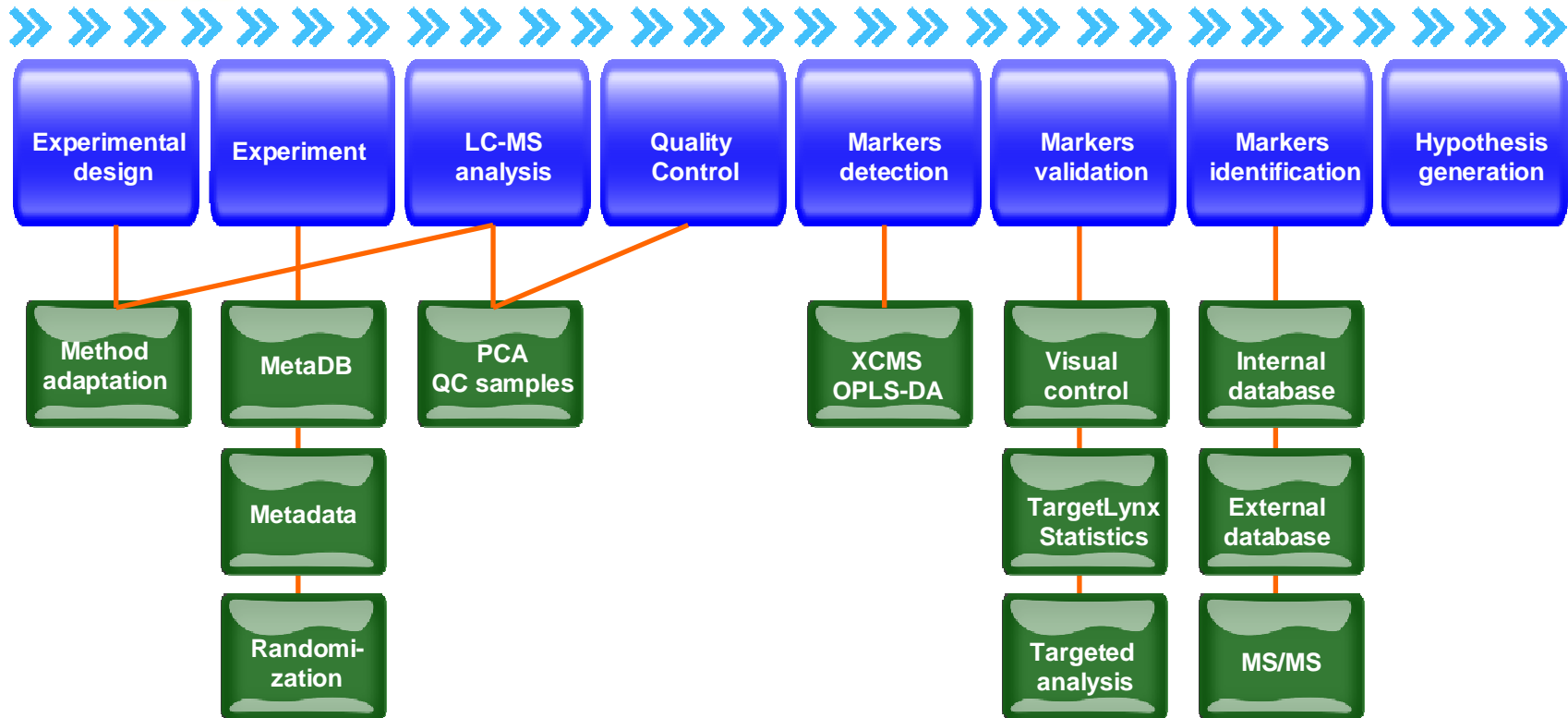


# LC-MS Wine Metabolomics: **experiment**



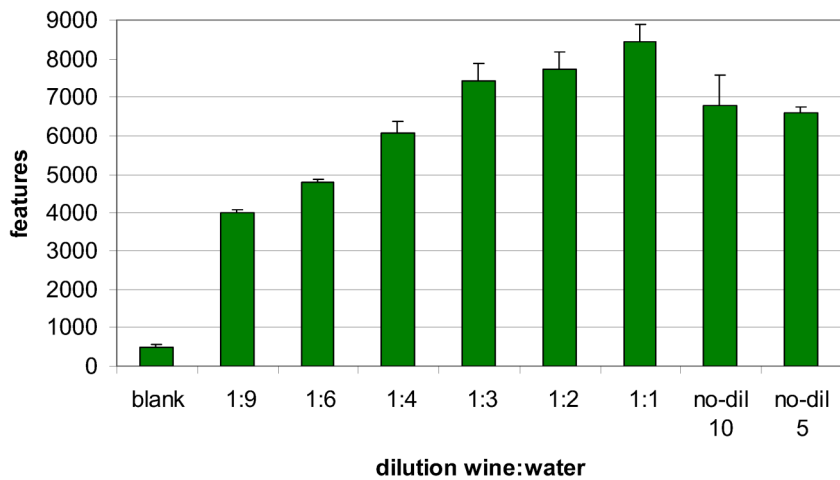
# LC-MS Wine Metabolomics: workflow



# LC-MS Wine Metabolomics: **method**



Method  
adaptation



# LC-MS Wine Metabolomics: markers



XCMS  
OPLS-DA

Visual  
control

TargetLynx  
Statistics

Targeted  
analysis

(tentative) bio-markers

false positives



false negatives



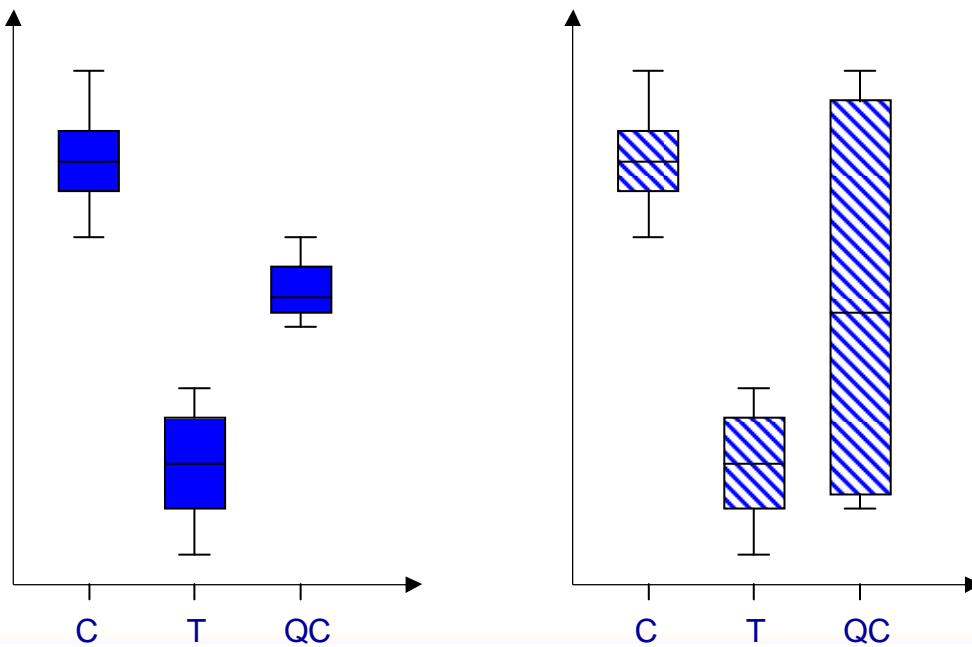
# LC-MS Wine Metabolomics: markers



1. Check chromatogram
