## A HANDHELD GUIDE: FUN & EASY MASS SPECTROMETRY EXPERIMENTS FOR YOUR TEACHING LAB

Advion Interchim



## A book of experiments for your students

The expression® CMS (Compact Mass Spectrometer) is the ideal instrument for the teaching lab thanks to its small size, ease of use, and one-click software. This pocket guide of classroom experiments offers students the ability to gain hands-on instrument experience by eliminating complex and difficult sample preparation.

The expression® CMS offers a wide range of sample introduction techniques, including:

- The Plate Express<sup>TM</sup> pushbutton TLC plate reader for results in <30 seconds</li>
- The ASAP® Atmospheric Solids Analysis Probe for one-touch sample analysis
- The Touch Express<sup>TM</sup> OPSI (Open Port Sampling Interface) for one-touch, prep-free ESI introduction
- ...and many more!

When class is not in session, the system is ideal for use for research projects, making this a versatile choice for university labs seeking state of the art equipment paired with streamlined teaching modules.

#### **RIGHT:**

The wide range of sample introduction techniques available with the expression® CMS.



## Who Stole my Chocolate? To Catch a Candy Thief

While the culprit may have consumed the evidence, some traces still remain: caffeine, as well as theobromine, a xanthine alkaloid, is present in chocolate. With the single swipe of a fingertip, students can use the CMS to identify patterns that match with a typical chocolate profile.

#### **Experimental Setup:**

- expression<sup>®</sup> CMS with ASAP<sup>®</sup> Atmospheric Solids Analysis probe
- Chocolate bar of your choice

**STEP 1:** Eat chocolate. Dark provides the best spectra.

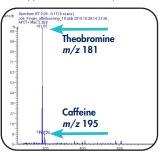


**STEP 2:** Touch the ASAP® probe to your fingers, insert in CMS.



STEP 3:

Compare fingerprint spectra with typical chocolate pattern.



#### **RESULTS:**

Did you find a match?! The fingerprint data can readily reveal abundant ions at m/z 181 and m/z 195, which are consistent with the presence of theobromine and caffeine; the marker molecules characteristic of chocolate.

## Caffeine m/z 196

## Mistletoe: Kiss of Love or Death? TLC/CMS to Find Out!

Mistletoe symbolizes a tradition of romance, however, mistletoe is also considered lethal. Named the "kiss of death," one species of mistletoe, Viscum, reportedly contains the poisonous alkaloid, tyramine, which can cause blurred vision, nausea, abdominal pain, and even death. So...kiss of love or?

#### **Experimental Setup:**

- expression<sup>®</sup> CMS with Plate Express<sup>TM</sup> TLC Plate Reader
- Tyramine & mistletoe herb/tincture

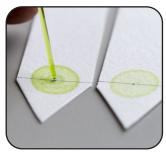
### STEP 1:

Derivatize a small aliquot of the tincture and tyramine.



#### STEP 2:

Spot on a TLC Plate: Mistletoe, Tyramine, & Mistletoe Tyramine



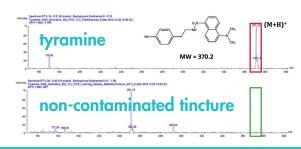
#### STEP 3:

Take developed TLC to the Plate Express<sup>TM</sup> to analyze spots.



#### **RESULTS:**

The results should suggest either that the level of tyramine in the tincture sample is very low and below detection limits or that tyramine is not present in the sample. It is common for chemists to employ TLC techniques as a quick, easy screen of a sample to determine the presence of an expected chemical. So, what should you do? This mistletoe is not deadly. But it can be hazardous, so don't eat it.



## Caffeine Levels in Fizzy Drinks: No Sample Prep

Feeling sluggish? In this experiment, students can test the caffeine levels in various beverages to learn where to find the strongest energy jolt! The best part? The sampling is done using the ASAP® probe: simply dip it in the drink and insert it directly in to the CMS for fun, prep-free analysis.

#### **Experimental Setup:**

- expression® CMS with ASAP® Atmospheric Solids Analysis probe
- Cola, energy drink, lemonade

#### STEP 1:

Dip the ASAP® probe in to a drink and then insert in CMS.



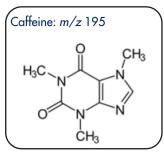
#### STEP 2:

Gather the mass spectra of each of the beverages.



#### STEP 3:

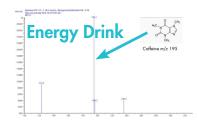
Compare each spectra with typical caffeine pattern.

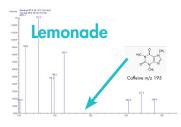


#### **RESULTS:**

#### How caffeinated are you?!

The ASAP/CMS analysis provided data in < 1 min with no sample preparation and no chromatography, making it ideal for reaction monitoring, compound identification, food safety, and analysis of natural products.





## **Drug Screening on Paper Currency: Touch Express™**

It is known that US paper currency in general circulation can contain cocaine residue due to contamination from handling during drug deals, the use of rolled up bills for snorting or inhalation, and cross contamination between bills in circulation. Touching a bill to the OPSI<sup>TM</sup> can screen for this.

#### **Experimental Setup:**

- expression<sup>®</sup> CMS with Touch Express<sup>TM</sup> Open Port Sampling Interface (OPSI)
- Currency in circulation, a new bill

#### STEP 1:

Obtain several bills, as well as an uncirculated paper bill.



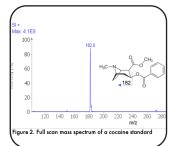
#### STEP 2:

Touch each bill to the OPSI<sup>TM</sup> port on the CMS, no prep.



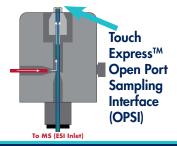
#### STEP 3:

Compare the spectra with typical cocaine pattern.



#### **RESULTS:**

Illegal or just rumor? In our studies, cocaine was detected on some US \$1 bills, \$10 bills as well as on a European €5 bill from a total of forty-nine bills. The European €5 bill had the lowest relative amount compared to all other bills whereas two of the US \$1 bills had the highest relative amount of cocaine. No cocaine was detected on a US \$2 bill that was obtained as a brand new bill from a local bank.



## **EXTRA CREDIT! Intelligent Flash Purification**

Ensuring successful synthesis of your product, setting up a flash purification method, and finally confirming ID of fractions can be a difficult and time consuming process. In this experiment, students can use Advion Interchim Scientific expression® CMS & puriFlash® flash chromatography system to speed up the synthesis, purification and characterization of a compound.

## Experimental Setup:

- expression<sup>®</sup> CMS with Plate Express<sup>TM</sup> & ASAP<sup>®</sup>
- puriFlash® XS 520 Flash System

#### STEP 1:

Confirm your reaction mixture in <30 seconds with TLC/CMS



#### STEP 2:

Photograph your developed TLC plate; send to puriFlash®



#### **STEP 3:**

Confirm flash fractions using ASAP/CMS



#### **RESULTS:**

# Imagine having real flash chromatography experience as an undergrad!

Enriching the teaching environment is a core mission at Advion Interchim Scientific. With the ability to create flash methods from your cell phone, to using fast sampling to cover reaction monitoring and fraction confirmation, flash chromatography is no longer a difficult or intimidating processit becomes yet another resume-building workflow that students can easily learn.



# HOW TO REQUEST MORE INFORMATION, A QUOTATION, OR TO PLACE AN ORDER

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