRD 3 Application Note

NBOMe Compounds

Introduction

NBOMe refers to a class of designer drugs discovered by Dr. Alexander Shulgin that contain and N-methoxybenzyl group. Of the NBOMe's that are used recreationally the most common are extensions of the 2C family of phenethylamines. In this paper we will be looking at how the IRD 3 can identify three of the most common NBOMe compounds 25I-NBOMe, 25C-NBOMe and 25C-NBOMe.

Varies counties throughout the world have enacted legislation to banned the sale and use of these dangerous compounds. In November 2014 the US DEA emergency schedule all three of the compounds listed above.

The similarities of these compounds make identification extremely difficult. When coupled with other laboratory techniques, the IRD 3 is extremely helpful in making a positive ID.

Results

For comparison purposes neat standards of all three compounds were prepped and injected. The goal was to see if any of the three compounds could be matched with entries in the ASAP IRD User Library to assist identification. The first sample run was 25C-NBOMe. A high quality library match of 99.3% (Figure 1) to 25C-NBOMe was obtained. Unfortunately the second match quality was 99.2% for 25B-NBOMe preventing positive identification. The second sample run as 25B-NBOMe. Once again when the sample was compared with the library entries (Figure 2) two libraries hits had quality matches of over 99.5%, making positive identification impossible. For the third and final sample, 25I-NBOMe a match quality of 99.7% was obtained. The second best library match was only 98% allowing for positive identification of the compound. Although the IRD was unable to positively differentiate the 25C from the 25I it was still able to give an accurate ID of the compound class. When coupled with retention time and GC-MS results positive identification is possible. In figure 4 all three compounds are overlaid to show there are small intensity differences in the spectra. Because the molecule is allowed to freely rotate in a low energy environment the molecular geometry is keep in tack, this provides a unique and highly reproducible spectra. Even with match qualities so close the analyst can be ensured that the highest match quality is truly the compound of interest.

Conclusion

For samples as similar as these NBOMe compounds, multiple laboratory techniques need to be used to aid in identification. GC-IRD is just one tool that can help the modern forensic laboratory obtain the needed information to make a positive ID.

Method Parameters

Oven:	150°C for 0 min, 25°C/min to 290°C for 10 min	Detector:	IRD 3
		Transferline A Temp:	290°C
Injection Volume:	1µL	Transferline B Temp:	290°C
Split Ratio:	5:1	Light Pipe Temp:	290°C
Carrier Gas:	Hydrogen	Resolution:	16cm-1
Column:	HP-5, 30m x 320µm x 0.25µm	Co-Add:	2

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Figure 1.

Sample	Metric	Top 3 Library Matches
25C-NBOME	99.3%	25C-NBOMe
GC R.T. = 6.45 mins	99.2%	25B-NBOMe
	98.2%	25I-NBOMe

Overlay of the Sample Spectra (in Green) and Highest Percentage Library Match (in Red)

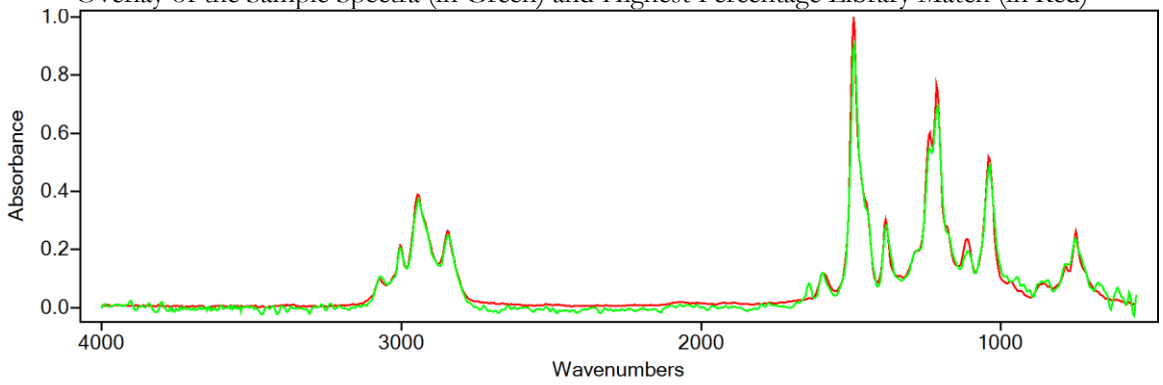


Figure 2.

