Determination of Quinine in Tonic Water and Caffeine in Coffee and Coke® using TLC-MS

Abstract

HPTLC–MS (High Performance Thin Layer Chromatography–Mass spectrometry) is a very useful analytical technique with low-level sample preparation shown in the example of determination of quinine in tonic water and caffeine in coffee and Coke®. Tonic water and Coke® were decarbonized by ultrasonic. The boiled coffee was extracted with a 0.45 µm syringe filter. After chromatographic separation the analyte was eluted with an TLC-MS Interface, transferred and finally detected with a mass spectrometer.

Results

Caffeine (hRf = 56, m/z = 195.2, 236.2, Fig. 2) and quinine (hRf = 37, m/z = 325.4, Fig. 4) were detected under UV light (254 nm, Fig. 1; 366nm, Fig. 3) and measured by TLC-MS.

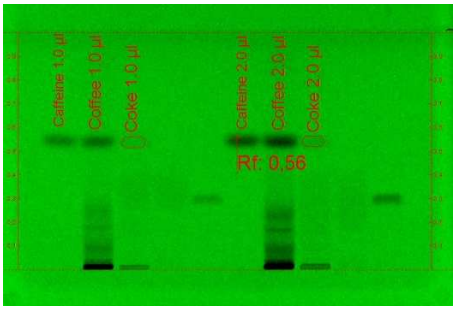

Fig. 1: Developed plate at 254 nm.
Chromatographic data shown on next page.

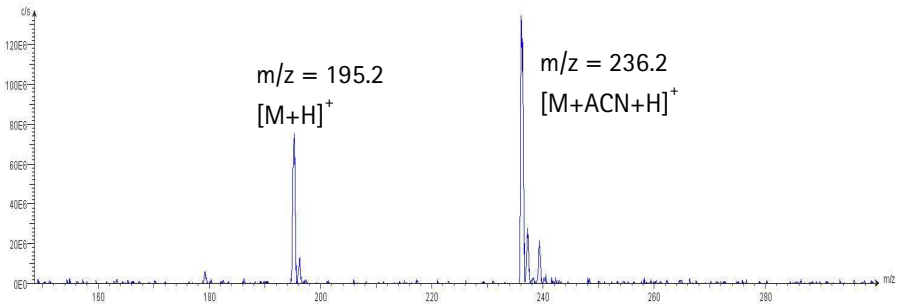

Fig. 2: mass spectrum of caffeine in coffee.

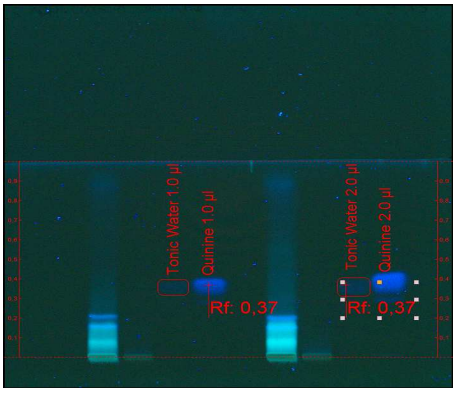

Fig. 3: Developed plate at 366 nm.
Chromatographic data shown on next page.

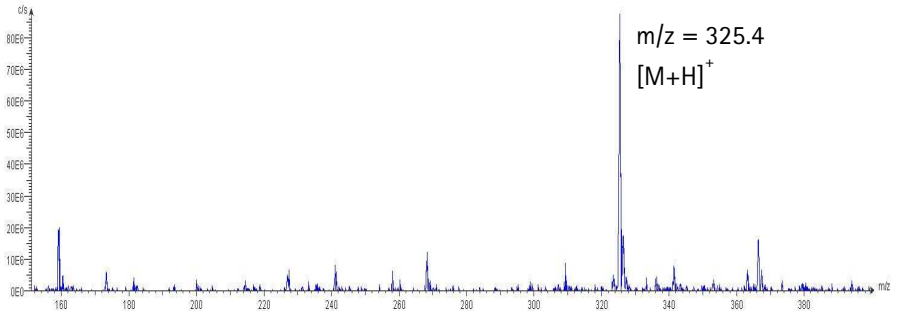

Fig. 4: mass spectrum of quinine in tonic water.

Conclusion

These results demonstrate that caffeine and quinine can easily be analyzed by HPTLC-MS with a minimum of sample preparation even in a complex matrix like coffee, Coke® or tonic water.

Chromatographic data

Track	Compound	Conc. [mg/mL]	Application volume [µL]	hRf	Detected mass m/z
1	Caffeine standard	1	1	56	195.2, 236.2
2	Coffee		1	56	195.2, 236.2
3	Coke®		1	56	195.2, 236.2
4	Tonic water		1	37	325.4
5	Quinine standard	1	1	37	325.4
6	Caffeine standard	1	2	56	195.2, 236.2
7	Coffee		2	56	195.2, 236.2
8	Coke®		2	56	195.2, 236.2
9	Tonic water		2	37	325.4
10	Quinine standard	1	2	37	325.4

Application data

Chromatography	Plate	HPTLC Silica gel 60 F_{254} MS-grade, 20x10cm
	Sample preparation	Caffeine and quinine standard diluted in Methanol; Coke® and tonic water were decarbonated; Coffee boiled and filtered with a 0.45 µm syringe filter.
	Sample application	ATS 4 sample applicator (Camag), 6 mm bandwise
	Application volume	1.0 and 2.0 µL
	Mobile phase	Isopropanol / n-Heptane / Water 7/3/1 + 1% Triethylamine
	Migration distance	5 cm
	Migration time	49 min
Extraction	Extraction equipment	TLC-MS Interface "Plate Express" (Advion)
	Extraction solvent	Acetonitrile / Water 95/5 (v/v) + 0.1% Formic acid
	Extraction flow	0.2 mL/min
Detection	Wavelength	UV light at 254 nm and 366 nm
	Staining	None
	MS equipment	expression CMS (Advion)
	MS detection	ESI (+) mode (m/z 150 - 400)

Ordering Information

HPTLC Si60 F_{254} MS-grade, 20x10 cm	1.00934
2-Propanol gradient grade for liquid chromatography LiChrosolv®	1.01040
n-Heptane for liquid chromatography LiChrosolv®	1.04390
Water for chromatography (LC-MS Grade) LiChrosolv®	1.15333
Triethylamine for synthesis	8.08352
Acetonitrile hypergrade for LC-MS LiChrosolv®	1.00029
Formic acid for analysis EMSURE	1.00264
Millex®-FH filter, 0.45 µm hydrophobic PTFE, 25 mm, non-sterile	SLFH025NS