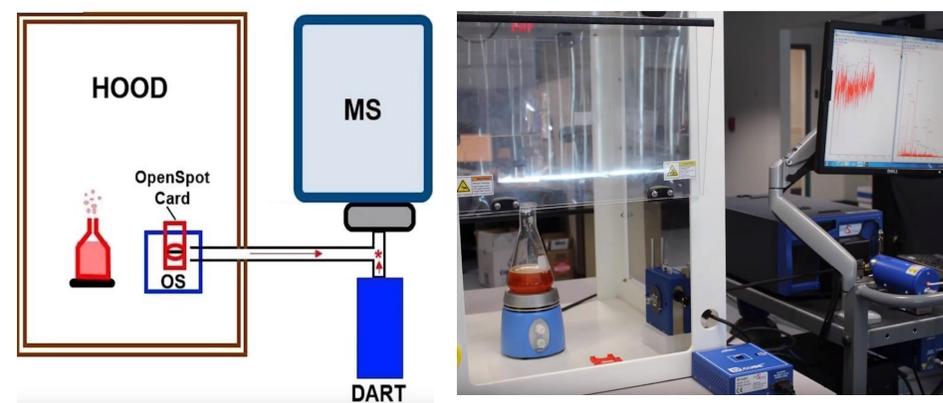


## Overview

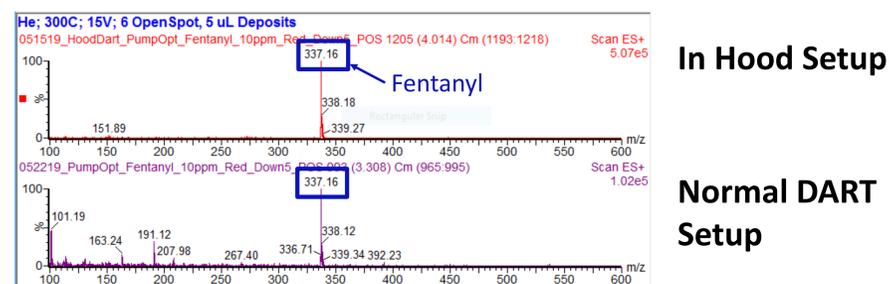
Analysis of hazardous chemicals or potent drugs with ambient ionization mass spectrometry, in organic synthesis, forensics, and other chemical industries, poses real dangers to the chemist responsible for their analysis. There have been recent efforts to move towards placing mass spectrometers into fume hoods for safer analysis; however, such close proximity the analyzed materials may also introduce instrument contamination. The ambient ionization source Direct Analysis in Real Time (DART) has remote analysis capabilities, allowing for a setup where sample desorption occurs in the hood and ionization by the DART occurs nearby, safely outside of the hood. We report here method optimization and proof-of-concept with this setup for safer analysis of several highly potent drugs.



## Experimental:

### Background Ions Decrease with In Hood Vaporization Setup

- Background ions are common in open air DART analysis
- Performing in-hood vaporization of samples prior to ionization can reduce the background intensity and variety of normal background ions

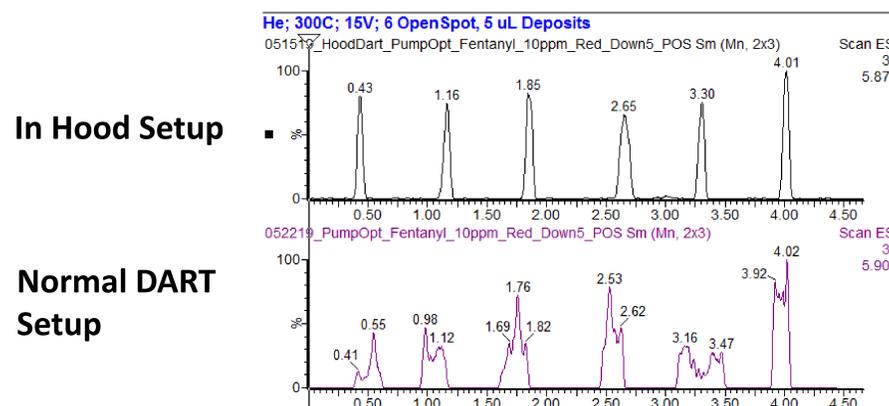


### Limit of Detection with Hood Vaporization Compared to Open Air Vaporization

	In Hood DART Setup	Normal DART Setup
Fentanyl	50 ng/mL	5 ng/mL
Codeine	50 ng/mL	5-50 ng/mL

