SACI in the analysis of coca in human urine

Keywords: Cocaine, urine, no sample preparation, high sensitivity

The abuse and consumption of drugs is an increasing problem in our modern society. In addition to the serious toxicological and social risks that users are subjected to, drugs also present a great threat toward nonusers in certain circumstances. For instance, in traffic or in the workplace, people under the influence of drugs can cause severe damage. The unfortunately wide diffusion of opiates, cocaine, amphetamines and other drugs has dramatically increased in recent years in the European illegal market.

This trend has been confirmed by the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA). Opiates, cocaine and their metabolites are usually detected in urine. Urine sampling is physically noninvasive and large volume of sample can be easily obtained. Moreover, it is a simple matrix with relatively high concentration of drugs and drug metabolites than other biological fluids.

Simultaneous determination of these drugs has practical applications on both pharmacokinetic studies and forensic assessment.

Figure 1 :SACI source on HCT ultra.

Surface Activated Chemical Ionization:

Surface-activated chemical ionization (SACI) is a new ionization technique operating with analyte solutions.

Insertion of a metallic surface in the ionization chamber [Fig.1], allowing for a better ion focalization and hence for an increase in ionization efficiency In particular, while in the case of ESI and APCI, high electrostatic potential (3–6 kV) are employed to lead to the sample ionization, in the case of SACI, the vaporized or sprayed analyte solution experiments employ a low voltage charged surface inserted (50 V) in an APCI ionization source. In this case, the corona discharge needle apparatus is not used but the ionization effect is activated only by the surface.

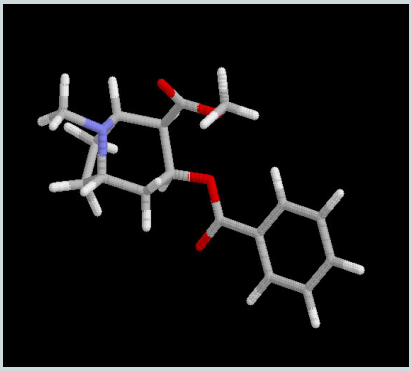
Experimental conditions and settings:

Analyte: Cocaine and its metabolite Benzoyletgonine

Sample: human urine

Sample Preparation and Analytical Conditions: Human urine diluted 1:100 in Water

LC-MS/MS conditions: C18 100 × 2.1 mm, 3.5 µm column was used. The chromatographic analysis was performed under gradient conditions.



Cocaine Molecular Structure

The mobile phases were: (A) H2O + 0.1% HCOOH and (B) CH3CN + 0.1% HCOOH. The gradient was used passing from 5% of B to 80% of B in 20 min. Flow rate: 0.25ml/min, injection volume 20 µL per sample.

Instruments Employed:

- HCT ultra, Bruker Daltonics
- HPLC Dionex Ultimate 3000

Experimental Results:

Cocaine and BEG chromatograms obtained by SACI ionization technique allow to detect an extremely clear signal even if present at very low concentration. Moreover, the low spectrum chemical noise makes possible to obtain high sensitivity (LOD=0.033, LOQ=0.1 pg/µl) by simple dilution of samples.

Cocaine and BEG tandem mass chromatograms (MS/MS) are shown in figure 2

SACI allows to detect Cocaine, Benzoyletgonine, in diluted human urine (as reported in Fig.3); precursor ions and respective product ion of these compounds are reported in table 1.

Drug	MW	Precursor	Product
Cocaine	304	305	182
BEG	289	290	168

Table 1:
MW, precursor and product ions of drugs analysed

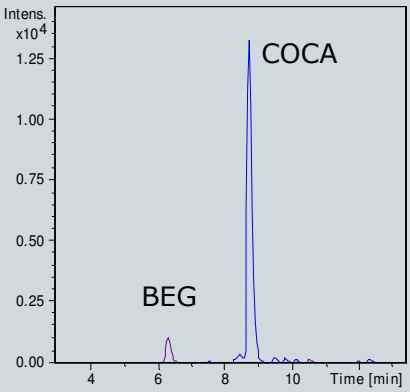


Figure 2: Chromatogram of 0.5pg/µl of a standard solution.

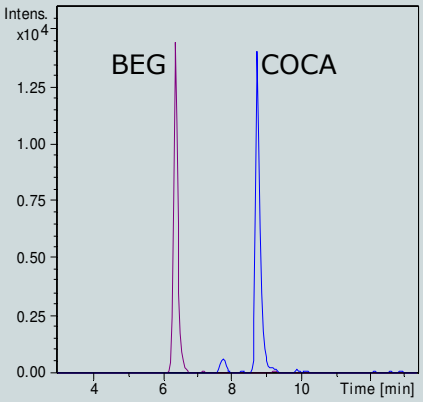


Figure 3: Chromatogram of human urine diluted before injection.

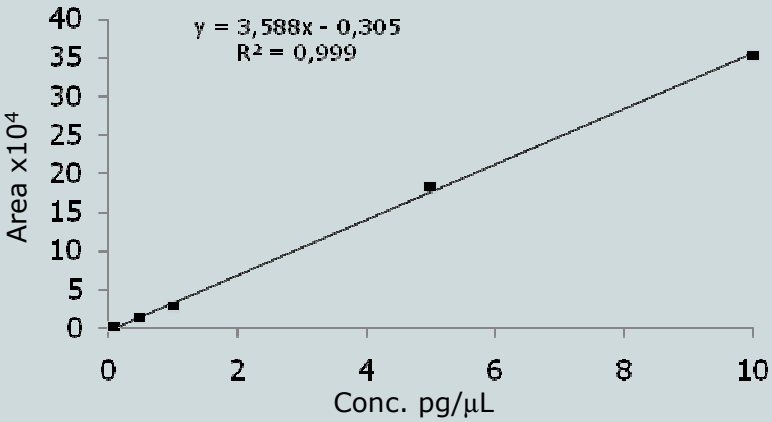


Figure 4: Cocaine Calibration Curve prepared in blanck urine (0.1 ÷10 pg/µL)

Good linearity (r^2 = 0.999) was achieved between 0.1 and 10 pg/µL [Fig. 4]

Conclusions:

SACI source and the instruments employed, allowed to achieve a significant results in drugs analysis even avoiding traditional purification steps (e.g. Solid Phase Extraction –SPE).

Acknowledgements and References:

Acknowledgements

1) ISB srl, via Fantoli 16/15, 20138 Milano.

2) Bruker Daltonics S.r.l., Macerata, Italy.

References

Cristoni S. “Surface Activated Chemical Ionization” Enciclopedia of Mass Spectrometry In Press

Cristoni S, Bernardi LR, Guidugli F, Tubaro M, Traldi P. “The role of different phenomena in surface-activated chemical ionization (SACI) performance” J Mass Spectrom. 2005 Dec;40(12):1550-7.

Cristoni S, Bernardi LR, Biunno I, Tubaro M, Guidugli F. “Surface-activated no-discharge atmospheric pressure chemical ionization” Rapid Commun Mass Spectrom. 2003;17(17):1973-81.

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