2. Check MS spectra
3. Peak integration
4. QC variability Vs. *p*-values

Visual control

TargetLynx Statistics



## LC-MS Wine Metabolomics: **annotation**



Sigma-Aldrich has **~55K** commercial available chemicals



Kegg contains **18K** metabolites



HMDB is based in **~42K** metabolites

Plant metabolome is estimated to cover **200K** metabolites



External databases



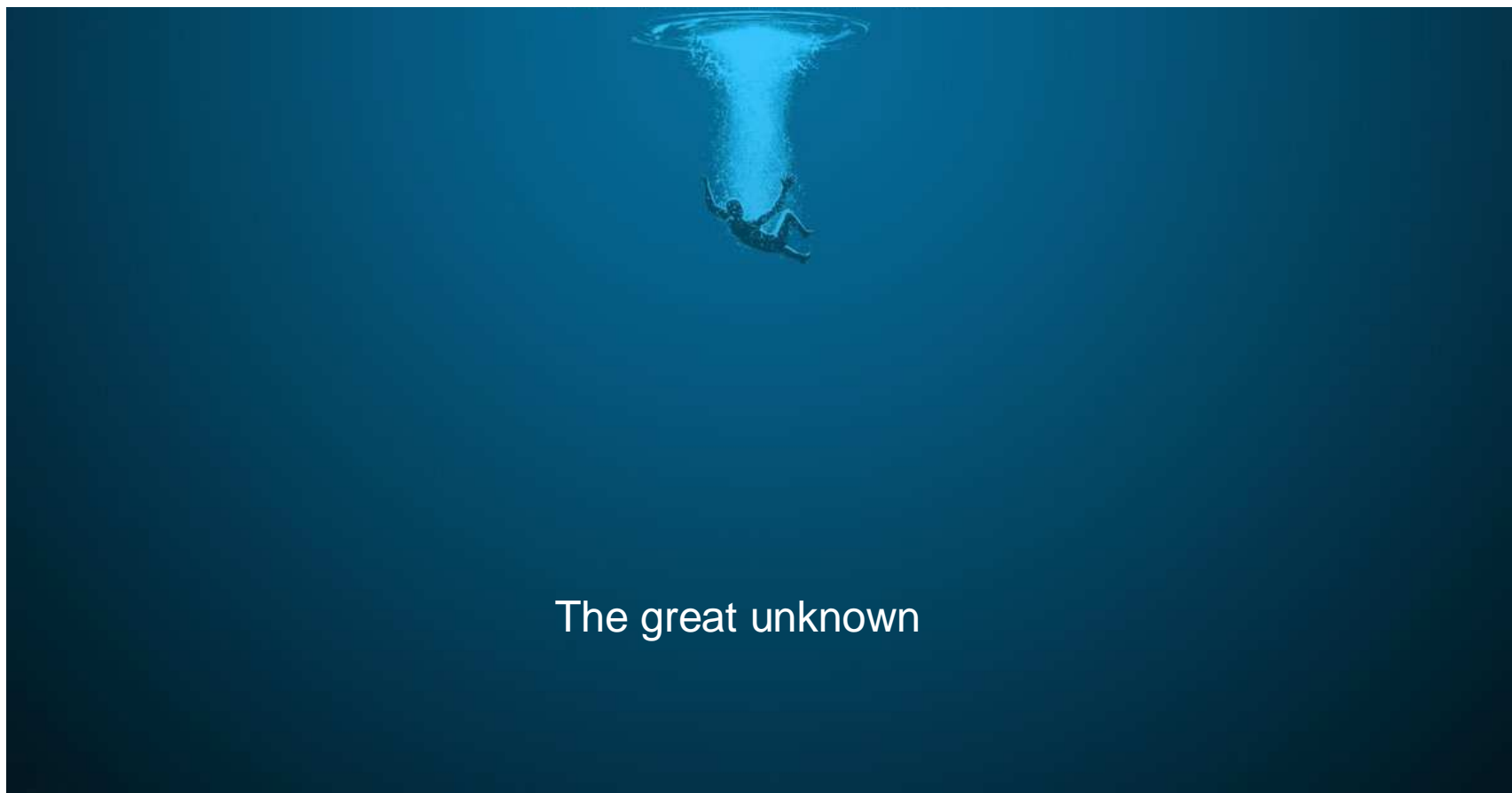
PubChem ID contains more than **10M** entries



