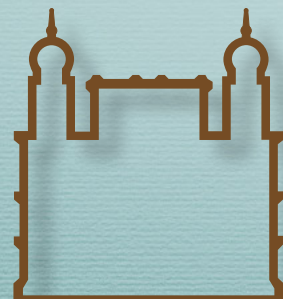


# Science in the Footsteps of Oswaldo Cruz

The CDTS Project



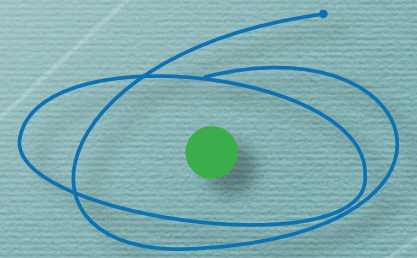
**inct-idn**  
instituto nacional de  
ciência e tecnologia  
de inovação em  
doenças negligenciadas



FIOCRUZ  
Fundação Oswaldo Cruz  
Ministério da Saúde



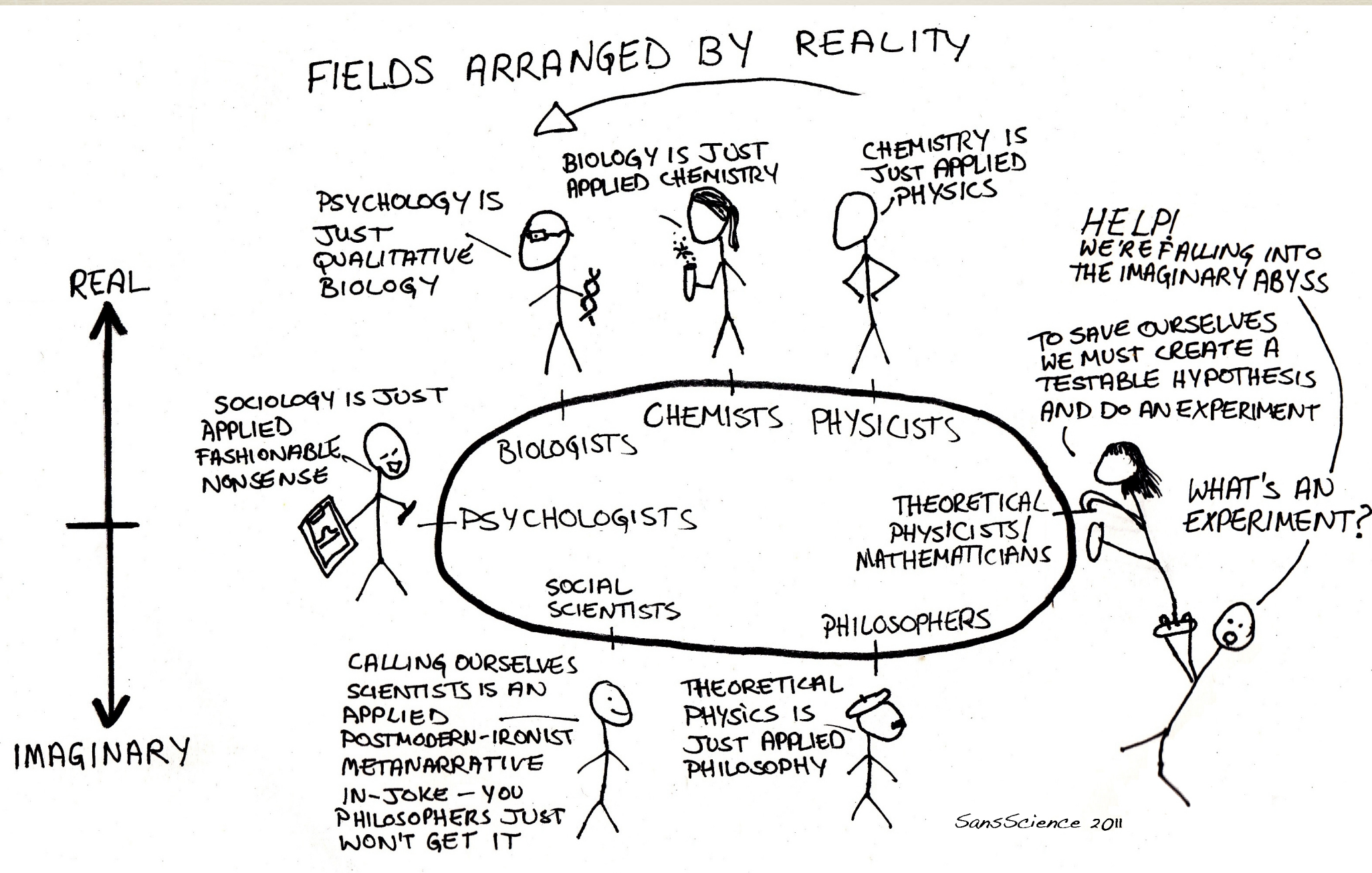
**manguinhos**  
Ministério da Saúde • Fundação Oswaldo Cruz



