

PHYTOCHEMICAL ANALYSIS OF TIMBERS
USING
**DIRECT ANALYSES IN REAL TIME,
TIME OF FLIGHT MASS SPECTROMETER
(DART TOFMS)**

Kristen Finch¹ and Edgard Espinoza²

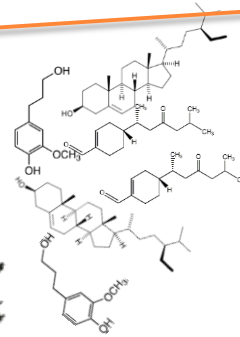
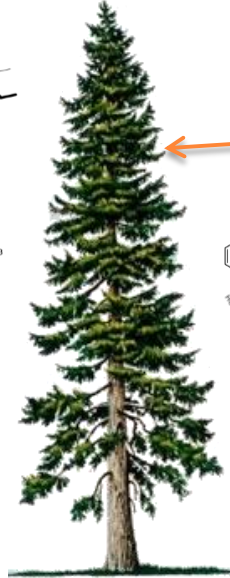
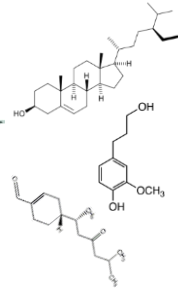
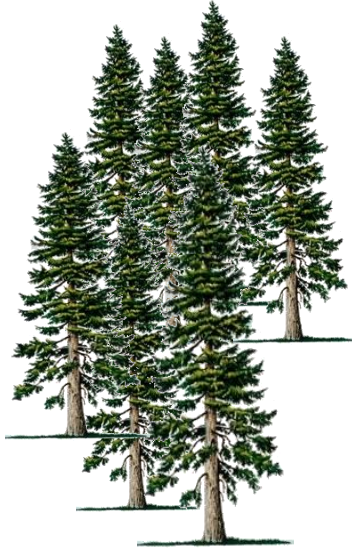
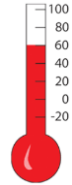
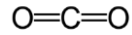
1 Botany and Plant Pathology at Oregon State University

2 National Fish and Wildlife Forensic Laboratory, Ashland, OR



VARIATION IN WOOD CHEMISTRY

Locked in Chemical Warfare



Defense

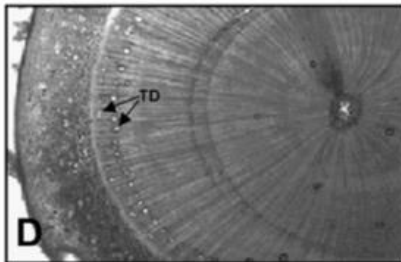
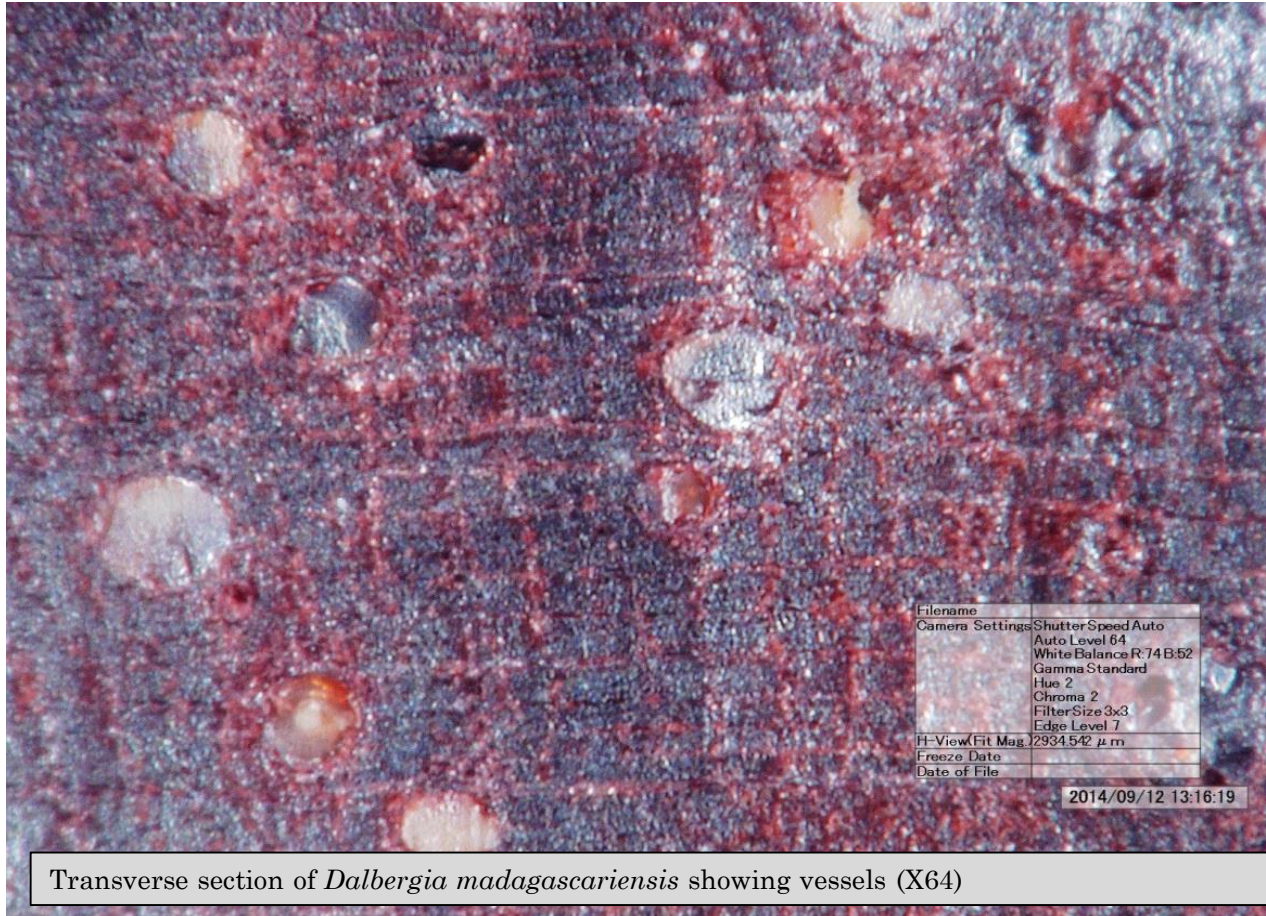