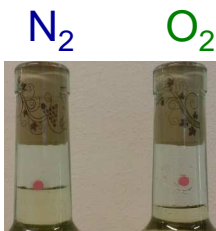
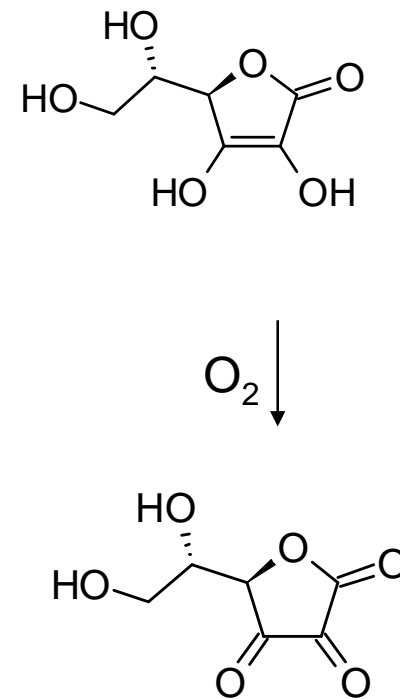
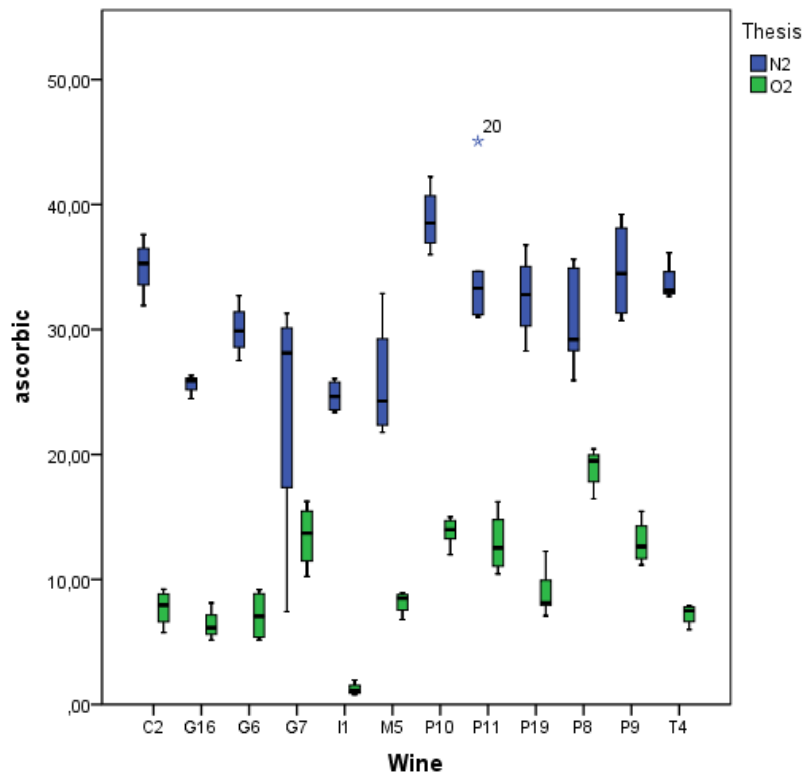
A division of the American Chemical Society

