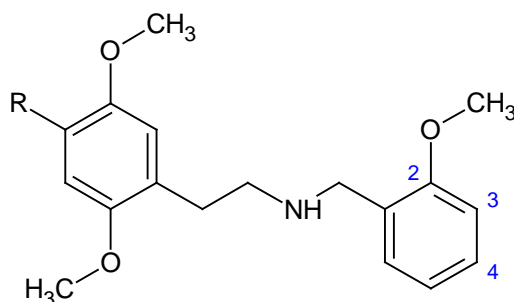


Analysis of NBOMe Isomers by Solid Phase GC-IR

A recent Microgram Journal paper by Casale and Hays at the US Department of Justice Drug Enforcement Administration (Volume 9, Number 2) reported the characterization and differentiation of eleven commonly encountered NBOMe derivatives via mass spectrometry and infrared spectroscopy. The authors noted that the NBOMe classes of compounds are high boiling late eluting compounds with respect to gas chromatography. The NBOMe's exhibit very low molecular ion abundance values ranging from 0.05 to 1% and also exhibit a very strong base peak at 121.

The ratio of 150 m/z to 226m/z has been reported as a differentiating factor between the n-propylthio (T7) and isopropylthio (T4) isomers. We found no consistency of the 150/226 ratio when comparing the data reported in the Microgram Journal with the data provided by Cayman Chemical, or with the GC/MS data obtained on our sample. The 150/226 ratio is dependent on the tuning of each mass spectrometer which may explain the lack of consistency between laboratories. The differentiation of NBOMe's and related isomers can be achieved with the infrared spectra.