Photo Huber et al. 2005



WHERE ARE THESE CHEMICALS?



Transverse section of *Dalbergia madagascariensis* showing vessels (X64)





WHAT IS DART TOFMS

**Direct Analyses in Real Time,
Time of Flight Mass Spectrometer (DART TOFMS)**

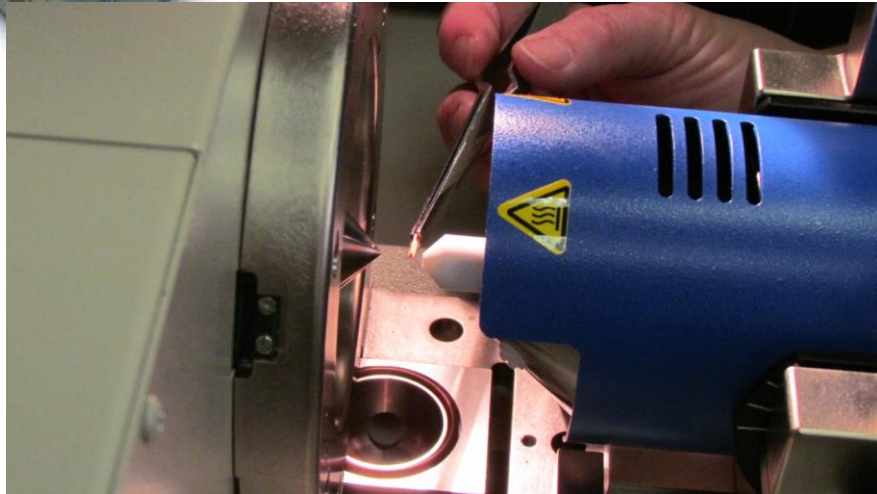




Photo by Ed Espinoza 2015

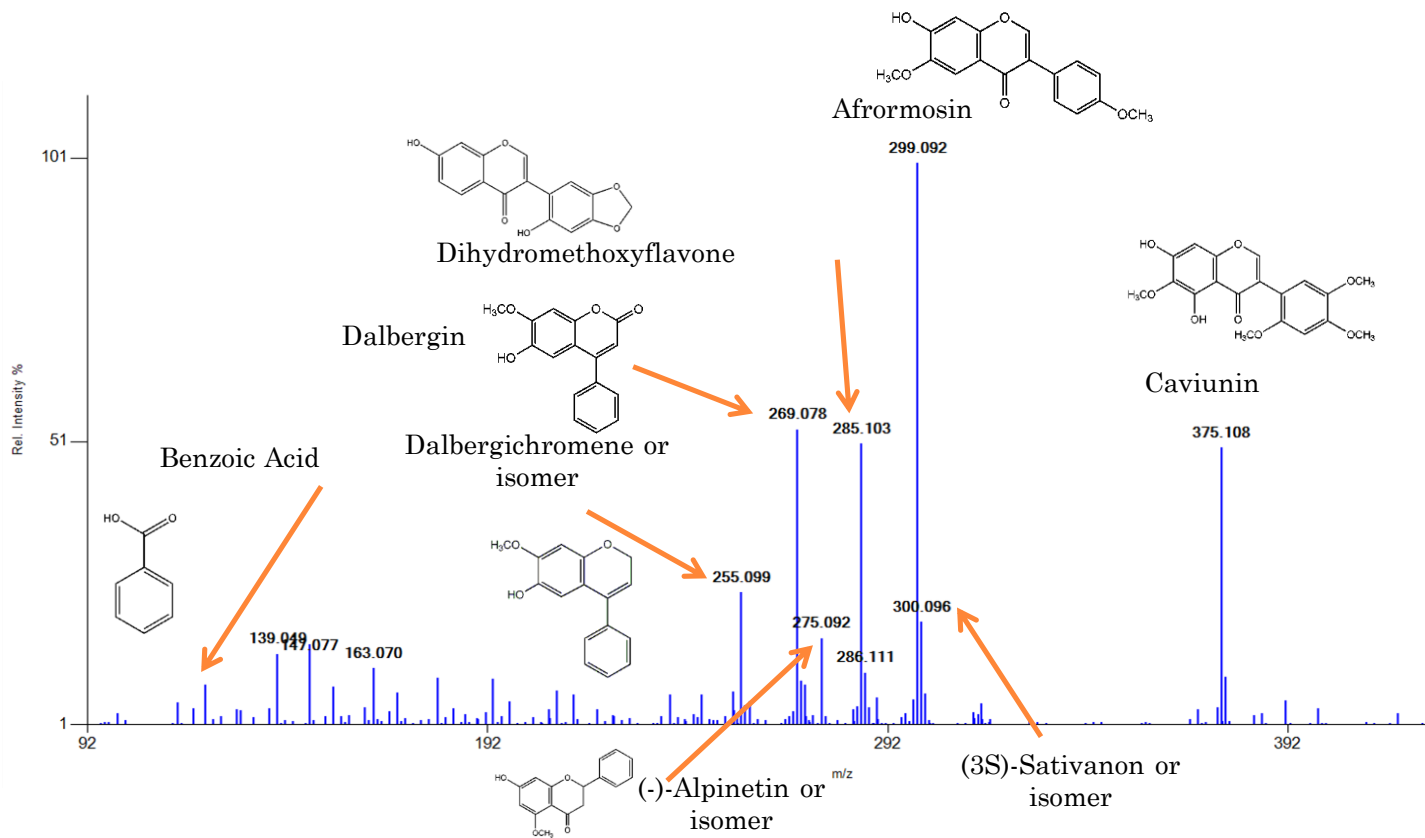


Photo by Kristen Finch 2015



Photo by Kristen Finch 2015

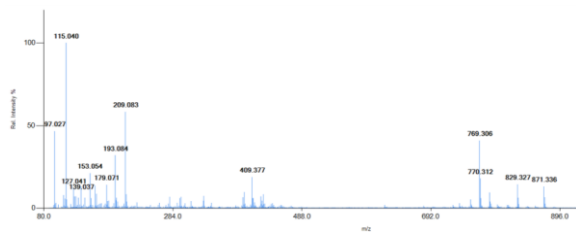
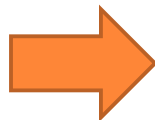




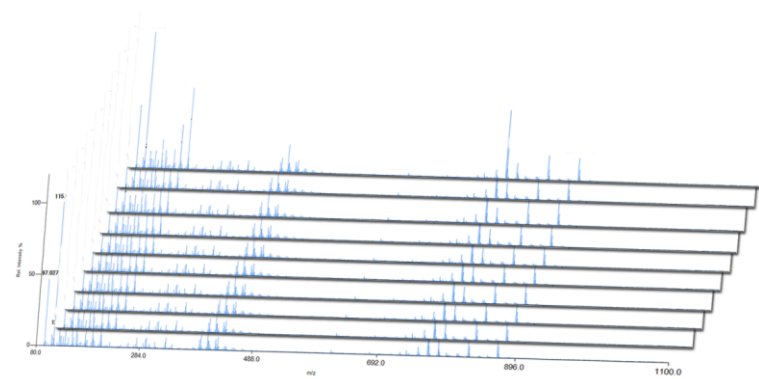
KNApSack: A Comprehensive Species-Metabolite Relationship Database

http://kanaya.naist.jp/knapsack_jsp/top.html



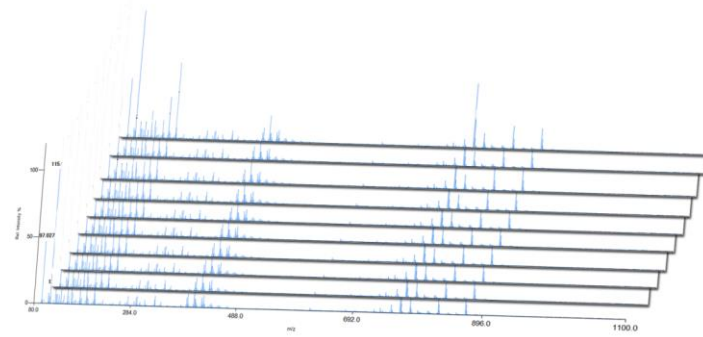