C A P E S



# A lost Chemist...





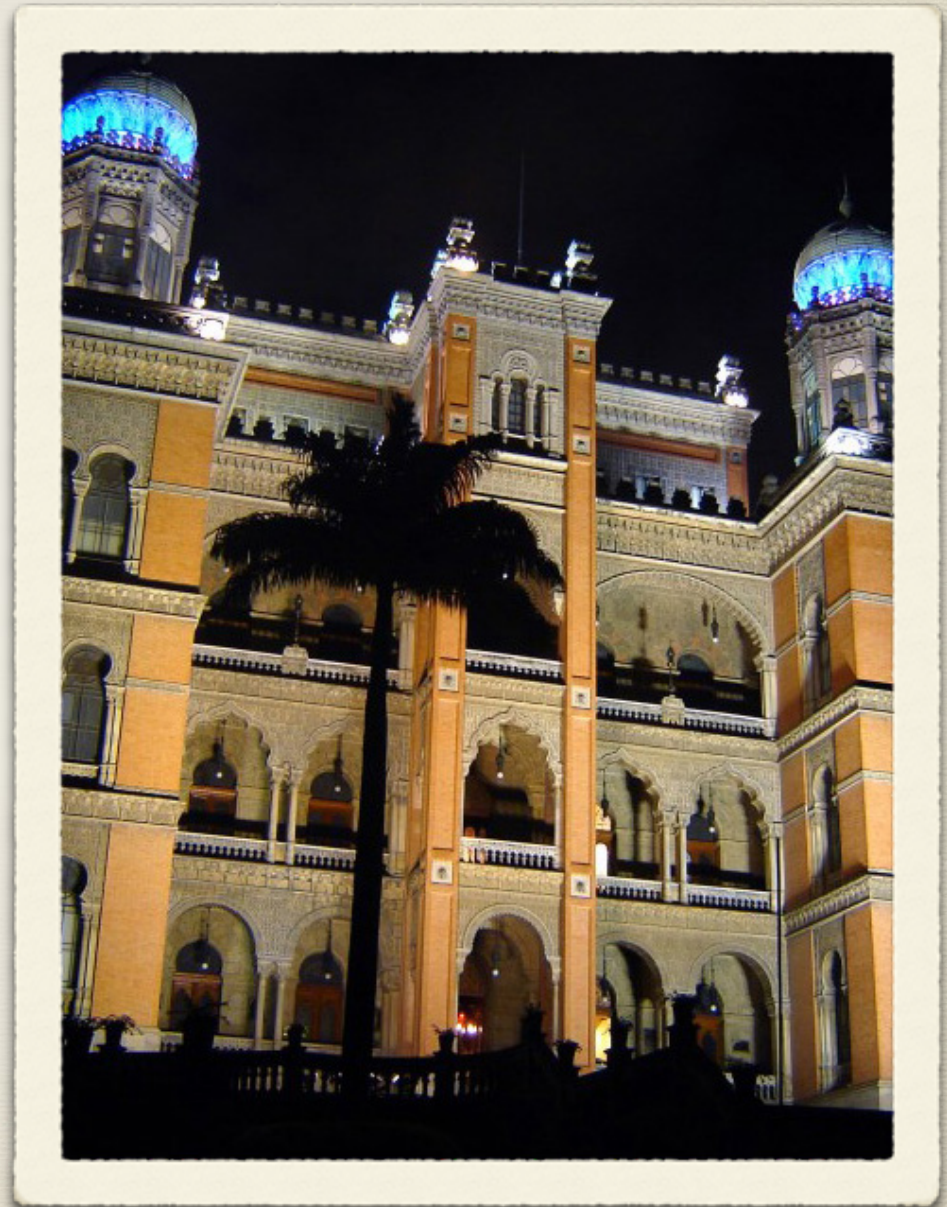
# The History of Fiocruz

*A single man making a difference*

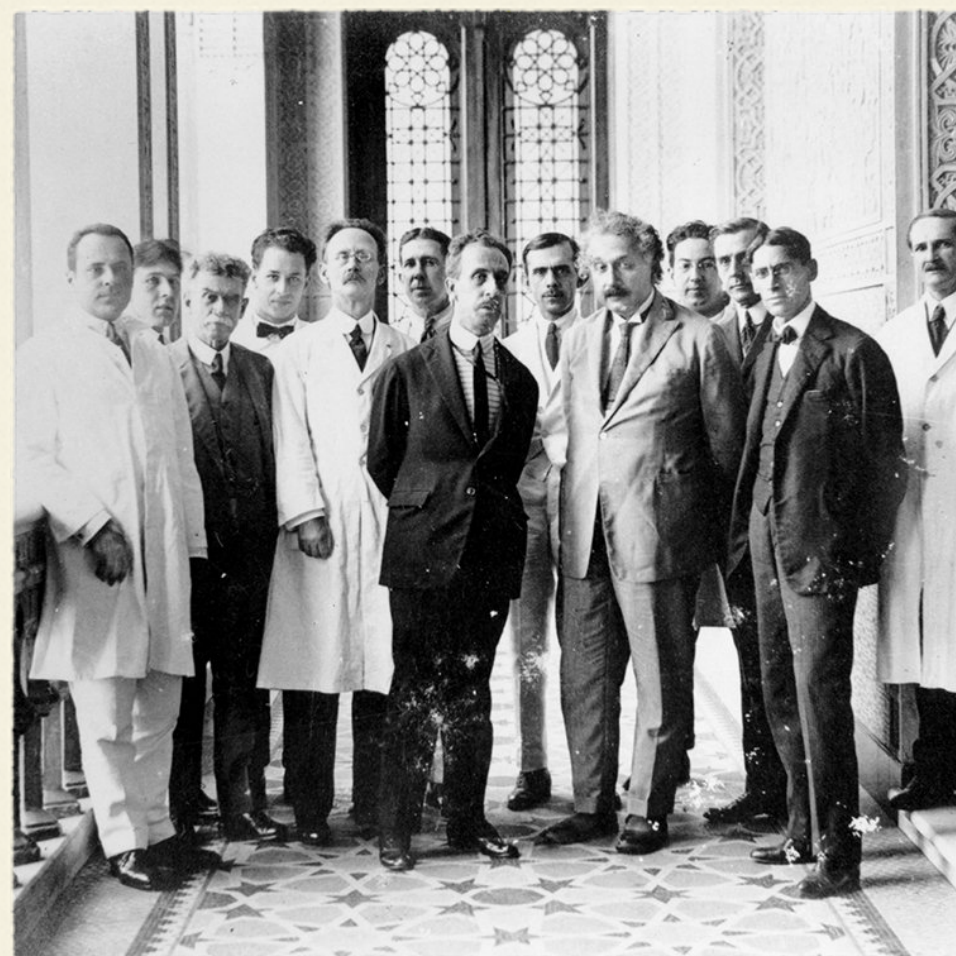
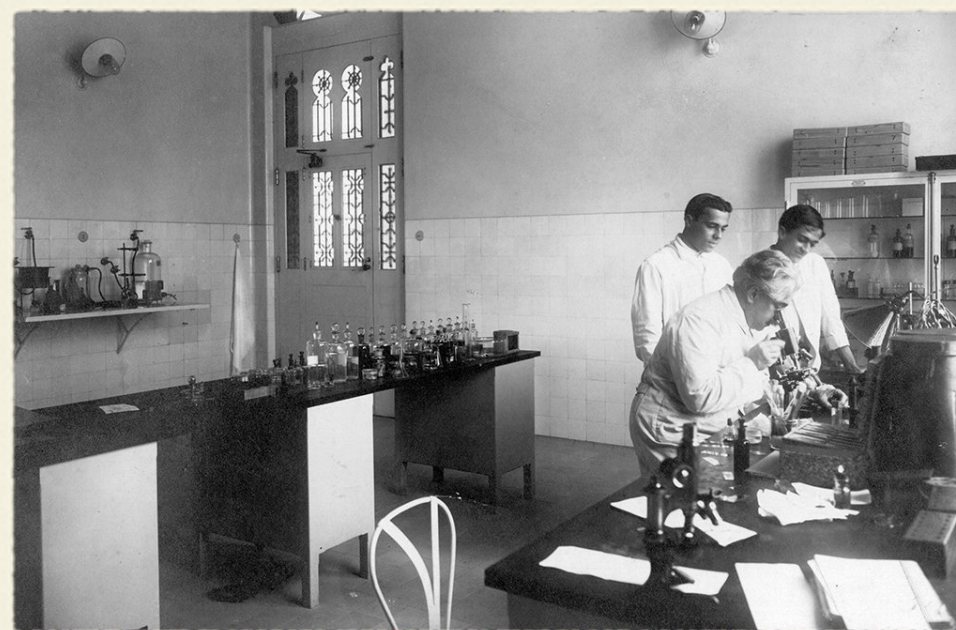


# Early years of Fundação Oswaldo Cruz

- \* Taken over in 1902 by Oswaldo Cruz
- \* Modeled after the *Institute Pasteur*
- \* Research for public health
  - \* Black Death
  - \* Yellow Fever Vaccine
  - \* Smallpox Vaccine
  - \* Malaria & Chaga's Disease