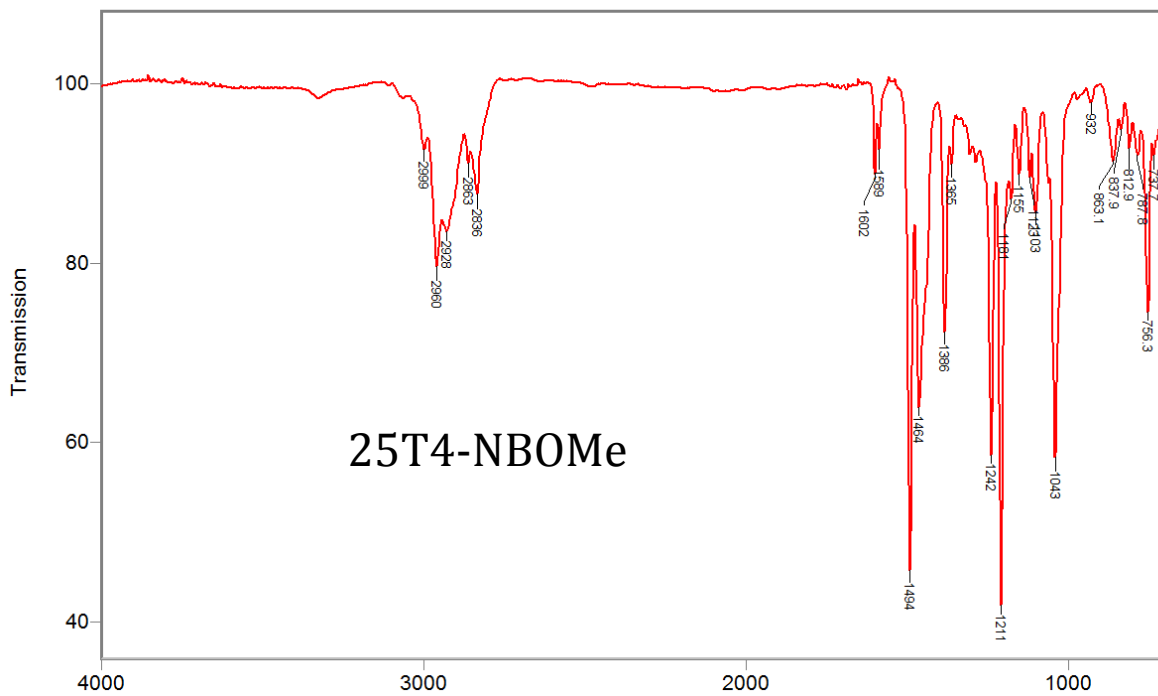
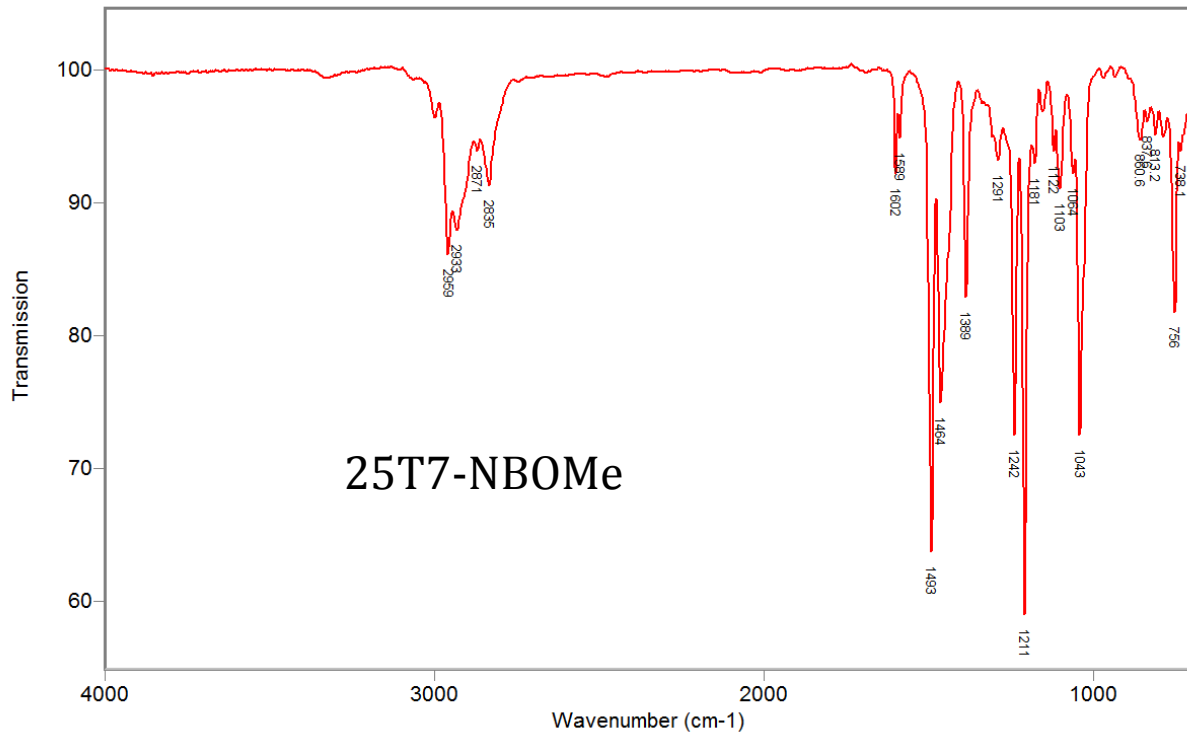


Basic Structure of a 2,5 methoxy NBOMe

In this application note we compare the infrared spectra of the available standards of the 2' methoxy benzyl compounds where the R group in the structure above is n-propylthio, or isopropylthio. The NBOMe compounds are highly potent, with dosage typically in the microgram range. Distribution on tabs of blotter paper has been observed (similar to LSD cases). The low dosage may require microgram sensitivity for detection with casework samples. The DiscovIR-GC[®] system provides high quality infrared spectra from nanograms of sample. The spectra of the standards are shown on the next page.