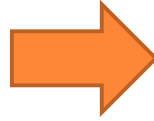


A single spectrum is useful for determining presence or absence of specific molecules and their relative abundance

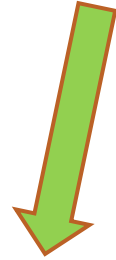
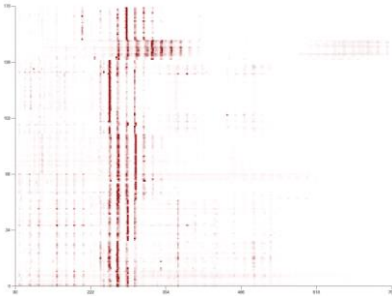


Many spectra are useful for characterizing species or populations

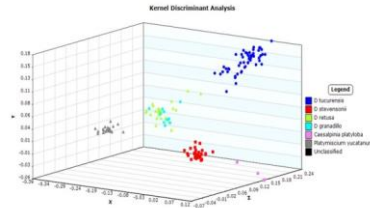




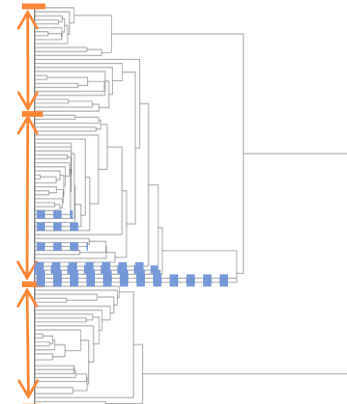
Heat Map



Multivariate Analysis



Hierarchical Cluster Analysis



DART TOFMS SPECTRA ON HAS BEEN USED FOR:

- Species identification
- Wild vs Plantation grown
- Geographic source assignment

- Inferences of rain fall
- Validation of Xyleria specimens
- Inferences of hybridization





SPECIES IDENTIFICATION

Cedrela spp.

