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Data Article

Data on ethyl glucuronide and cocaethylene concentrations in the hair of cocaine users

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ABSTRACT

We present data on ethyl glucuronide and cocaethylene concentrations from the hair of cocaine users. Head hair from 64 subjects, previously tested for cocaine, cocaethylene, benzoylecgonine and anhydroecgonine methyl ester (AEME), were subsequently analysed for Ethyl Glucuronide (EtG). Samples were prepared by solid phase extraction and analysed using gas chromatography coupled to tandem mass spectrometry. The dataset is made available to allow analysis of possible correlation between cocaethylene and ethyl glucuronide or between other metabolites presented in the data.

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Specifications table

Subject area	<i>Chemistry</i>
More specific subject area	<i>Forensic toxicology</i>
Type of data	<i>Table, figure</i>
How data was acquired	<i>Head hair samples were analysed using gas chromatography coupled to tandem mass spectrometry to acquire identification and concentration of alcohol and cocaine metabolites.</i>

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Data format	Analysed
Experimental factors	Hair sample length, hair preparation and analysis methodology is consistent throughout.
Experimental features	Hair samples from 64 subjects were previously analysed for cocaine, cocaethylene, benzoylecgonine and anhydroecgonine methyl ester (AEME). The same hair samples were subsequently tested for ethyl glucuronide (EtG) to allow observation of possible correlation between cocaethylene and EtG.
Data source location	TrichoTech Ltd, Cardiff, U.K.
Data accessibility	Data is with this article
Related research article	n/a

Value of the data

- Data is provided from 64 subjects showing cocaine, cocaethylene and other metabolite concentrations in head hair, alongside ethyl glucuronide concentrations from the same hair section.
- Trends and positive / negative correlation may be evaluated from the data.
- Data provides insight into the range of concentrations that may be observed in hair for the detected compounds.

1. Data

Data were obtained from TrichoTech Ltd for hair samples from 64 subjects previously analysed for cocaine, cocaethylene, benzoylecgonine and anhydroecgonine methyl ester (AEME). The same hair samples (B samples) were subsequently tested for ethyl glucuronide (EtG) to allow observation of possible correlation between cocaethylene and EtG. A dataset of hair concentrations for these drugs and metabolites is presented. (Figs. 1 and 2 and Table 1).

2. Experimental design, materials, and methods

Hair samples from the 64 subjects were split lengthways, into two samples, creating an A and B sample. Sample A then continues through the testing procedure whilst sample B, which is identical in length and weight, remains sealed and is stored in case a sample needs to be re-analysed.

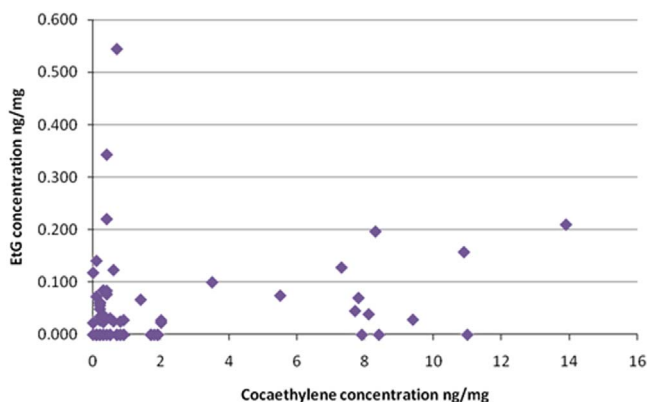


Fig. 1. Cocaethylene concentration versus EtG concentration in 64 hair samples.

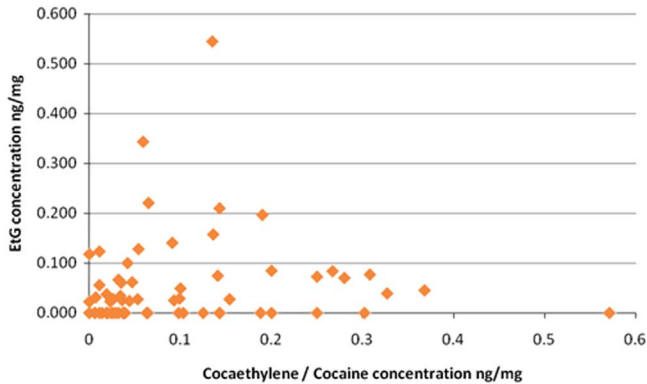


Fig. 2. Cocaethylene/cocaine concentration versus EtG concentration in 64 hair samples.

Table 1

Correlation between EtG and cocaethylene.

	Cocaethylene negative	Cocaethylene positive	Total (EtG)
EtG negative	3	25	28
EtG positive	0	36	36
Total (Cocaethylene)	3	61	64

The B hair samples from 64 subjects which had been previously tested for cocaine and its metabolites were cut into 1 cm sections from the root end of the hair. These hair sections were then analysed to determine EtG concentration. By using the B sample it was possible for the data from the newly tested EtG hair samples to match the time period of their corresponding A sample which was tested for cocaine and metabolites, allowing the possibility of concentration correlation to be examined. The analysis of cocaine and metabolites was conducted at TrichoTech Ltd, a UKAS accredited facility using a SPE clean-up stage, followed by GCMS confirmation.

3. Preparation and analysis of hair samples

Methodology for the hair preparation, extraction and analysis is described by Paul et al. [1].

4. Dataset

Quantitative data from EtG, cocaine, benzoylecgonine, cocaethylene and AEME are presented. Cocaethylene / cocaine data are also presented for analysis. Hair section weights are provided. EtG concentration within the 64 subjects ranged from 0.02 ng/mg to 0.54 ng/mg with a mean concentration of 0.05 ng/mg (standard deviation 0.09 ng/mg). Cocaethylene concentrations ranged from 0.1 ng/mg to 13.9 ng/mg with a mean concentration of 2.19 ng/mg (standard deviation 3.41 ng/mg). EtG concentration plotted against cocaethylene concentration is demonstrated in Fig. 1.

Illustrating the data in this manner can lead to the incorporation of error by not separating the effect a high cocaine concentration would have on the corresponding amount of cocaethylene. For instance, if on average 17% of cocaine is converted to cocaethylene *in vivo*, then someone who consumes a very high dose of cocaine may in turn produce a larger concentration of cocaethylene. To avoid this error the ratio of cocaethylene to cocaine can be plotted against EtG concentration. A graph representing this is shown in Fig. 2.

A qualitative comparison of EtG and cocaethylene is shown in [Table 1](#). Sixty one samples tested positive for cocaethylene whereas 36 tested positive for EtG.

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2018.09.043>.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2018.09.043>.

References

- [1] R. Paul, R. Kingston, L. Tsanaclis, A.J. Berry, A.J. Guwy, Simultaneous determination of EtG and GHB in hair by GCMS/MS, *Drug Test. Anal.* 3 (2011) 201–205.