Vaping misuse of 'liquid X' – a vibrational spectroscopy study

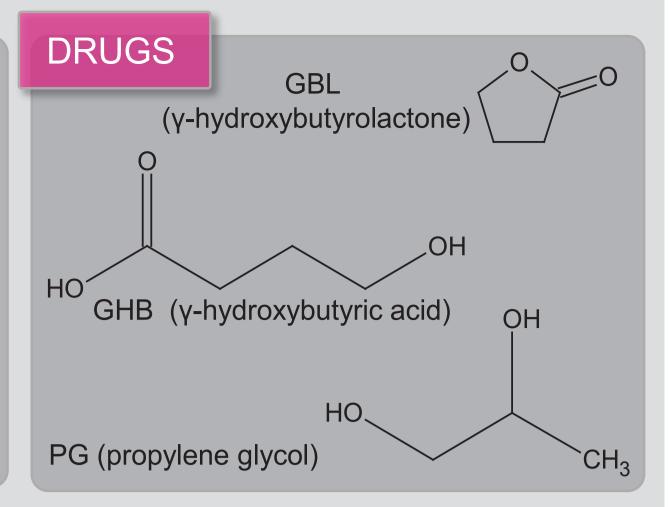
INTRODUCTION

Recently, there has been a huge growth in vaping, i.e. the use of electronic cigarettes for the consumption of both nicotine-containing and nicotine-free liquids ('e-liquids') that are vaporised to be inhaled. There are variety of eliquids for intended use available on the market with the base carrier of propylene glycol (PG), however, news reports reveal that vaping has become a vehicle for vaping misuse of illegal drugs, such as cannabis and synthetic cannabinoids. Recipes for e-liquids involving illegal substances are easily accessible on the internet for any user.

AIMS AND OBJECTIVES

Vibrational spectroscopy analysis of clandestine eliquids containing 'liquid X' aka GHB (γ-hydroxybutyric acid) and its chemical precursor GBL (γ-hydroxybutyrolactone), before and after vaping.

- Build a new trapping system for vapour and aerosol collection during vaping.
- Use vibrational spectroscopy to analyse collected samples.
- Characterise spectra of e-liquid base PG as well as above compounds.



METHODOLOGY

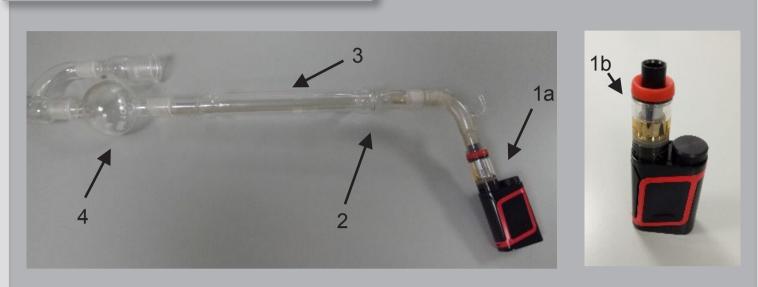


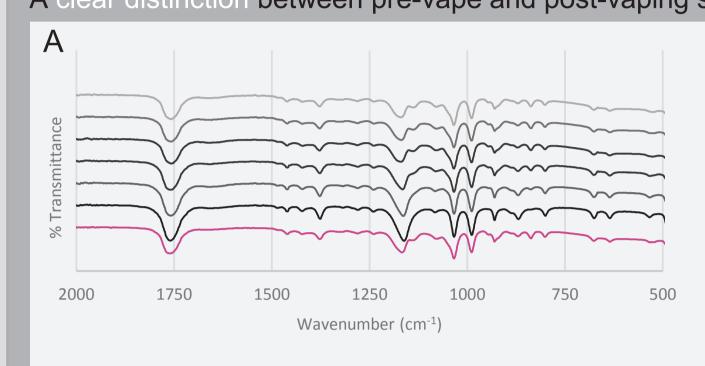
Fig 1: 1a E-cigarette with tank, 1b e-liquid changed colour during vaping; 2 glass wool for trapping vapour/aerosol; 3 condenser to aid collection; 4 bulb to prolong vapour exposure to traps

Clandestine mixed e-liquids were analysed using both Raman and Infrared spectroscopy (IR) pre- and post-vaping. Each e-liquid type was vaped for a maximum of 10 tanks (2 mL of e-liquid/tank) to mimic realistic vaping behaviour. Sample collection was glass wool as a physical trap placed in the apparatus. Samples were collected and analysed by IR and Raman spectroscopy pre-vaping, and after vaping of 1, 2, 4, 6, 8 and 10 tanks. A total of 32 scans was collected for each IR spectrum. Data evaluation was performed using MS Excel 365 and Tanagra (1.4.50).

Fig 2: Vaping simulation apparatus. E-cigarette is connected via glass tubing to vacuum pump with adjustable pressure. Condenser and ice bath aid collection of liquefied vapour and aerosol.

RESULTS

Analysing the spectra obtained from GBL and PG mixtures a close similarity between all vaping repeats using the same coil for up to 10 tanks can be seen (**Fig 3A**). Therefore, cluster analysis was performed. A clear distinction between pre-vape and post-vaping samples can be seen.