Collaborators

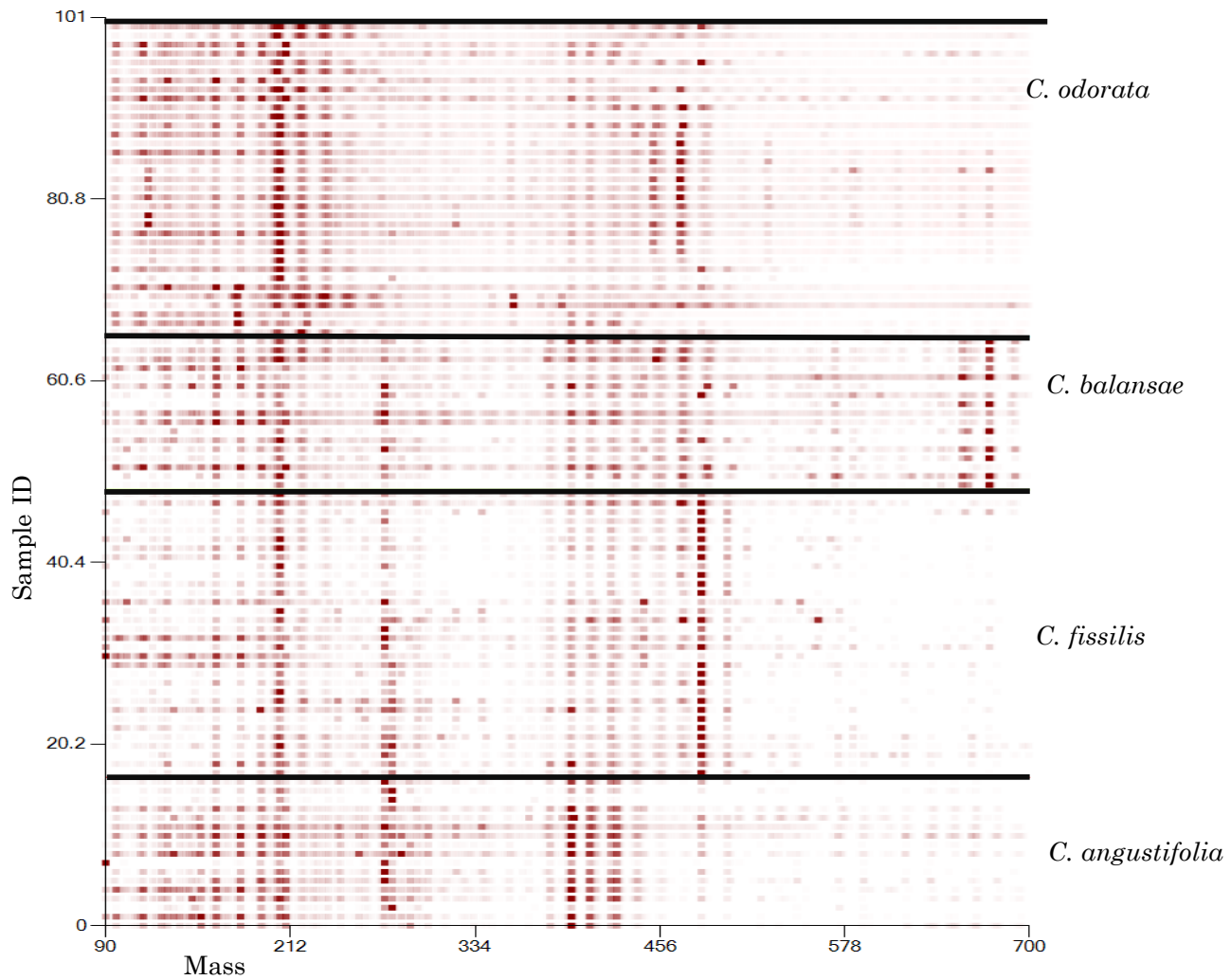
Kathelyn Paredes and Pieter Zuidema,
Wageningen University
The Netherlands