CAS contains over **90M** unique organic and inorganic chemicals

## LC-MS Wine Metabolomics: **annotation**



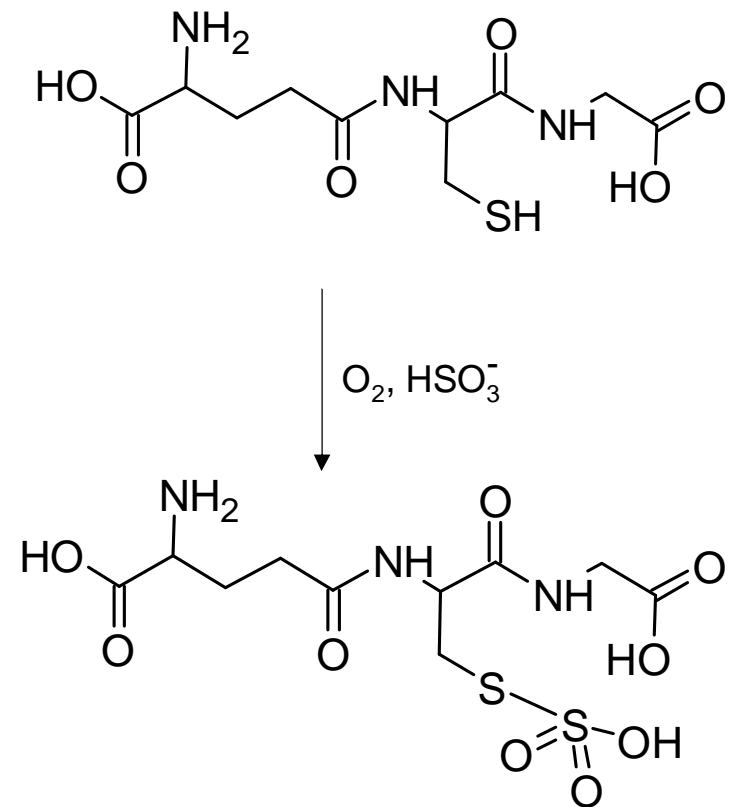
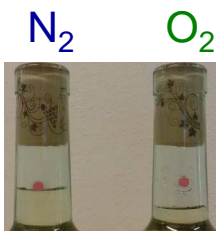
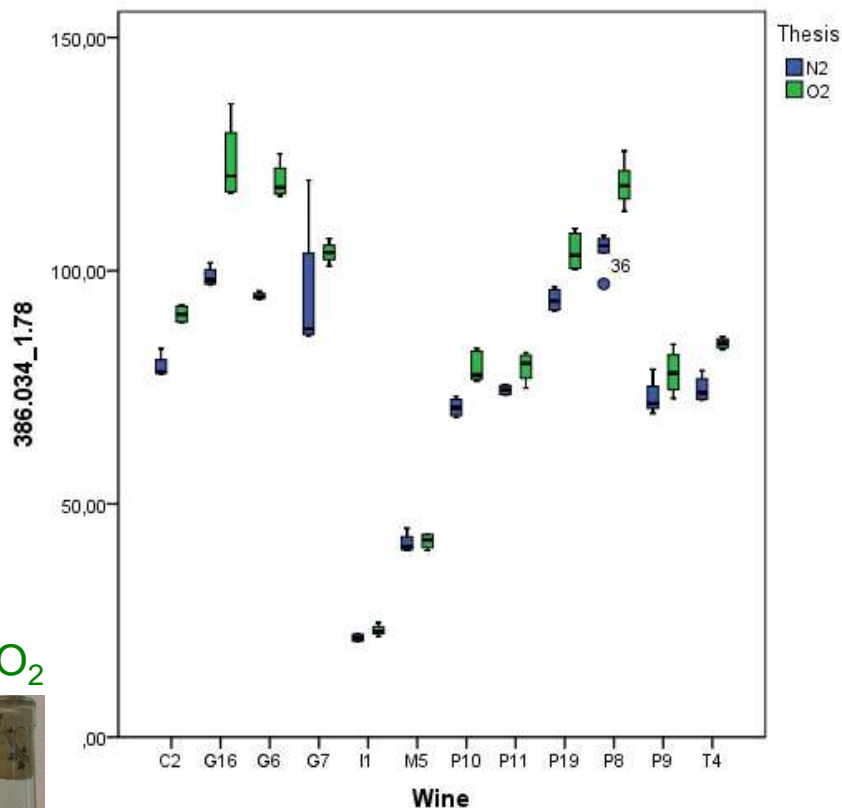
# LC-MS Wine Metabolomics: Hypothesis





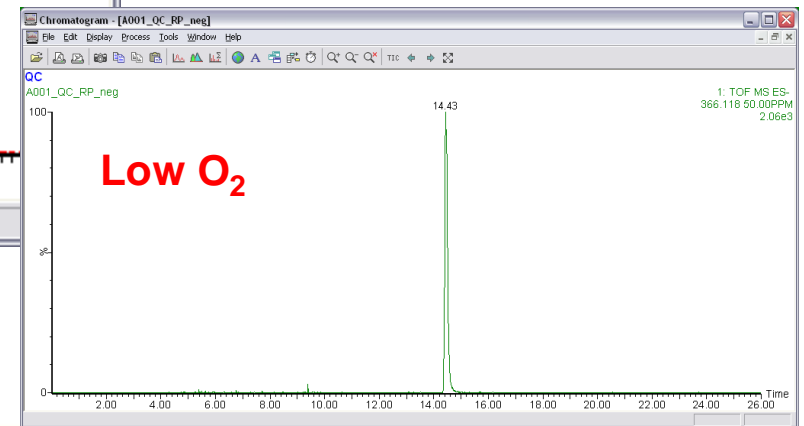
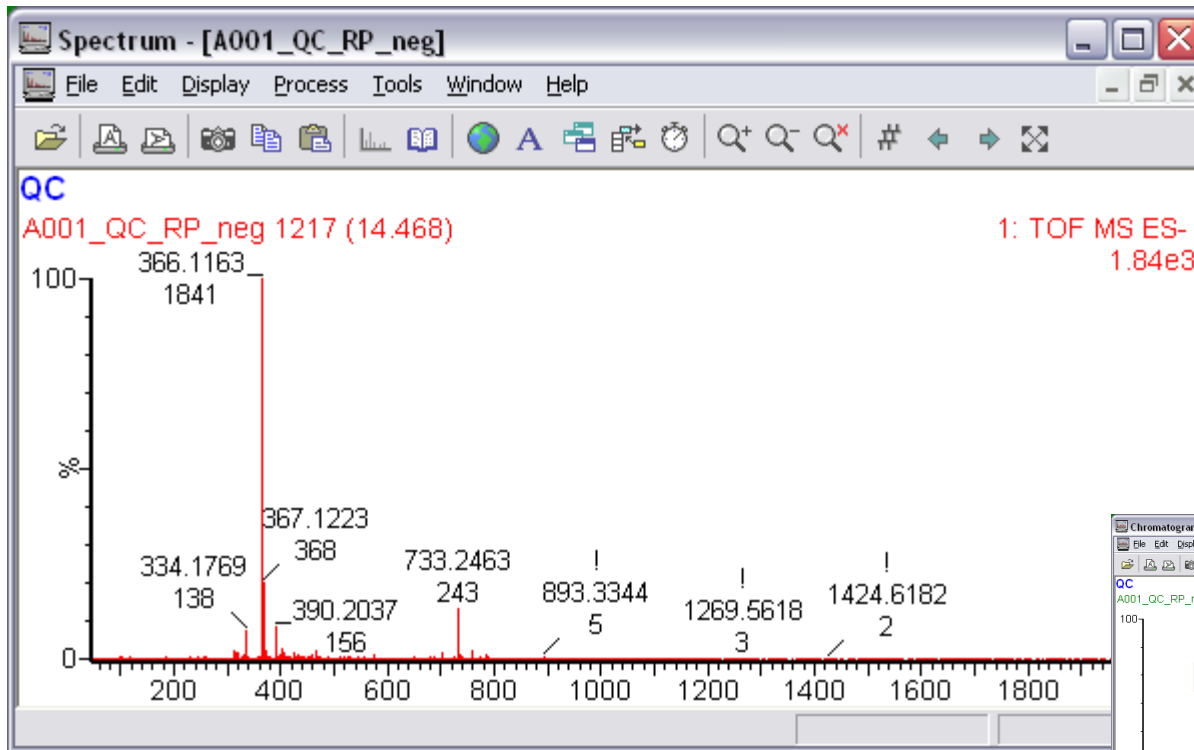


