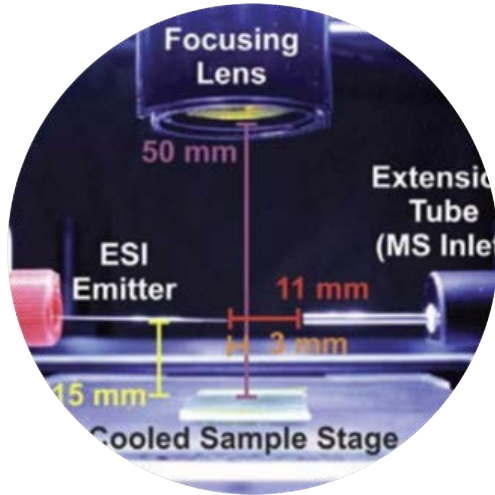


# LAESI MSI of foods and food ingredients

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October 5, 2017



# Outline

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- Spatially-resolved food analysis
- Initial application studies
  - Pesticides on citrus fruits and rose leaves
  - Mycotoxins on rye
  - Glycoalkaloids on tomato
  - Unknown on maize
- Conclusion and perspectives

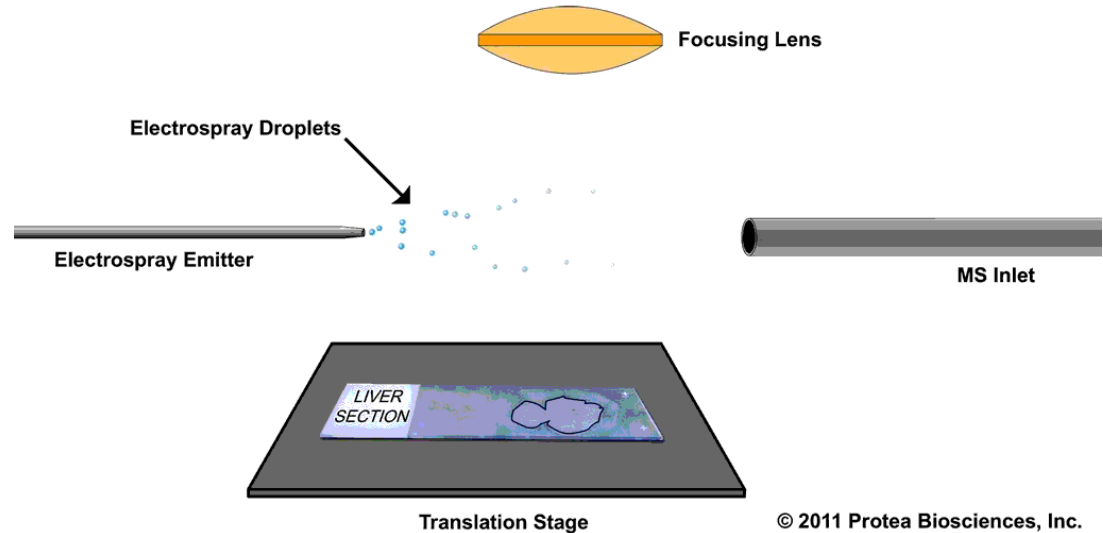
# Why spatially-resolved food analysis?

- Food contaminants usually measured in a single averaged dimension
- Levels may vary locally to a large extent: average-based data hardly useful when specific parts are being used and consumed
- 2D and 3D food analysis methods needed that can deal with large and irregular sample surfaces
- Also relevant for: surface contamination, surface defects, search for early ripening markers, options for re-use of off-spec foods, in agriforensics, etc.