FOUR SPECIES TESTED

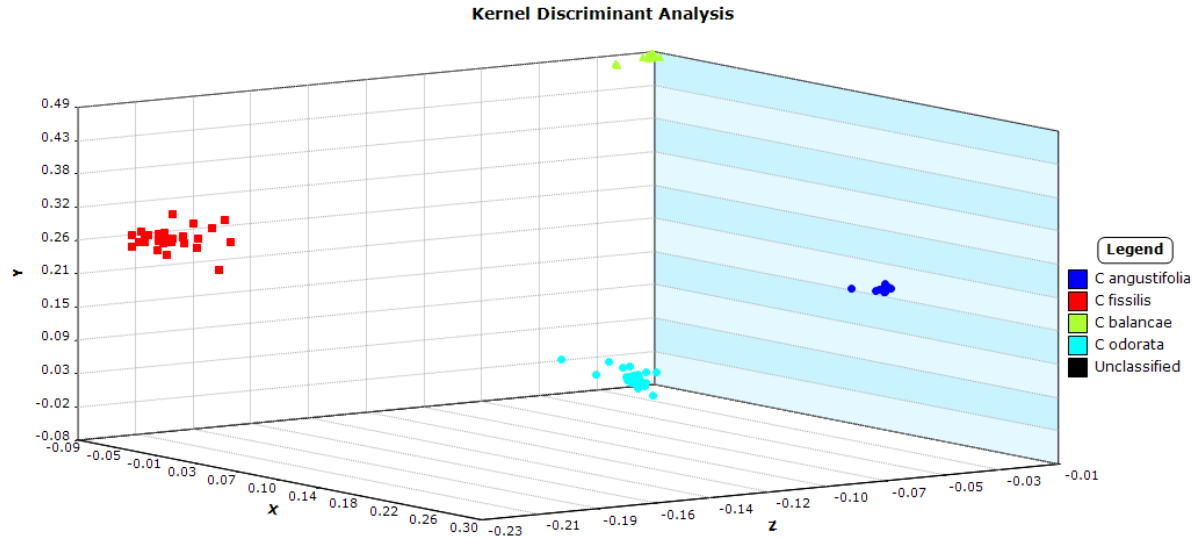
Species	CITES	n	Origen
<i>Cedrela angustifolia</i> Sesse & Moc		17	Bolivia
<i>Cedrela balansae</i> C.DC.		17	Bolivia
<i>Cedrela fissilis</i> Vell.	App III	32	Bolivia
<i>Cedrela odorata</i> L.	App III	35	C & S America
		$\Sigma = 101$	

Ask me about my dissertation- *Cedrela* phylogenomics!





KERNAL DISCRIMINANT ANALYSIS OF *CEDRELA* SPP.



Leave-One-Out Cross-Validation = 83.2%



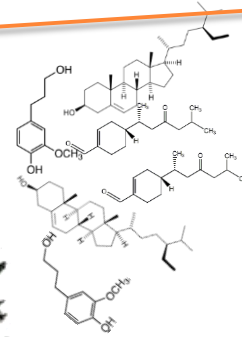
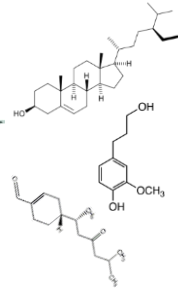
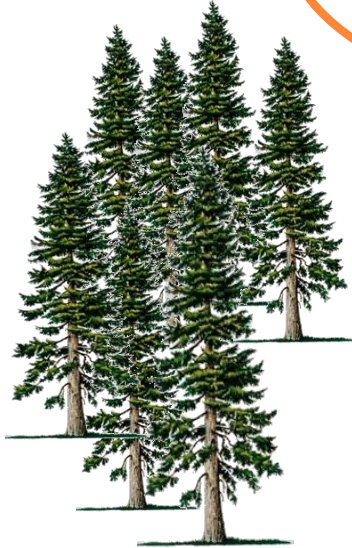
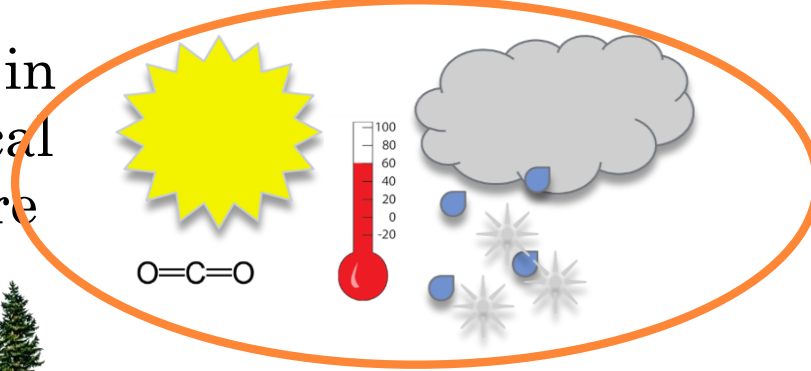


INTRASPECIES VARIATION WILD VS. CULTIVATED

Aquilaria spp.

E. O. Espinoza, C. A. Lancaster, N. M. Kreitals, M. Hata, R. B. Cody, R. A. Blanchette. Distinguishing wild from cultivated agarwood (*Aquilaria* spp.) using direct analysis in real time and time of-flight mass spectrometry. *Rapid Commun. Mass Spectrom.* **2014**, 28, 281.