Sample	Metric	Top 3 Library Matches
25B-NBOME	99.7%	25B-NBOMe
GC R.T. = 6.92 mins	99.5%	25I-NBOMe
	99.2%	25C-NBOMe

Overlay of the Sample Spectra (in Green) and Highest Percentage Library Match (in Red)

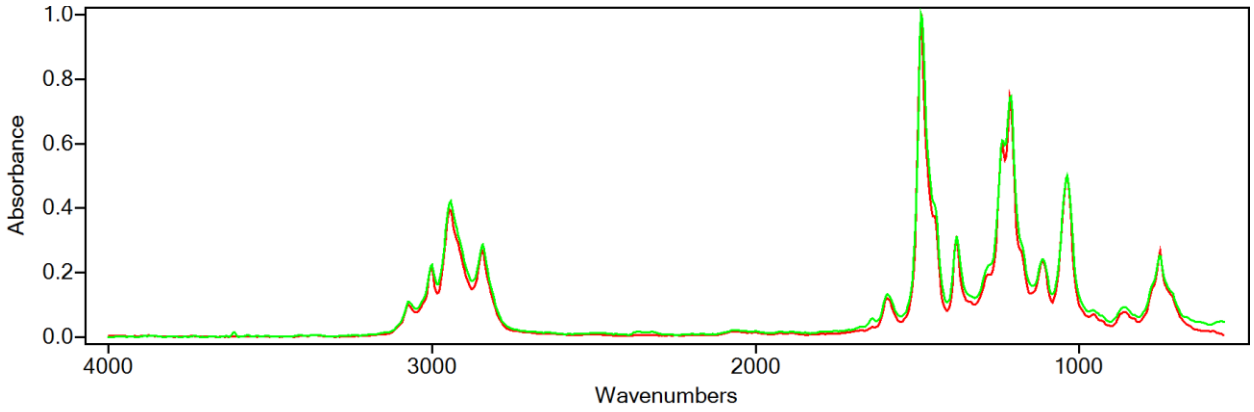


Figure 3.

Sample	Metric	Top 3 Library Matches
25I-NBOME	99.7%	25I-NBOMe
GC R.T. = 7.54 mins	98.9%	25B-NBOMe
	97.5%	25C-NBOMe