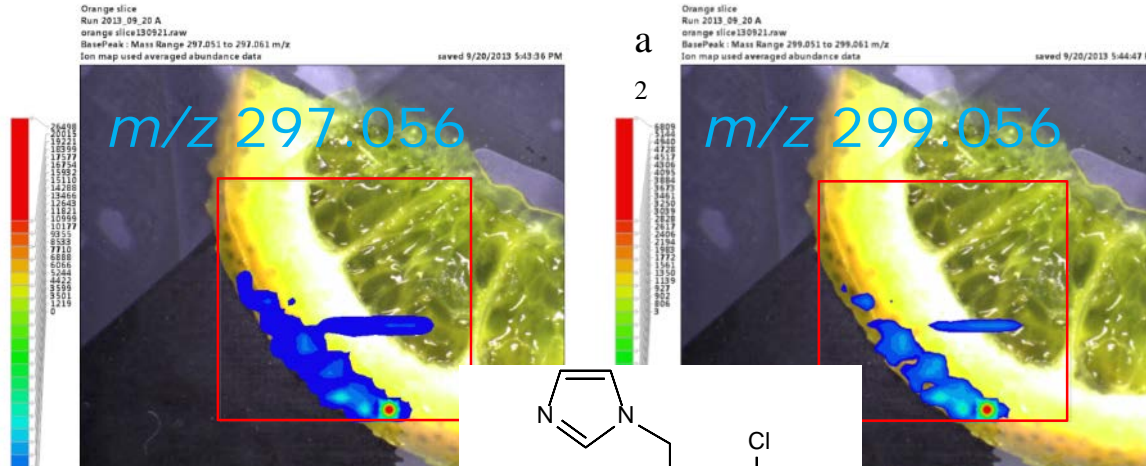


# LAESI MSI

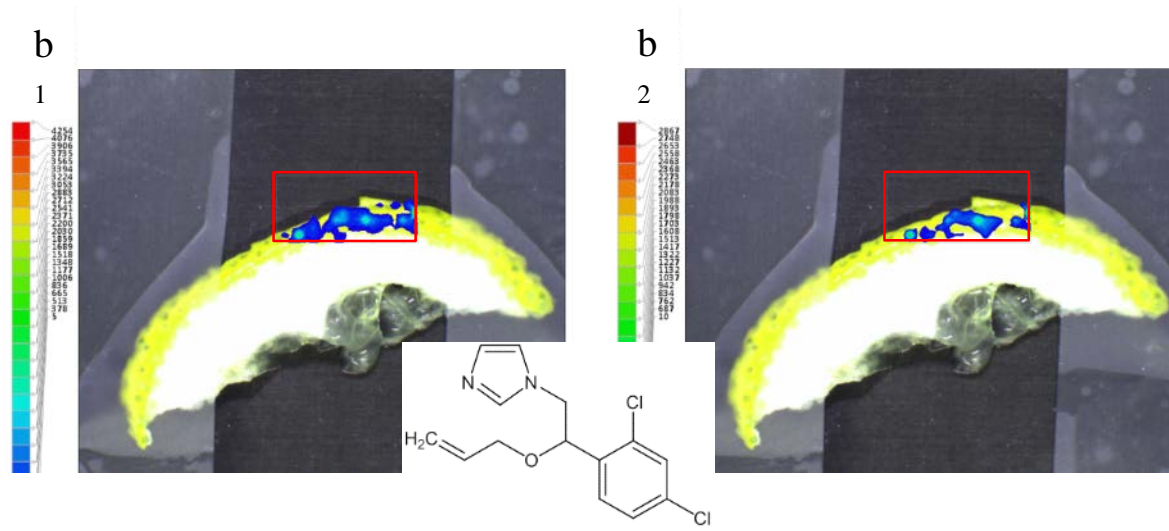
- Accommodates large objects
- No precise tissue slicing needed
- No MALDI matrix application
- (sub-)mm spatial resolution