Locked in Chemical Warfare



Defense

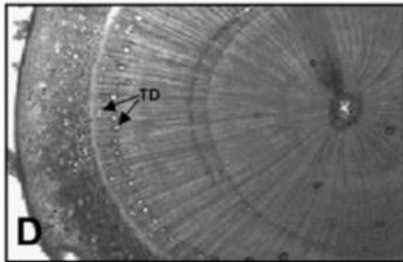


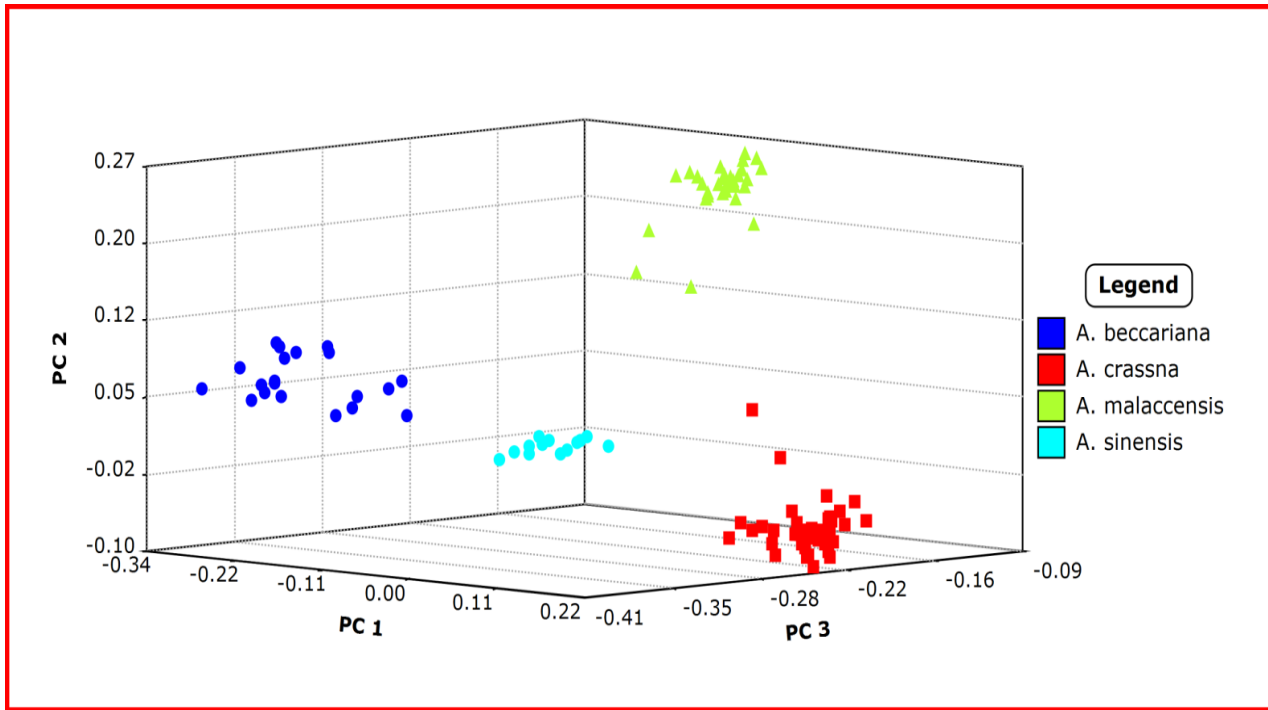
Photo Huber et al. 2005



GEOGRAPHIC SCALE

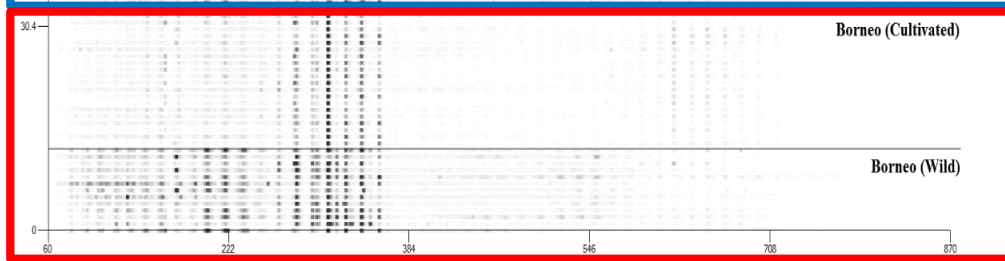
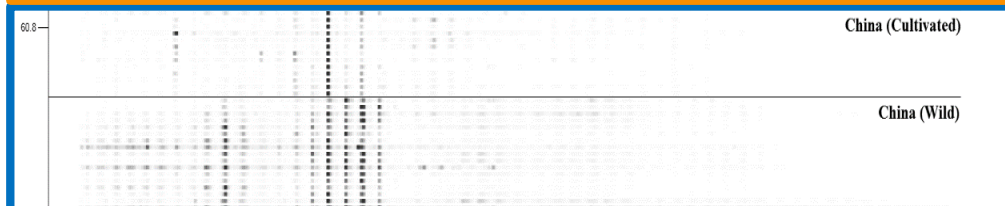
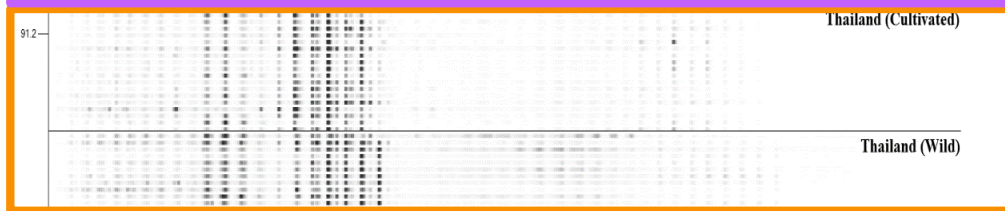
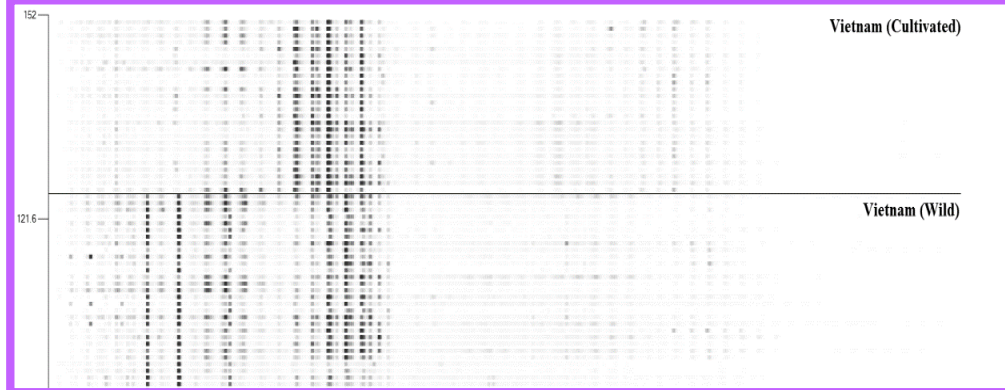