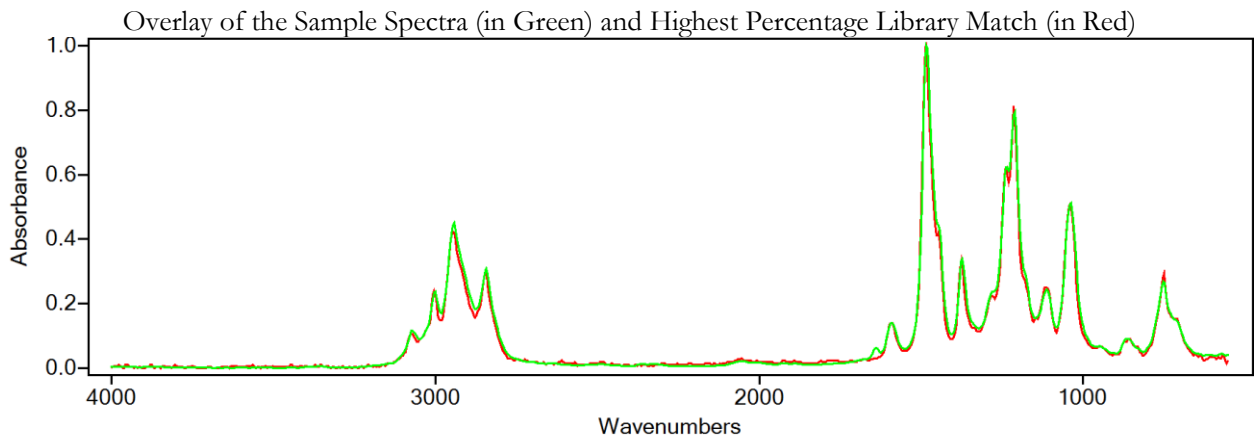
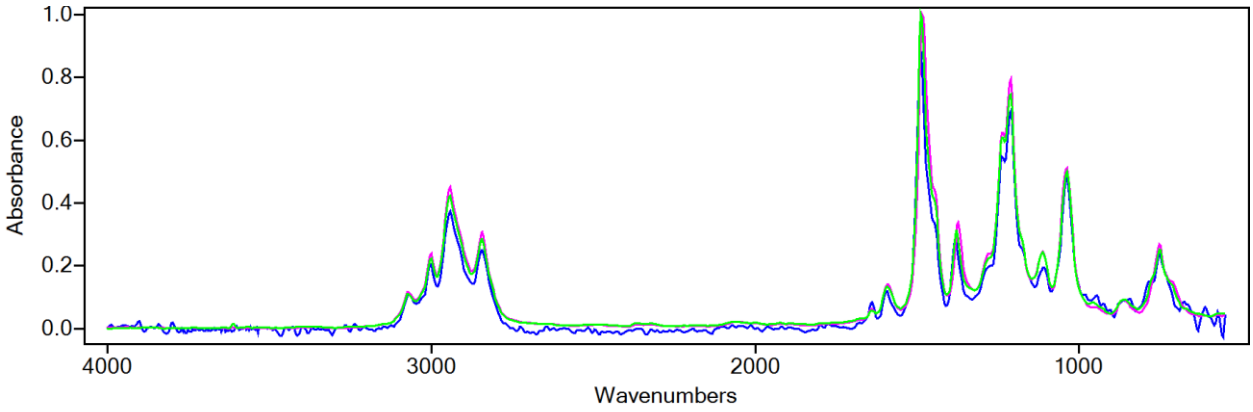
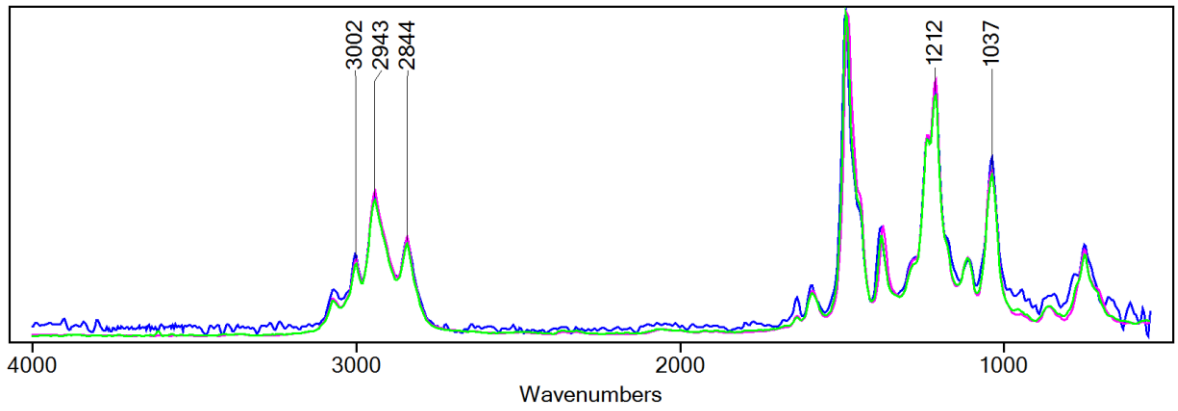


Figure 4.

Sample	Metric	Top 3 Library Matches
25C-NBOMe		
25B-NBOMe		
25I-NBOMe		
Conclusion		





Conclusion

These samples all produce spectra that are very similar, and provide very close library match percentages. Despite the similarities, the library search algorithm consistently picked the correct match. The overlays below show the spectra, and identify the main peaks that vary slightly between isomers

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