# LAESI MSI of regular citrus fruits

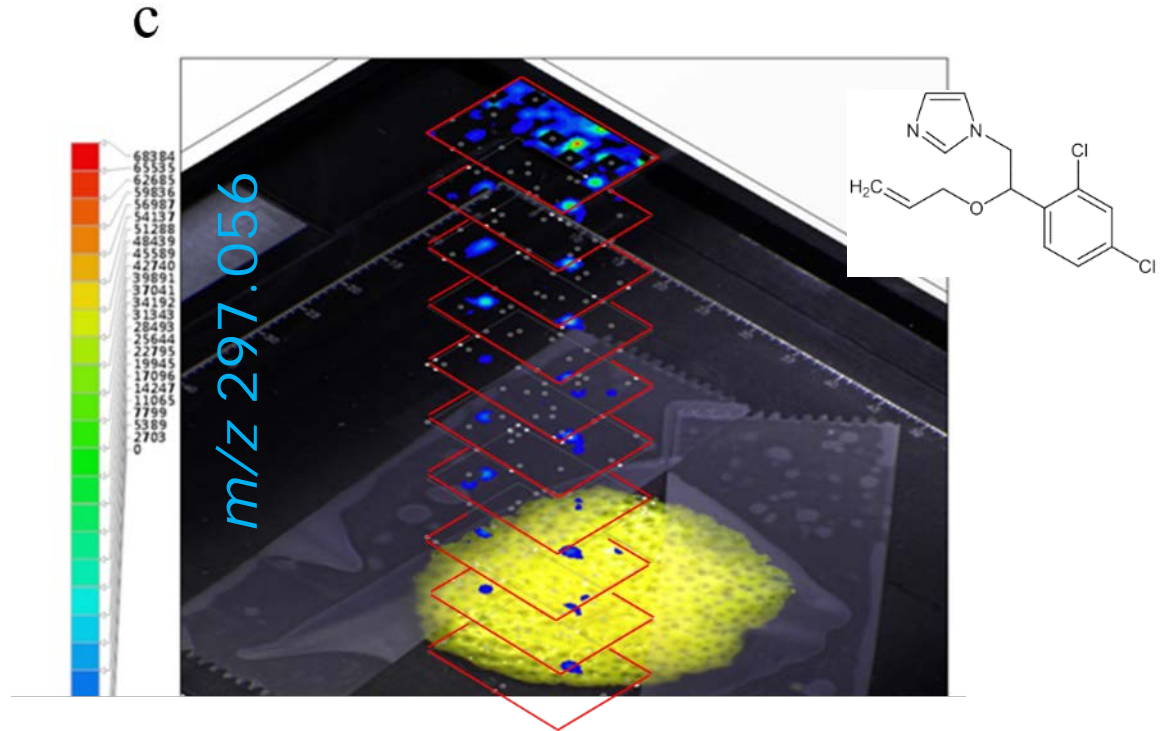


# LAESI MSI of regular citrus fruits

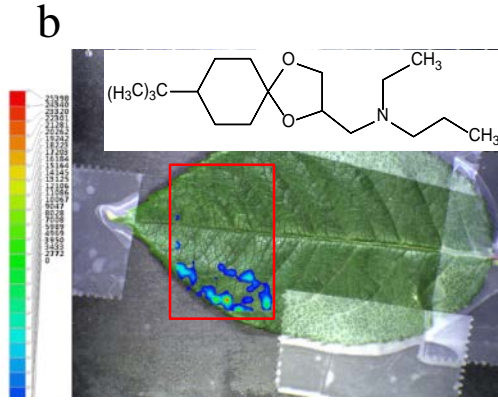
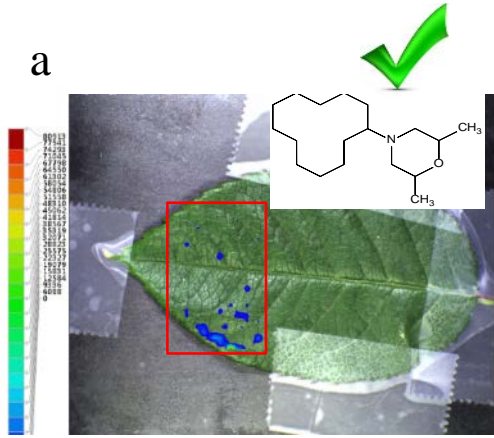