# LC-MS Wine Metabolomics: Hypothesis





# LC-MS Wine Metabolomics: Annotation





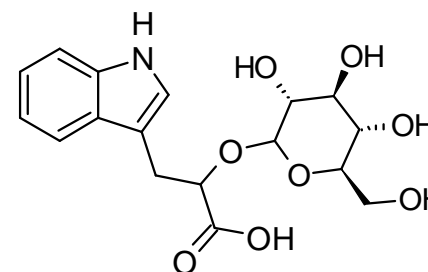
Anal Bioanal Chem (2014) 406:1201–1208  
DOI 10.1007/s00216-013-7244-z

RESEARCH PAPER

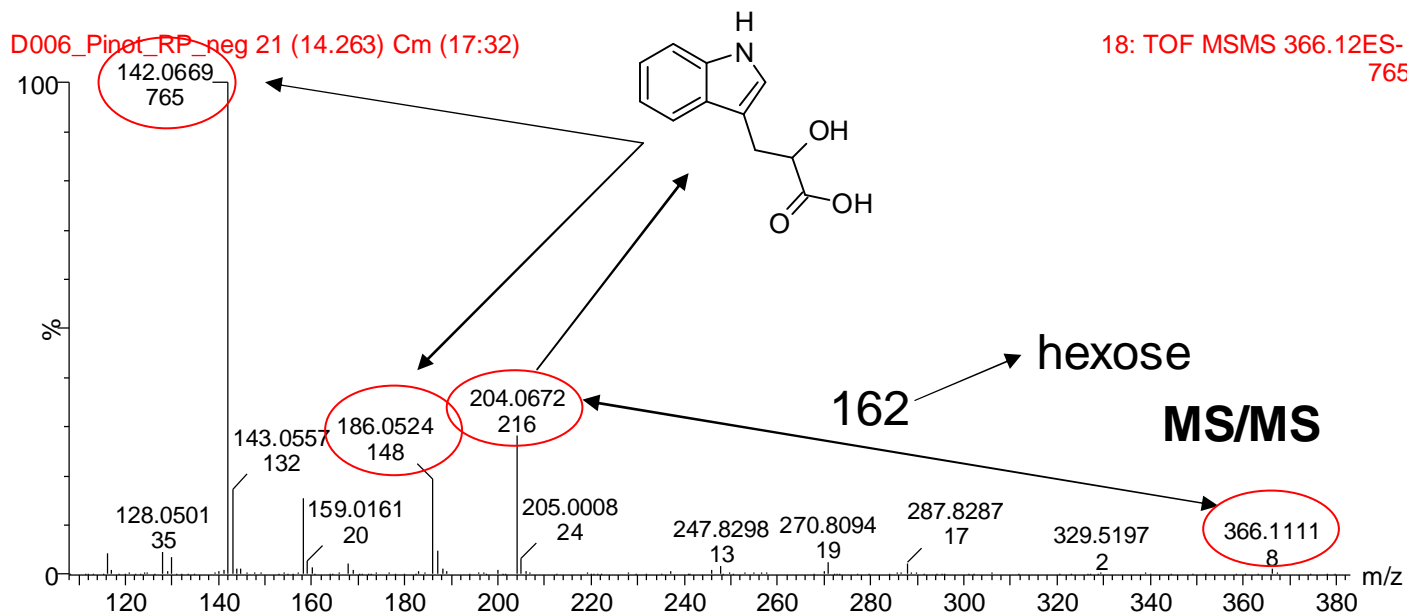
## Isolation, characterization, and determination of a new compound in red wine

Sandy Fabre · Christelle Absalon · Noël Pinaud ·  
Christiane Venencie · Pierre-Louis Teissedre ·  
Eric Fouquet · Isabelle Planet