- The normal DART ionization setup shows lower limit of detection values and better sensitivity than when performing in-hood vaporization

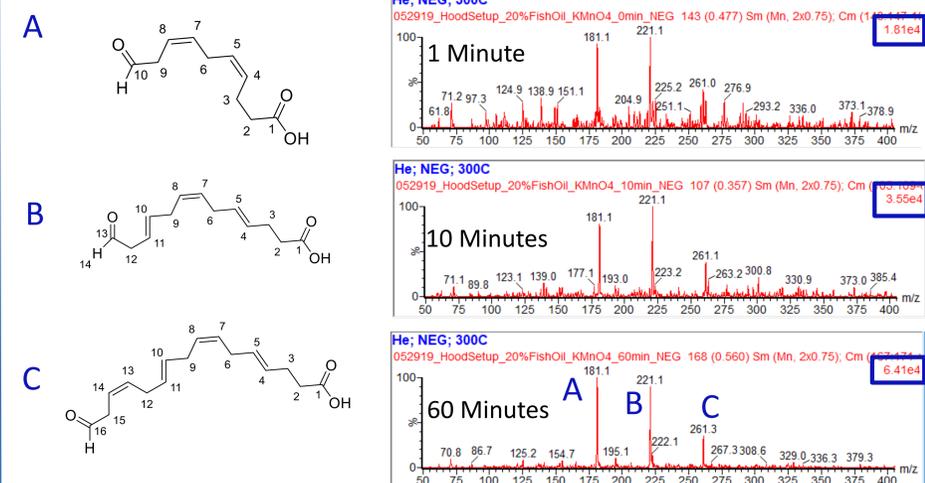
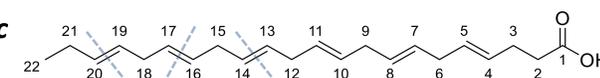
### Sharper Peaks with Less Peak Splitting is Observed Using the In Hood Vaporization Setup with DART



## Real-Time Reaction Monitoring with In Hood Setup

- Cleavage of the fatty acids DHA and EPA in odorous fish oil with the potassium permanganate reagent was achieved with the in hood vaporization setup
- Real-time monitoring of the reaction was performed showing the progression of the reaction at 1, 10, and 60 minutes
  - Cleaved product ions 181 m/z, 221 m/z, and 261 m/z (parent structures shown below) increase in intensity over time showing the progression of the DHA oxidation reaction over time.

### Docosahexaenoic Acid (DHA)



## Conclusion

- The in hood vaporization setup with DART-MS allows for safer ambient analysis of harmful samples such as fentanyl, or real-time reaction monitoring with odorous samples like fish oil
- Analysis with this hood setup shows sharper peaks with less peak splitting than is seen with the normal DART setup. The common DART background ions also decrease with the in-hood vaporization analysis.
- The in hood setup has low LOD's of drugs of abuse at 50 ng/mL, but the normal DART setup still achieves better LOD's and sensitivity
- **Despite potentially sacrificing some sensitivity, which is compound dependent, the in hood DART setup offers many advantages over DART analysis in open air especially when analyzing potentially harmful or odorous chemicals best handled in the hood.**

## Methods

### In Hood Vaporization of Followed by DART Ionization

A DART-SVP ionization source is interfaced to a Waters QDa single quadrupole mass spectrometer.

- 1) A small amount of sample is spotted onto a wire mesh card, which is inserted into a modified OpenSpot Vaporizer unit tethered from the hood.
- 2) A current is applied to heat up the sample carrier, vaporizing the chemicals
- 3) Vaporized sample is then transferred from the hood environment to the DART ionization region by passing through the tether.
- 4) Once the vaporized sample enters the DART ionization region, the sample is ionized and is pulled into the MS for analysis.