# 3D-LAESI MSI of regular citrus fruits, 10 pulses

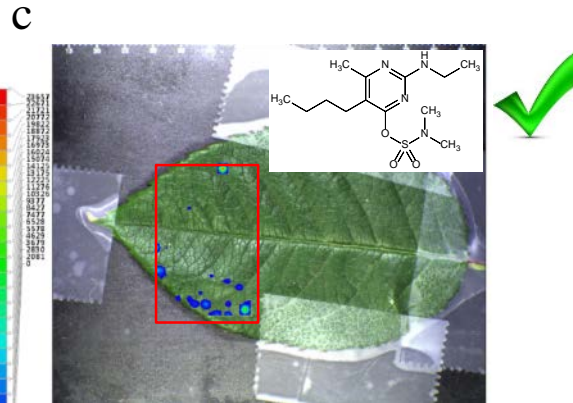
*penetration into lemon peels*



# LAESI MSI of rose leaves



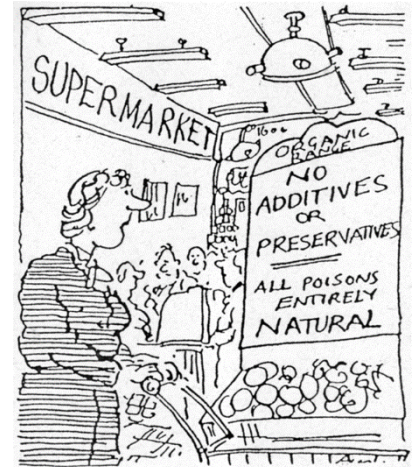
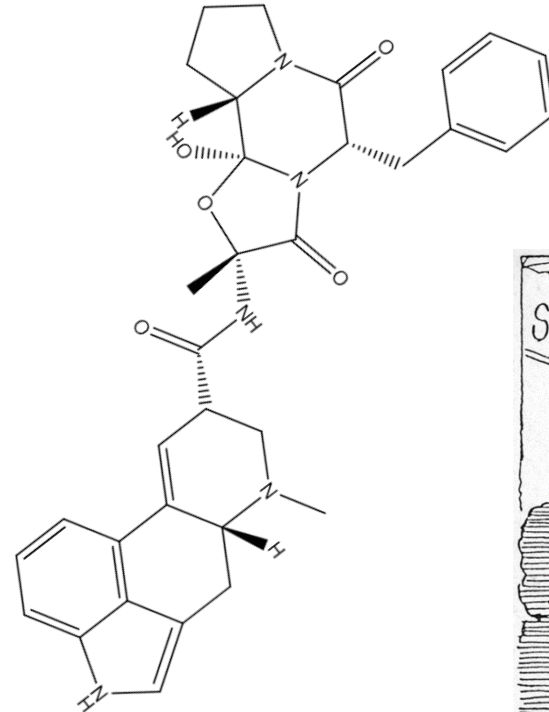
*Co-application of licensed and banned pesticides?*