Name	R Group
25T7-NBOMe	CH ₃ CH ₂ CH ₂ S-
25T4-NBOMe	(CH ₃) ₂ CHS-

DiscovIR-GC[®] Infrared Spectra



Specific Spectral Features of 25T7-NBOMe (black) and 25T4-NBOMe (red)

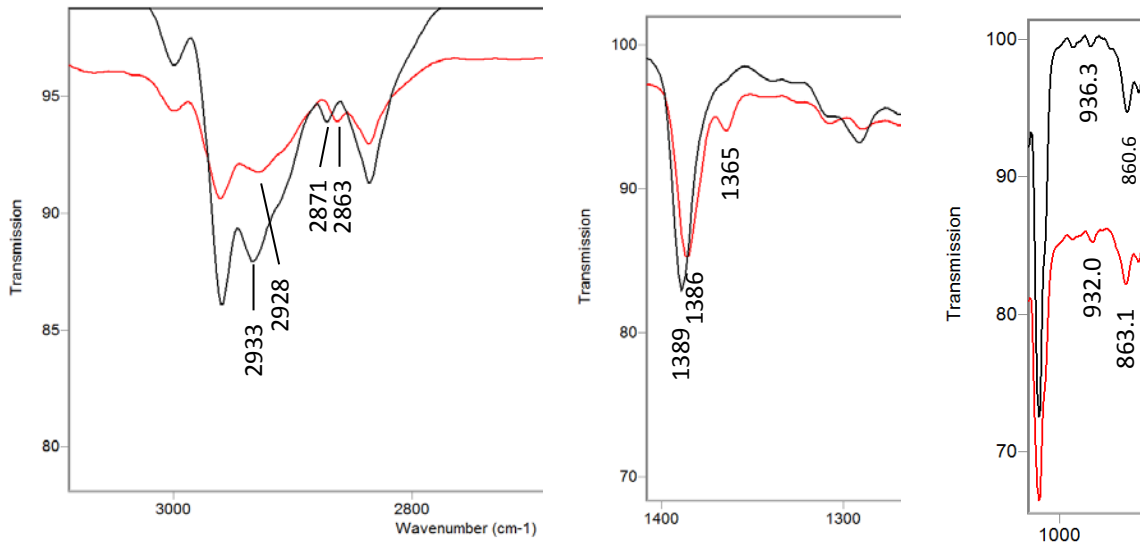
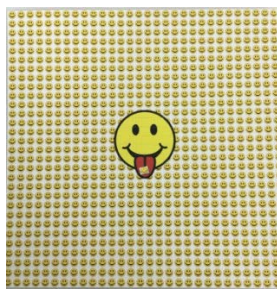


Table of Differentiating Bands						
25T7-NBOMe	2933	2871	1389	n/a	936.3	860.6
25T4-NBOMe	2928	2863	1386	1365	932.0	863.1