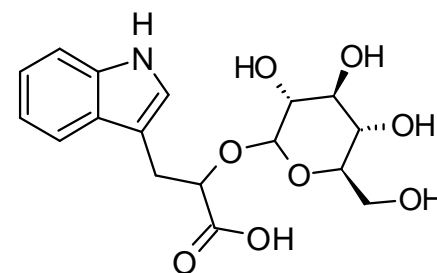
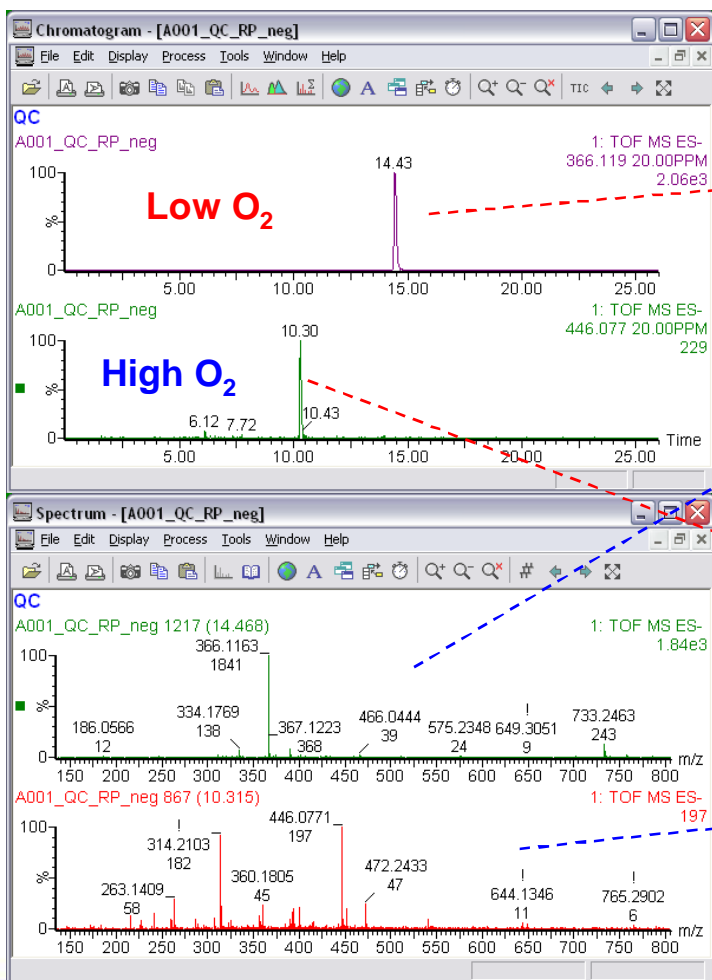
Received: 23 April 2013 / Revised: 27 June 2013 / Accepted: 10 July 2013 / Published online: 4 August 2013  
© Springer-Verlag Berlin Heidelberg 2013



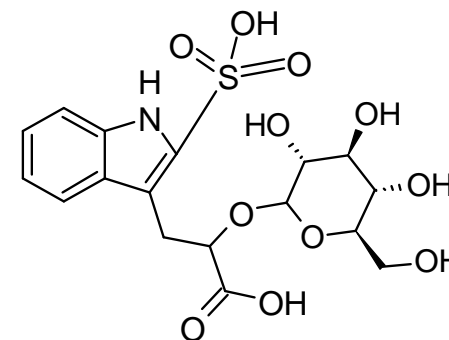
18: TOF MSMS 366.12ES-765



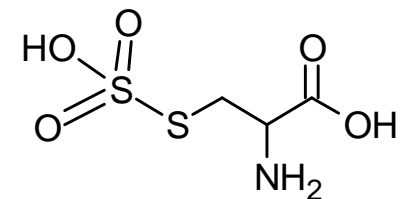
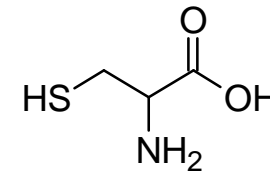
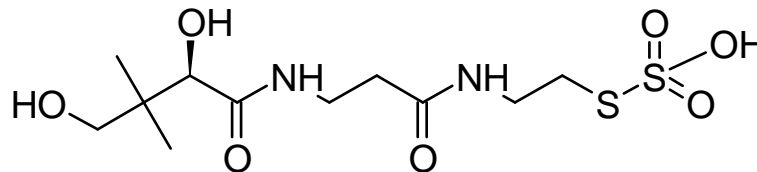
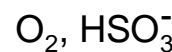
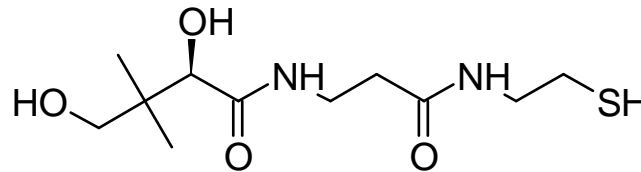
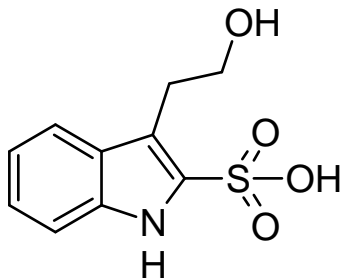
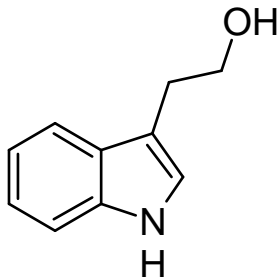
# LC-MS Wine Metabolomics: Annotation