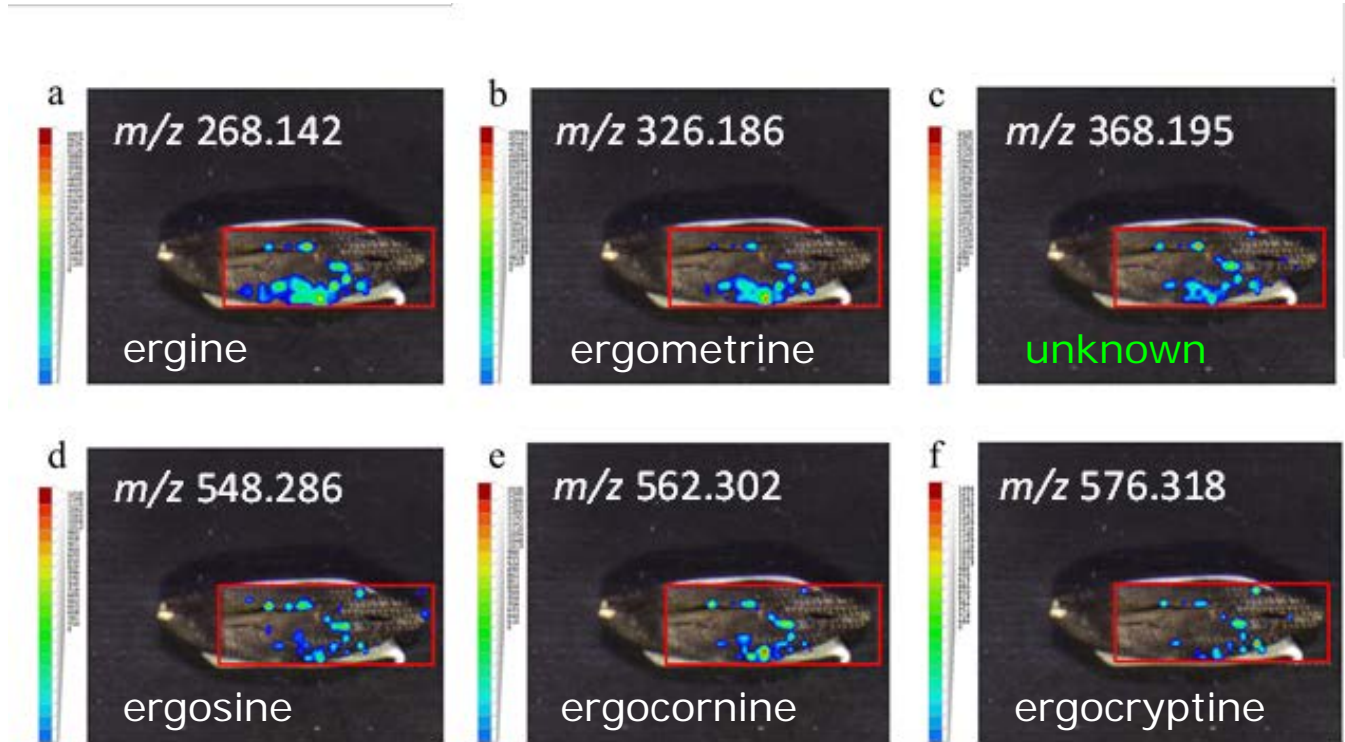


# LAESI MSI of mycotoxins on rye

- *Ergotism is the effect of long term ergot poisoning, traditionally due to the ingestion of alkaloids produced by the Claviceps purpurea fungus that infects rye*

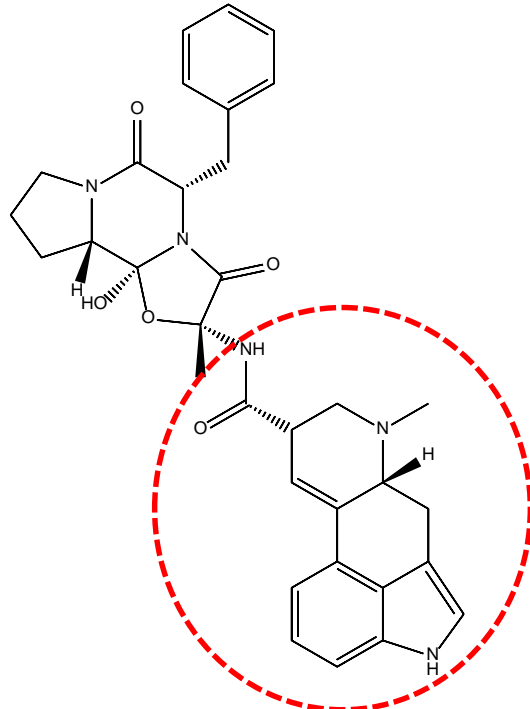


# LAESI MSI of ergot body



*Localization of mycotoxins: ergot alkaloids on rye*

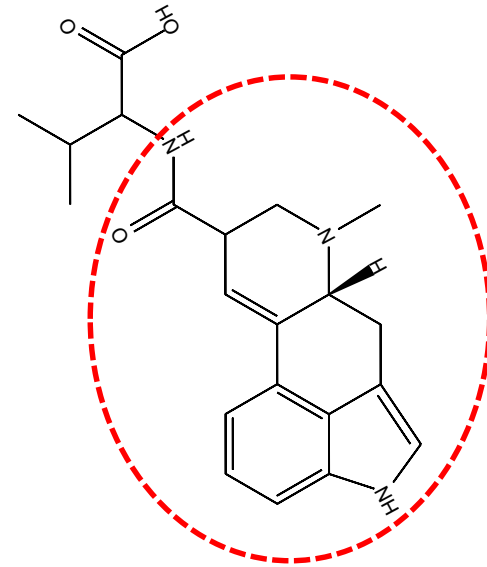
# LAESI MSI of ergot rye: discovery unknown