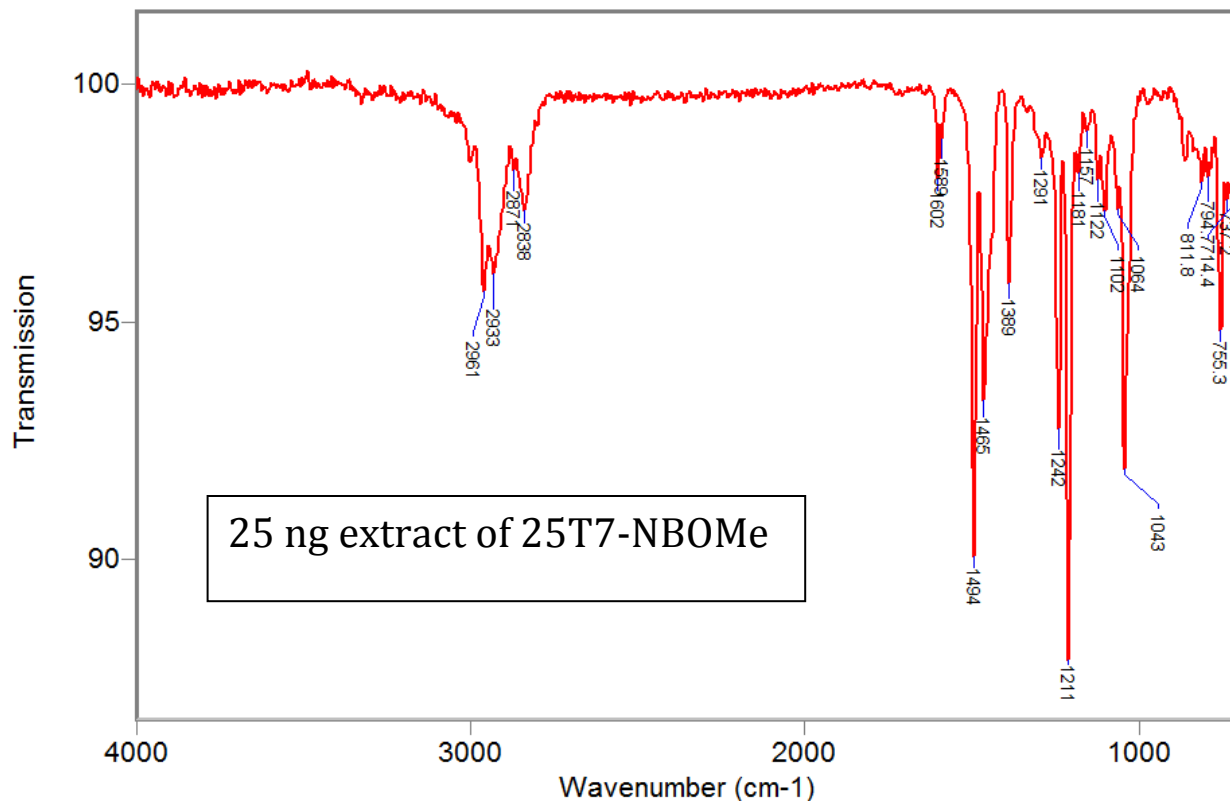
One of the street names for NBOMe's is "Smiles". A "Smiley Face" blotter art sheet with 900 perforated tabs was purchased to simulate "street samples". Alleged dosages on the Erowid internet drug user site ranged from 250-1000 micrograms per blotter tab. Individual blotter tabs were spiked with controlled amounts of compounds in chloroform. Five micrograms of 25T7-NBOMe was spiked onto a blotter tab to test the sensitivity of the DiscovIR® with blotter exhibits.



The individual tabs were placed in low volume insert and with 100 microliters of solvent. A spectra from a blotter tab spiked with 5 micrograms of 25T7-NBOMe is shown on the next page. The 100x dilution and 2:1 split ratio resulted in 25 nanograms being injected on column.



The spectra of the 25 ng injection is shown below. The bands at 2933, 2871, 1389 and the absence of the band at 1365 confirm the compound is 25T7-NBOMe. The library search software also identifies the correct isomer.



Conclusion: The DiscovIR-GC[®] system is capable of obtaining high quality infrared spectra from NBOMe compounds distributed on blotter tabs with 5 micrograms per blotter tab, or 25 nanograms injected on column. These high boiling compounds elute from the GC at temperatures above 290°C. High temperatures such as these present a challenge for GC-IR which can only be overcome by condensing the sample to the solid phase. The subtle structural differences in the molecules require high resolution solid phase infrared spectra to differentiate between isomers.

The continued appearance of new psychoactive substances challenges chemists to make correct identifications. Interpretation of subtle differences in complex analytical data to verify the identification of the unknown compound is difficult. It is increasingly apparent that multiple sophisticated technologies are needed to ensure confidence in identifications. The DiscovIR-GC[®] is an excellent addition to the forensic analytical laboratory tasked with identifying new psychoactive substances.