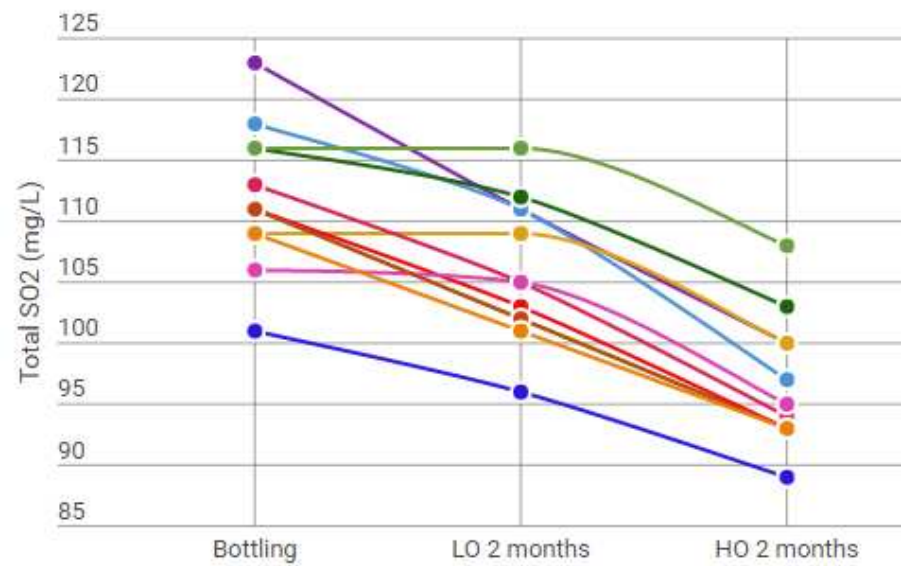
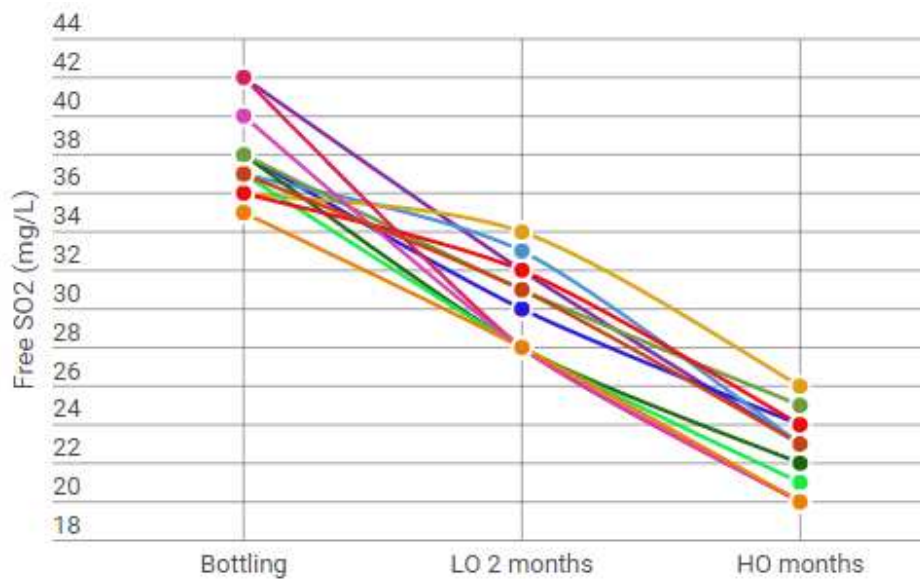
O<sub>2</sub>, HSO<sub>3</sub><sup>-</sup>



# LC-MS Wine Metabolomics: Hypothesis



# LC-MS Wine Metabolomics: Hypothesis Confirmation



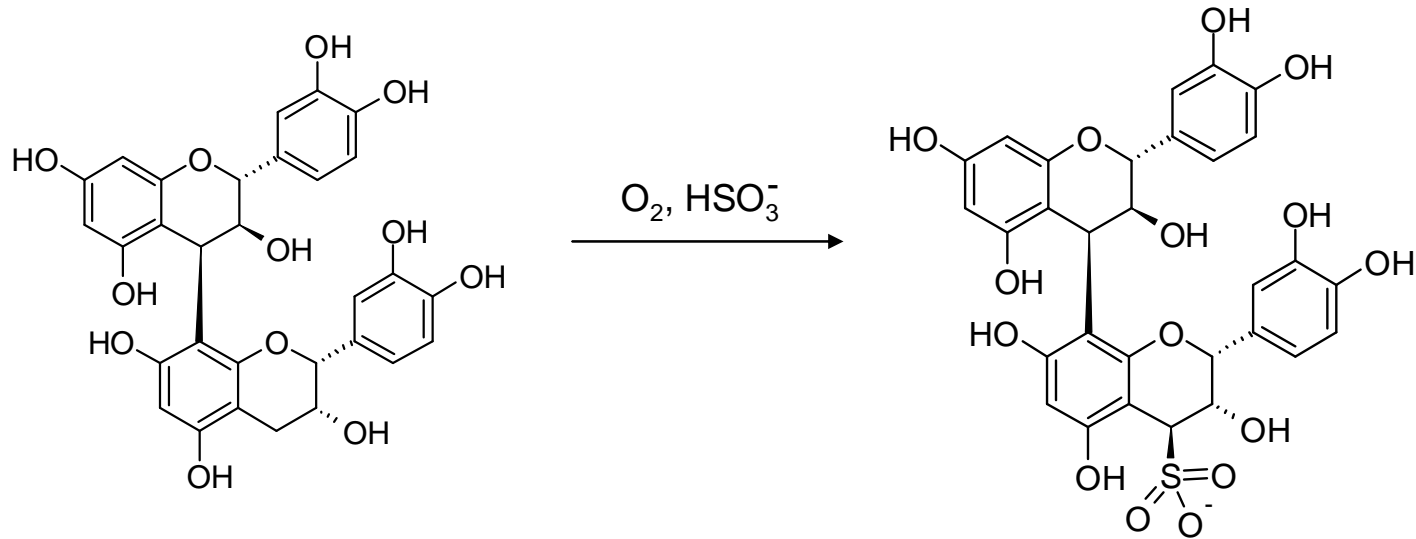
- Inzolia
- Muller Thurgau
- Chardonnay
- Traminer
- Grillo 1
- Grillo 2
- Grillo 3
- Pinot gris 1
- Pinot gris 2
- Pinot gris 3
- Pinot gris 4
- Pinot gris 5

- Inzolia
- Muller Thurgau
- Chardonnay
- Traminer
- Grillo 1
- Grillo 2
- Grillo 3
- Pinot gris 1
- Pinot gris 2
- Pinot gris 3
- Pinot gris 4
- Pinot gris 5

LO: Low O<sub>2</sub>  
HO: High O<sub>2</sub>



# LC-MS Wine Metabolomics: Old work



# LC-MS Wine Metabolomics: Public Repositories



## MetaDB a Data Processing Workflow in Untargeted MS-Based Metabolomics Experiments

Release date: 10-Nov-2014

### Organism

- Vitis vinifera (Grape)