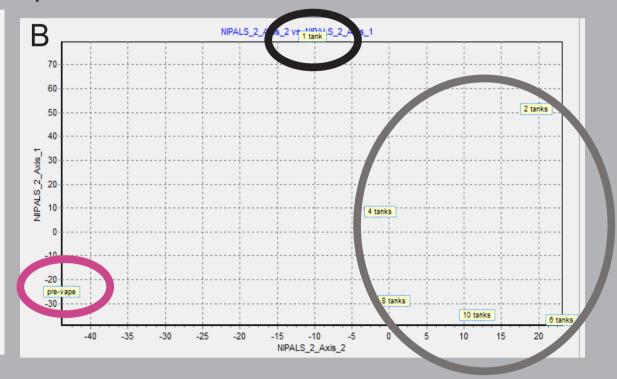
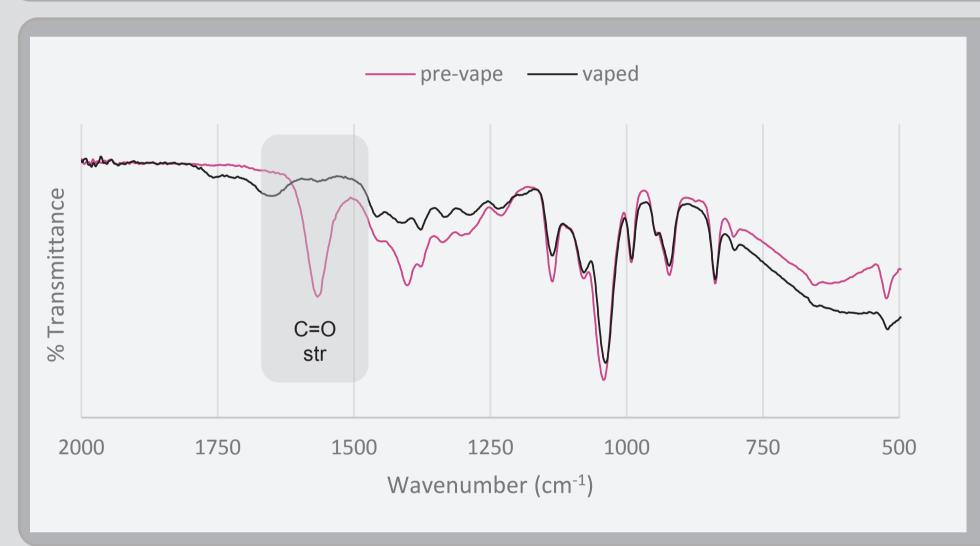
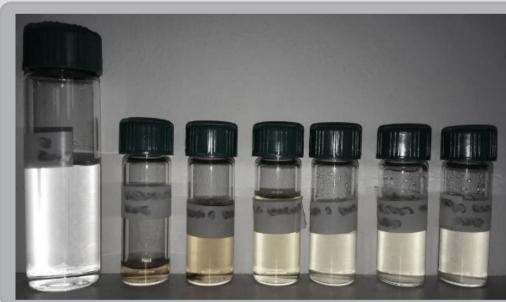


Figure 3: Collection of IR spectra and Principal Component Analysis (PCA) **A:** Infrared spectra of GBL and PG (1:1) both pre-and post-vaping. **B:** Visualisation of cluster analysis showing PC1 vs PC2 (78% of variability) of GBL and PG (1:1) using NIPALS



GHB showed a significant change in its IR spectrum post vaping with the disappearance of carbonyl stretching band around 1570 cm⁻¹. Contact of e-liquids to the heated coil could lead to the creation of harmful substances.

Figure 4: Comparison of GHB in PG pre- and post-vaping (2 mL vaped).



The PG carrier e-liquid showed a colour change from colourless to brown by vaping one tank (2 mL). Further vaping using the same coil yielded in gradually lighter coloured post-vape PG samples.

Figure 5: Comparison of PG e-liquid pre- and post-vaping. Left to right: pre-vaping, tank 1 (2 mL) vaped, 2 tanks, 4 tanks, 6 tanks, 8 tanks and 10 tanks vaped.

CONCLUSION

The change in colour of vaped and condensed e-liquids could indicate a potentially harmful change in the composition of e-liquids due to close contact to a heated metallic wire, i.e. the coil. The most extreme change in both colour and odour was observed when vaping GHB mixed with PG. IR analysis of the samples corroborated a structural change of the active ingredient through the disappearance of key band in the spectrum.

Vaping misuse of legal and illegal substances is becoming more popular, yet very little research has been done to this date towards understanding the chemical effects the vaping process has on those substances used, and the potential harm that could result from such change. This project came a step closer to shedding light onto the subject, potentially aiding to understanding the harmfulness of vaping misuse.

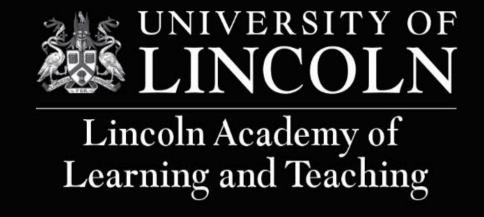
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