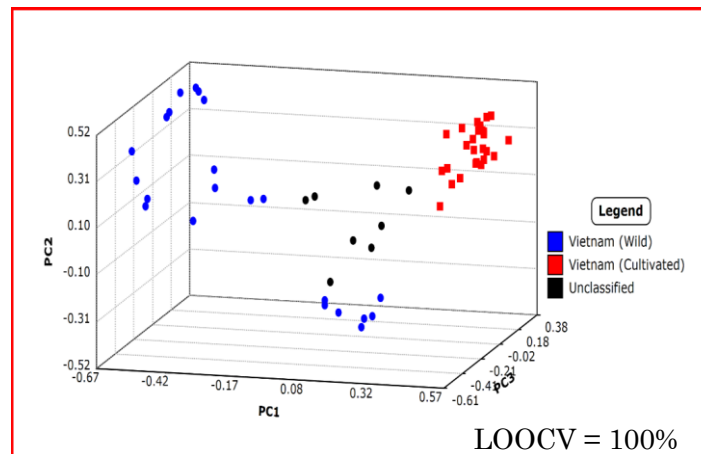
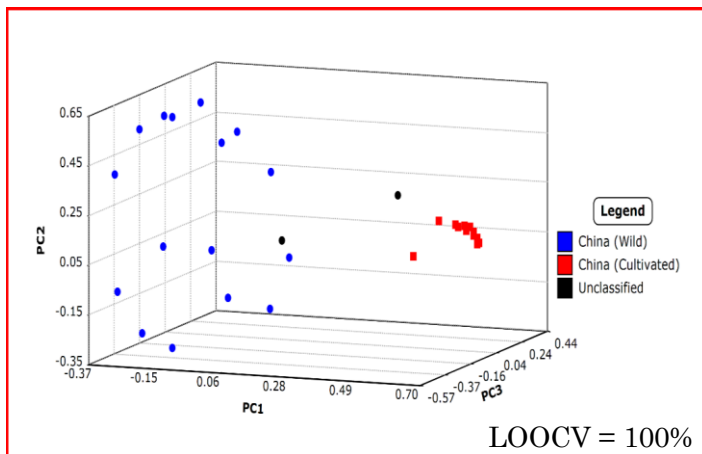
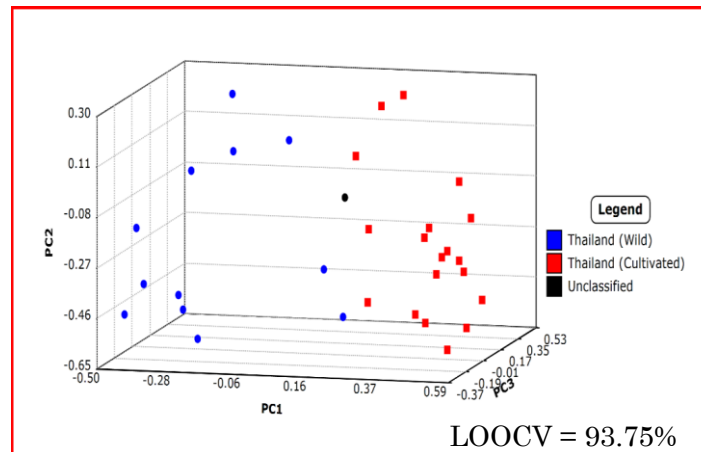
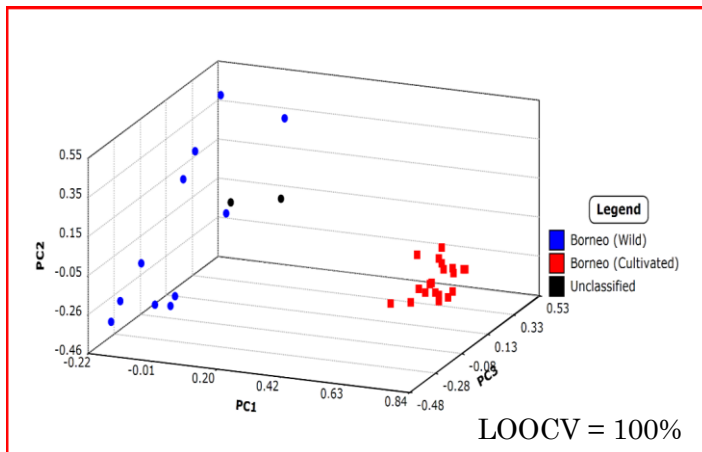
AQUILARIA TAXONOMIC CLASSIFICATION



