Analysis of Fluorinated Anesthetics Using Laser Spectroscopy
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Introduction
One of the purposes behind this study of fluorinated anesthetics was to provide a link between laser spectroscopy and our interest in the medical field. Laser photo-acoustic spectroscopy provides a way to identify and quantify molecules in the gas-phase. Common gases found in the medical field include such fluorinated anesthetics, administered via inhalation.

Inhaled anesthetics, such as isoflurane, enflurane, and sevoflurane, are used during various medical procedures to produce an anesthetic state, which is done by setting a specific concentration of the molecules in the central nervous system via the lungs and bloodstream (1). These molecules provide the desired physiological response by binding to GABA, receptors (2, 3).

The use of anesthetics in the medical field can affect not only patients but also operating medical teams through leaks in the system (4). Current spectroscopic methods for monitoring these volatile anesthetics take advantage of the infrared (IR) region (5, 6).

Our work illustrates the potential of laser photo-acoustic spectroscopy in the near-IR region to distinguish the different anesthetics, and to contribute to the large goal of monitoring volatile compounds in medical settings.

Experimental
The gas-phase samples were analyzed by laser photo-acoustic spectroscopy. Laser dye (a mixture of LDS 867 and LDS 925), excited by pulsed 532 nm photons from a Nd:YAG laser (10 ns pulses, 10 Hz), acted as a medium to generate light at the selected wavelengths (10-20 mJ/pulse).

Liquid anesthetics were obtained via SynQuest Laboratories and the Hall lab at Smith College. The anesthetics were chosen for the similarities in their ester structure (Table 1). Air was removed from the photo-acoustic cell (Fig. 1), and the liquid evaporated from a glass vacuum flask to fill the cell until its vapor pressure.

The pulsed laser beam hit the gaseous anesthetics by passing through the cell lengthwise. The absorption was monitored using a hearing-aid microphone in the center of the cell. When the molecules absorbed the light, they generated a pressure wave that was sensed by the microphone and processed as an electronic signal. As the laser wavelength was scanned in small steps (0.05 nm), observed large signals indicated optimal wavelengths for the anesthetics to absorb energy from the laser.

Results and discussion
Photo-acoustic spectra that we obtained in the near-IR region (Fig. 2) represent absorption to generate vibrationally excited molecules, with four quanta of C-H stretch. The multiple peaks in each spectrum arise from the different types of C-H bonds.

Isoflurane, enflurane, and sevoflurane each have a unique absorbance pattern. Such differences could be useful to identify these anesthetics in the near-IR region.

Future computational analysis and comparison with similar molecules will elucidate the assignment of the peaks, to show which C-H bonds are responsible for each signature. Preliminary assignments here are based on similarities in spectra and on relative peak intensities.

Isoflurane and sevoflurane both feature a peak around 862 nm; this could be due to their similar C-H bond, on the carbon sandwiched between the terminal C and the O. Similarly, isoflurane and enflurane both have a peak near 880 nm and a single H atom on the fluorinated methyl group. Sevoflurane’s two similar C-H bonds are likely to give rise to a single peak with twice the intensity, consistent with the half peak at 885 nm.

The appearance of additional peaks is not surprising, since these molecules are each likely to exist in more than one conformer at room temperature. Different conformations place the C-H bonds in different environments, thus changing the wavelengths required to excite them. Also, isoflurane and enflurane have chiral isomers that could have distinct spectral signatures.

Conclusion
By seeing into the ability of each anesthetic to absorb energy at different wavelengths, one can make use of near-IR technology to monitor these volatile compounds not only in medical settings, but also in other fields that deal with volatile substances.

Further experimentation to understand these spectra could include comparing isoflurane, enflurane and sevoflurane with other anesthetics, such as halothane or desflurane, all which have a similar structure.

This study of analyzing different anesthetics and their absorption properties in the near-IR region is an example of the interdisciplinary nature of research. By starting this particular bridge between laser photo-acoustic spectroscopy and the medical field, we found that there are many links between the different areas of the sciences.

References

Acknowledgements
Prof. Hsieh for helping our exploration of connections with the medical field, AEMES, Smith College Department of Chemistry and Collaborations, and Prof. Hall for expanding our knowledge of anesthetics.

Table 1. Structures and relative pressures of each anesthetic

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<tr>
<td>Enflurane</td>
<td>F F F O H</td>
<td>172</td>
</tr>
<tr>
<td>Sevoflurane</td>
<td>F F F H F</td>
<td>157</td>
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Fig. 1. A microphone attached to the cell transmits wavelength absorption information to the computer.

Fig. 2. Laser photo-acoustic spectra for isoflurane (top), enflurane (middle), and sevoflurane (bottom).

Fig. 3. Photo-acoustic cell used to interact excited laser dye with anesthetics. A microphone attached to the cell transmits wavelength absorption information to the computer.

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