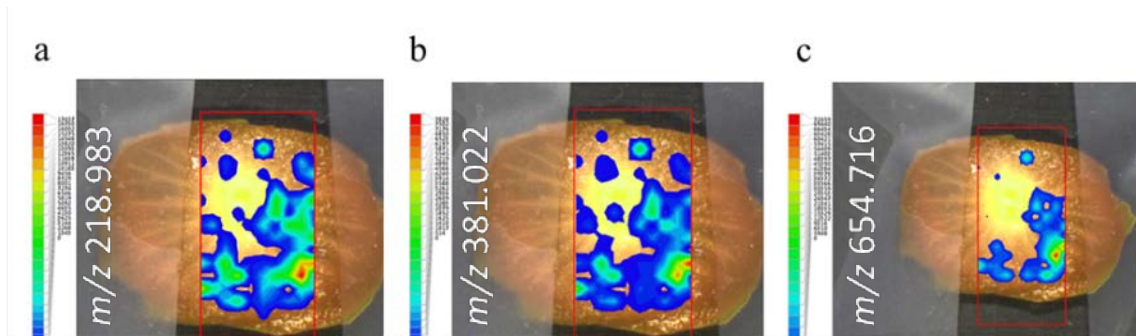
Ergotamine

## Ergoval found

Chemical Formula:  $C_{21}H_{25}N_3O_3$   
Exact Mass: 367.1896

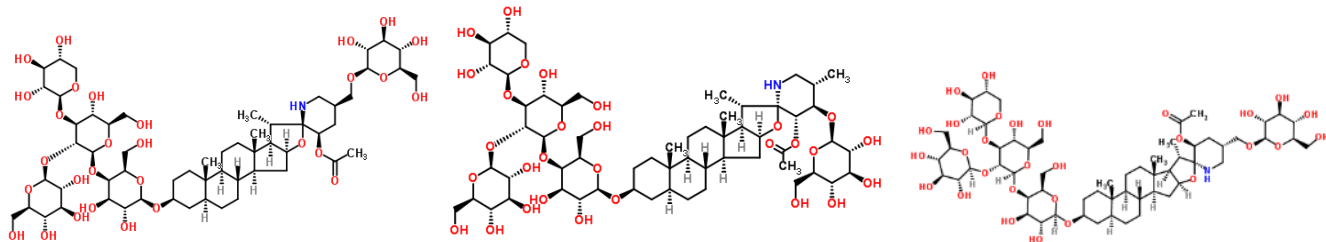


# LAESI Ion Mobility MSI of cherry tomato



*Very high water content: lower laser power!*

Glycoalkaloid isomers separated in ion mobility cell during MSI



Lycoperside F  
CCS<sub>calc</sub> 271 Å

Lycoperside G  
256 Å

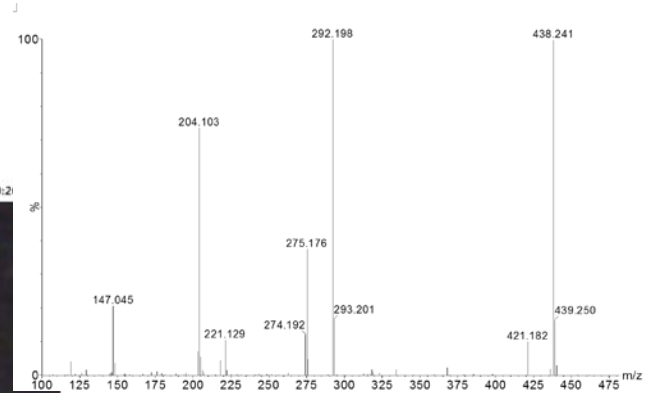
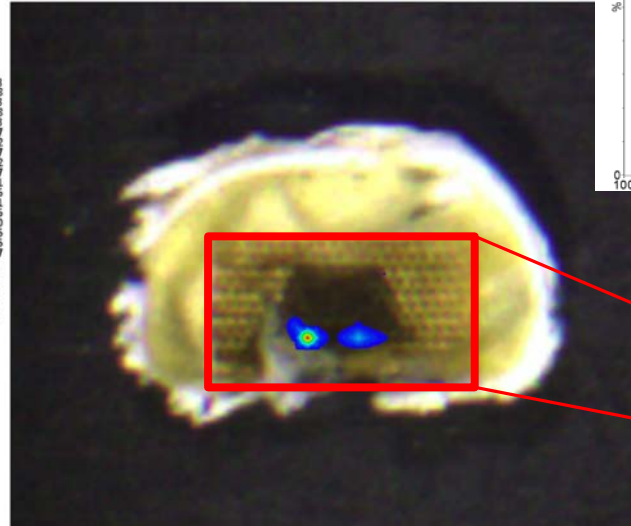
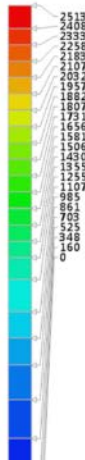
Esculeoside A  
268 Å