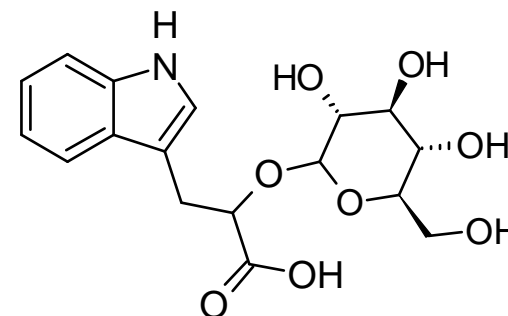
### Study Factors

- Variety: [QC, Phoenix, Regent]
- Country: [QC, Germany, Italy]

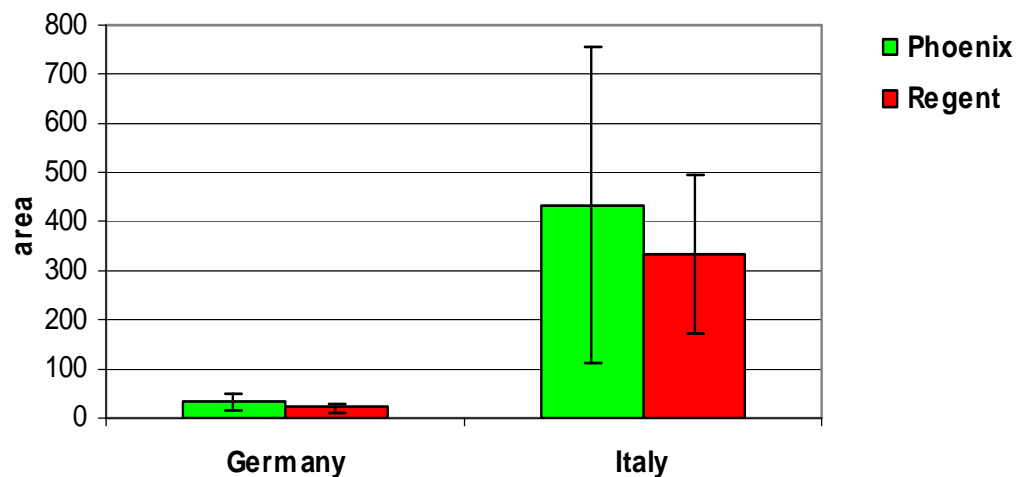
### Assay

- mass spectrometry (50)

Study identifier: **MTBLS137**  
Submitted  
by [Panagiotis Arapitsas](#)



indole-3-lactic glucoside



## Top 30 red grape cultivars

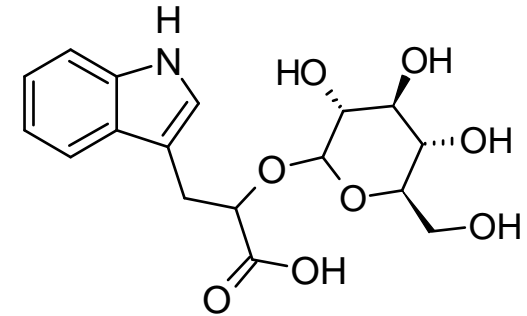
1	2010	Cabernet Sauvignon	←
2	2010	Nero	
3	2010	Couderc	
4	2010	Isabella*	
5	2010	Marzemino	
6	2009	Cabernet Sauvignon	←
7	2010	Nebbiolo	
8	2010	Casetta N.	
9	2008	Cabernet Sauvignon	←
10	2009	Carmenere	
11	2010	Girelli PnxMe*	
12	2010	Ancellotta	
13	2010	Schiava lombarda	
14	2010	Carmenere	
15	2010	Uva di Troia	
16	2010	Landal	
17	2010	Schioppetino	
18	2009	Cabernet franc	
19	2010	Negro Amaro	
20	2008	V. Champini*	
21	2007	V. Champini*	
22	2008	Carmenere	
23	2010	Pinot noir	
24	2009	Calabrese	
25	2010	Pinot noir	
26	2007	Cabernet Sauvignon	←
27	2008	Merlot noir	
28	2010	Montepulciano	
29	2010	Xarello	
30	2009	Lambrusco salamino	


271 entries

## Top 30 white grape cultivars

1	2010	Verduzzo Friulano	←
2	2007	Verduzzo Friulano	←
3	2008	Greco bianco di Tufo	
4	2009	Verduzzo Friulano	←
5	2009	Sauvignon blanc	←
6	2010	Xarello	
7	2010	Sauvignon blanc	←
8	2010	Perla di Csaba	
9	2007	Welschriesling	
10	2007	Montagna*	
11	2010	Grechetto bianco	
12	2007	Perla di Csaba	
13	2009	Grechetto bianco	
14	2009	Xarello	
15	2007	Garganega	
16	2008	Girelli PnxMe*	
17	2009	Biancaccia*	
18	2007	Ribolla gialla	
19	2010	Biancaccia*	
20	2009	Prosecco	
21	2008	Biancaccia*	
22	2010	Montagna*	
23	2009	Nosiola	
24	2008	Biancaccia*	
25	2009	Biancaccia*	
26	2010	Italia	
27	2008	Kozma Palne Muskotaly	
28	2010	Prosecco	
29	2008	Prosecco	
30	2009	Valderbara*	

181 entries





Fulvio Mattivi  
Daniele Perenzoni  
Andrea Angeli

Maurizio Ugliano

Paolo Pangrazzi  
Umberto Pichler







**Pinot noir**  
Naousa  
Rapsani

**Chardonnay**  
Malagouzia

**Cabernet Sauvignon**  
Nemea

**Gewurtztraminer**  
Mantinia

**Riesling**  
Assyrtico