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Automatic identification and semi-quantitative analysis of psychotropic drugs using GC-MS

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Introduction

Accidental poisoning due to the abuse and excessive intake of stimulants and other illegal drugs or psychotropic drugs continues to be a troublesome social issue. In particular, when death occurs due to acute drug poisoning, identifying the specific drug responsible and determining its concentration in blood are essential subjects in clinical and forensic laboratories. For this purpose, we developed a database (Forensic toxicology database) and applied this database to automatic detection of barbiturate, phenobarbital, and chlorpromazine.

Experimental

GC-MS analysis was performed on a GCMS-QP2010 Ultra (Shimadzu) equipped with a Rxi®-5Sil MS (30 m × 0.25 mm I.D. df=0.25 µm, Restek). The data were processed using GCMSsolution software and Forensic Toxicology Database (Shimadzu). These three compounds were added to blank serum, and the concentration adjusted to 10 µg/mL. The actual samples were obtained from a psychiatric patient who had been administered these three compounds.

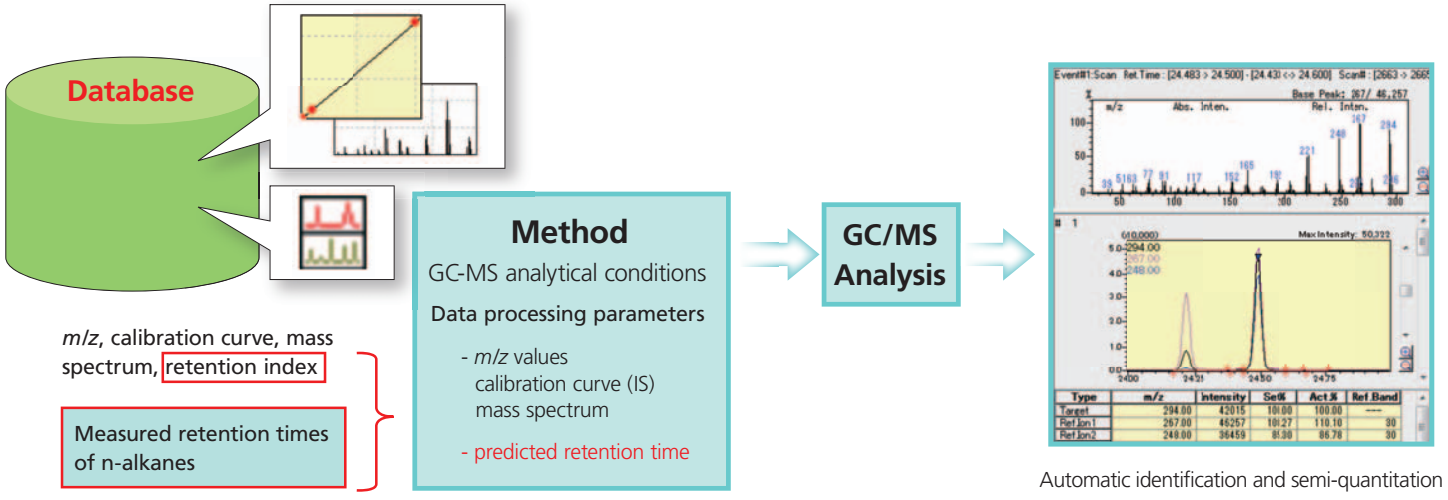
Forensic toxicology database

Forensic toxicology database consists of mass spectra, retention indices, *m/z* values for mass chromatograms and the relative response factors for compounds in forensic toxicology for automatic identification and semi-quantitation.

Registered compounds

1011 spectra for 502 compounds were registered.

Category	Compound number	Spectral number
Drugs of abuse	218	Free 208, TMS 204, TFA 179
Psychotropic drugs	182	Free 158, TMS 111, TFA 7
General drugs	66	Free 52, TMS 58
Pesticides	36	Free 36