# LAESI MSI of maize kernel caps

## Tip cap of maize kernel unknown $m/z$ 438.244 +/- 5 mDa

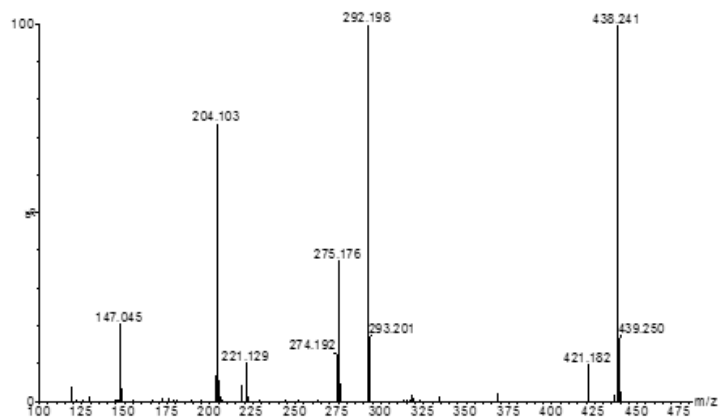
Run 2013\_12\_20 A  
20131220\_LAESI TIPCAP MAISENHANCEF2.RAW  
BasePeak : Mass Range 438.239 to 438.249 m/z  
Ion map used averaged abundance data

saved 2/3/2014 10:2



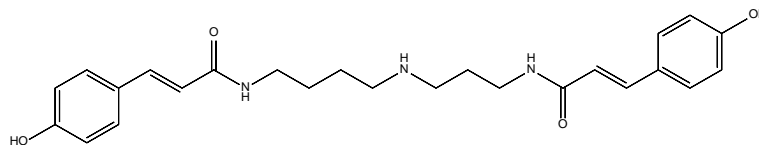
*Dark-coloured tip caps*

# LAESI MSI of maize kernel caps



At dark spots more from this compound

Structure elucidation by MS/MS during LAESI MS/MS



Neutral loss (Da)	Elemental composition	Theor. mass	Mass error (mDa)	Proposed (sub)structure
146.043	C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>	146.037	+6	
17.022	NH <sub>3</sub>	17.026	-4	NH <sub>3</sub> (neutral loss from ion 292)
74.087	C <sub>3</sub> H <sub>10</sub> N <sub>2</sub>	74.084	+3	H <sub>2</sub> N-C <sub>3</sub> H <sub>6</sub> -NH <sub>2</sub> (neutral loss from ion 292)
88.095	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub>	88.100	-5	H <sub>2</sub> N-C <sub>4</sub> H <sub>8</sub> -NH <sub>2</sub> (neutral loss from ion 292)
57.058	C <sub>3</sub> H <sub>7</sub> N	57.058	0	C <sub>3</sub> H <sub>6</sub> -NH (neutral loss from ion 204)

# Conclusions and perspectives

- LAESI MSI is exciting
- LAESI under native conditions; does not require precision slicing, nor labelling or matrix addition, just tape or sticky gum
- Differentiation between isomers feasible during MSI
- MS/MS structure elucidation feasible during MSI
- Like in any MSI technique: data handling and quantitation are major challenges

# Acknowledgements

- Patrick Mulder
- Theo de Rijk
- Eric van Bennekom

- More details?

**Open  
Access**

*Anal. Bioanal. Chem.*  
406 (2014) 6805-6815



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- TI-COAST
- Shared Research Facilities



# Questions?

*Thank you for your  
kind attention!*