Leave-One-Out Cross-Validation = 96.33%









Photos by Kristen Finch 2015

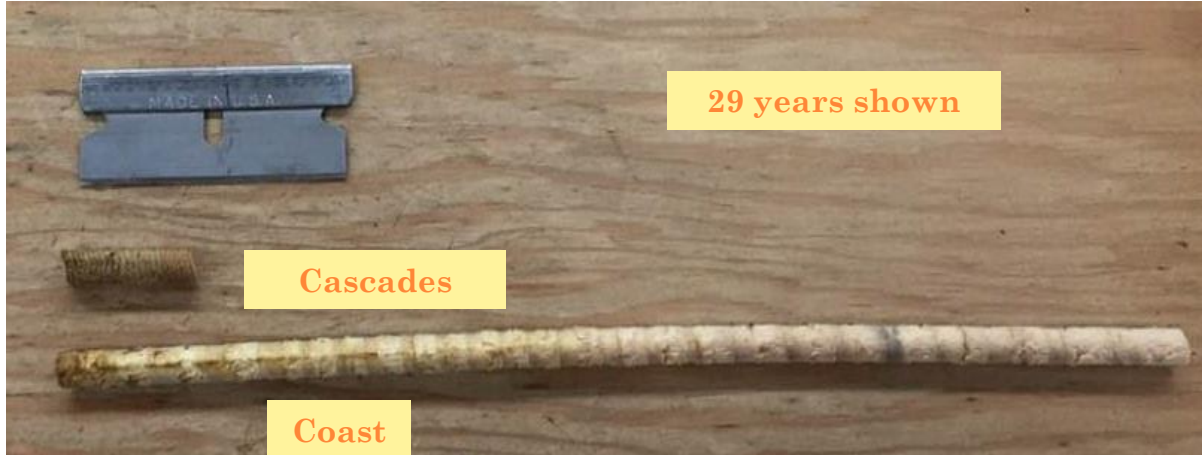
FINE SCALE GEOGRAPHIC SOURCE ASSIGNMENT

Pseudotsuga menziesii var. *menziesii*

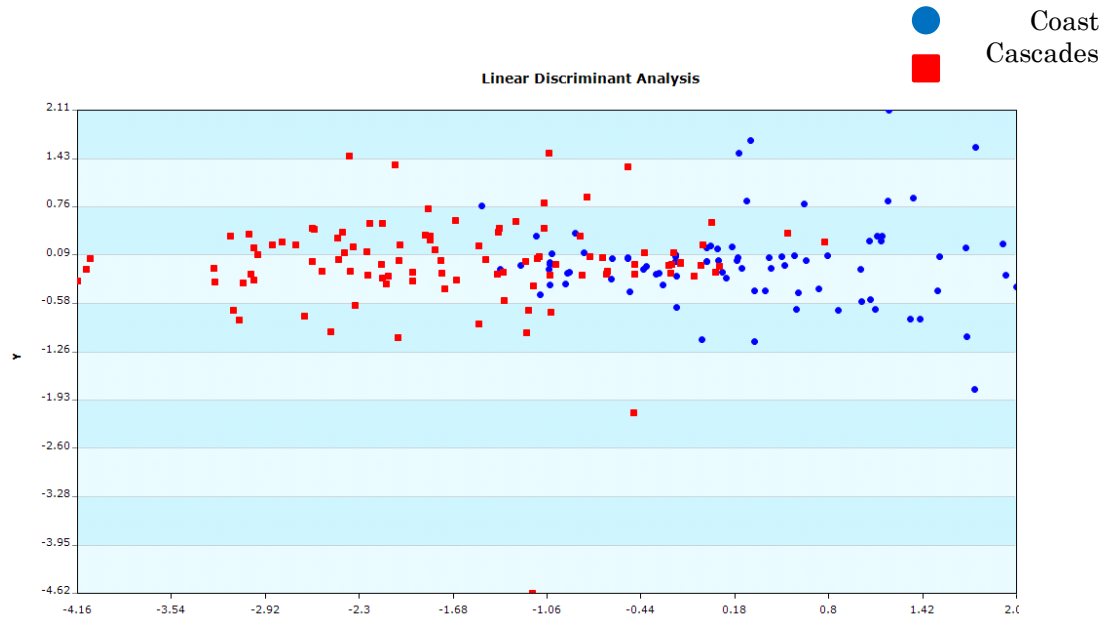
Coastal Douglas-fir

Kristen Finch, Ed Espinoza, Rich Cronn

Environmental differences typically lead to obvious differences in growth rate.



RESULTS



Leave-one-out cross-validation: 74.33%^x



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- Inferences of hybridization

Please contact us with your questions:

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REFERENCES

- E. O. Espinoza, C. A. Lancaster, N. M. Kreitals, M. Hata, R. B. Cody, R. A. Blanchette. Distinguishing wild from cultivated agarwood (*Aquilaria* spp.) using direct analysis in real time and time of-flight mass spectrometry. *Rapid Commun. Mass Spectrom.* **2014**, 28, 281.
- FINCH, K. N., ESPINOZA, E., CRONN, R. C. In Preparation. Direct Analysis in Real Time (Time of Flight) Mass Spectrometry differentiates wood chemotypes of *Pseudotsuga menziesii* (Douglas-fir) from two regions in Oregon.