Automatic identification and semi-quantitation

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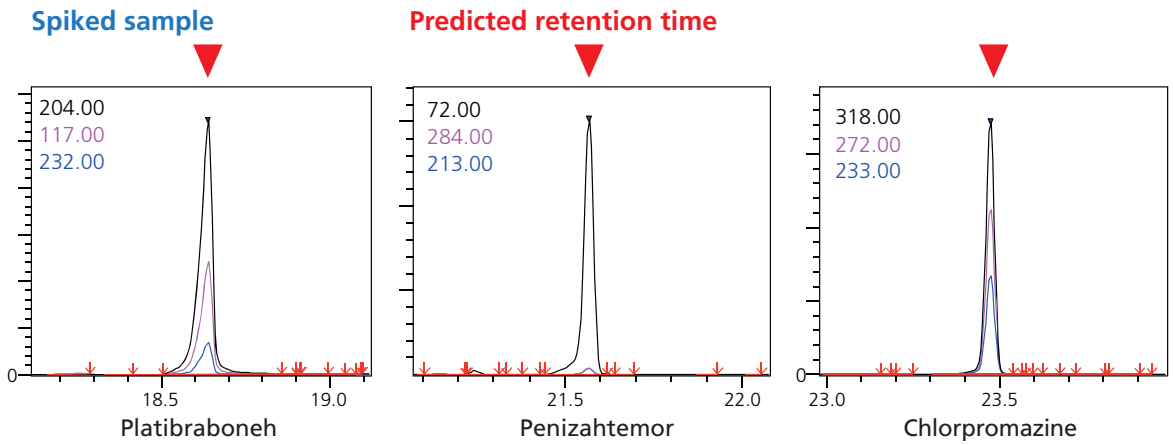
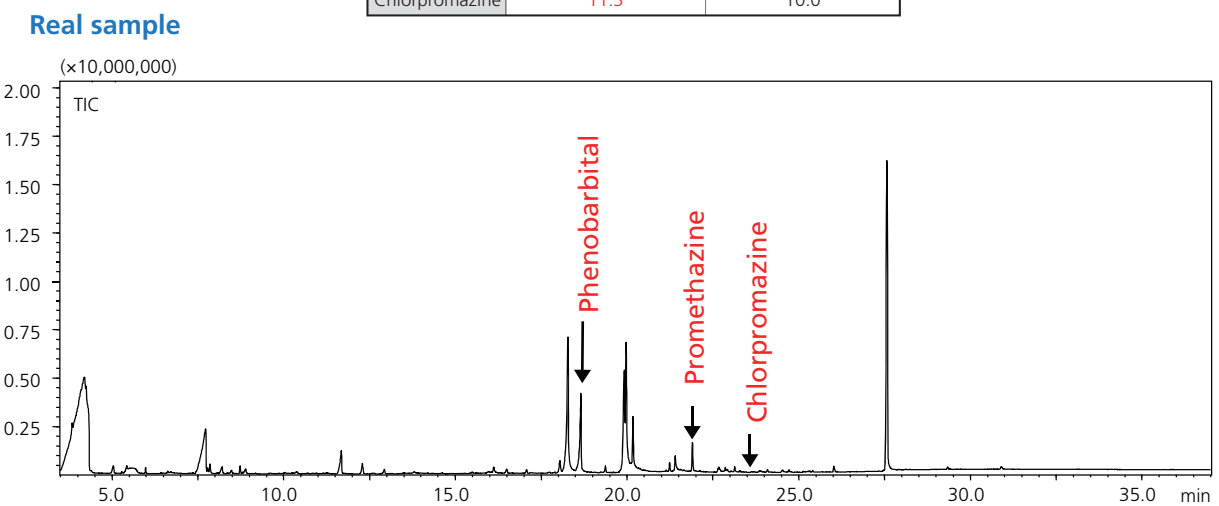
Results and discussion

Whilst chlorpromazine and promethazine showed excellent quantitative results in both samples, phenobarbital indicated a value of 2 to 3 times higher compared to actual values. The semi-quantitation feature of the Forensic Toxicological Database generates a semi-quantitation value which provides a rough estimate of "the drug concentration in the final sample" based on the response factor obtained from the previously analyzed standard sample. The semi-quantitation value can vary considerably depending on the pretreatment procedure, the GC injection port, and the column condition. It is therefore necessary to regard the measured amount only as an approximate value. For quantitative analysis requiring great accuracy, standard samples must be used.



Semi-quantitation and additive amount [ug/mL]

	Semi-quantitation	Additive amount
Phenobarbital	17.6	10.0
Promethazine	11.4	10.0
Chlorpromazine	11.3	10.0



Semi-quantitation and calibration method [ug/mL]

	Semi-quantitation	Conventional method
Phenobarbital	33.2	11.6
Promethazine	0.15	0.13
Chlorpromazine	0.02	0.03

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Conclusion

(1) Automatic qualitative and semi-quantitative analyses using the database were conducted for three psychotropic drugs.
(2) This allows automatic identification and a rough estimate of a drug's concentration.
(3) This was optimal for quick screening analysis of these compounds in clinical and forensic laboratories.

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