# And today?

- \* Research for Public Health
  - \* Malaria
  - \* Chaga's Disease
  - \* Dengue
  - \* Cancer & Alzheimer's
  - \* many others
- \* **Vaccines**









# CDTS

Center for Technological  
Development in Health:  
All in one place

- \* Technological Platforms
- \* Animal Experimentation
- \* Support Laboratories
- \* Flexible Laboratories
- \* Technological Management  
and Administration





# NMR in Fiocruz

Daily Routine, improved



# Motivation

“Chasing molecules that were never there: Misassigned natural products and the role of chemical synthesis in modern structure elucidation”

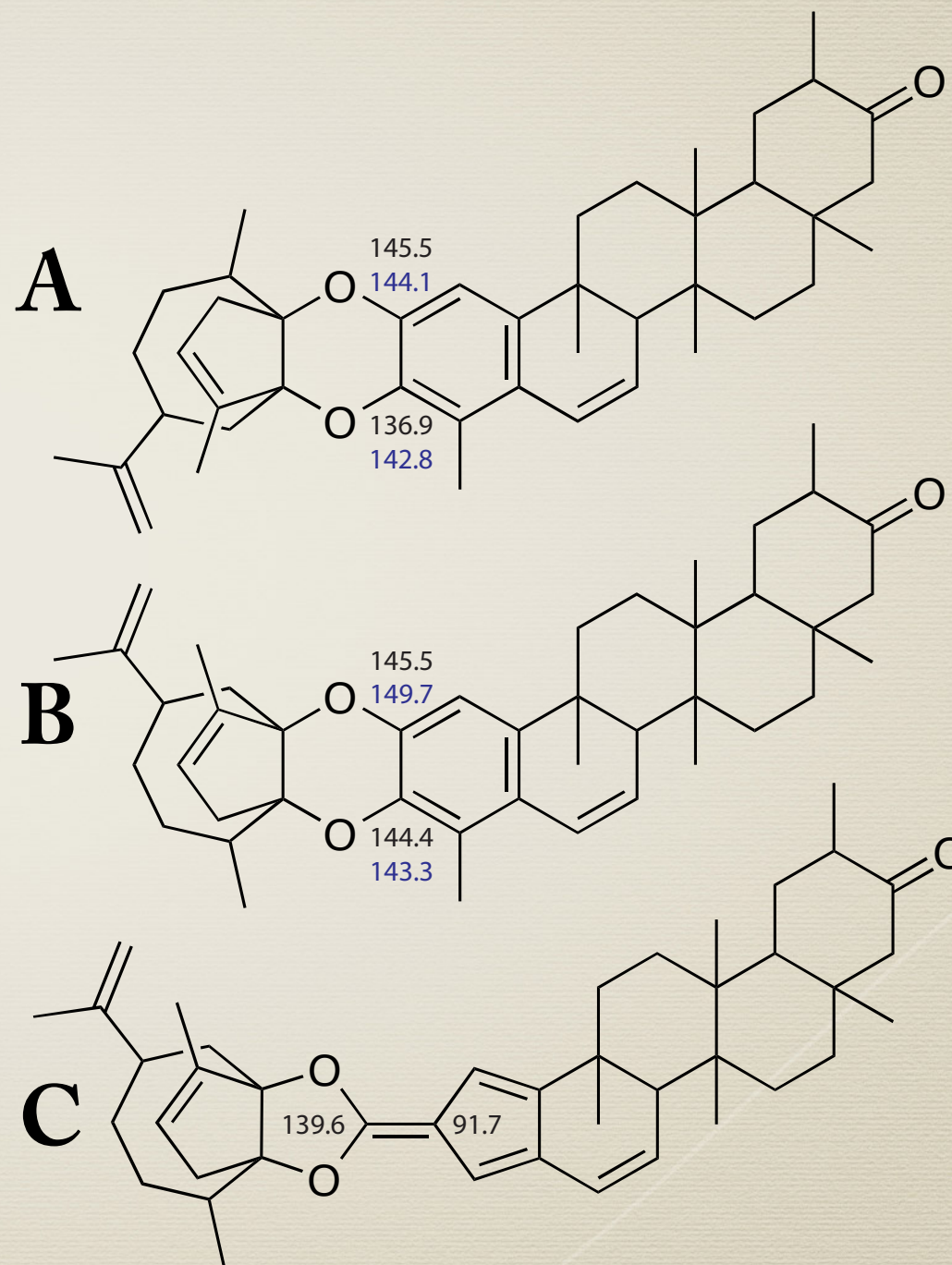
- \* ~30% of the published structures are wrong, but it is never discovered
- \* In general, only synthesis discovers error
- \* Synthesis is done only for interesting molecules





# Discussion of Structures

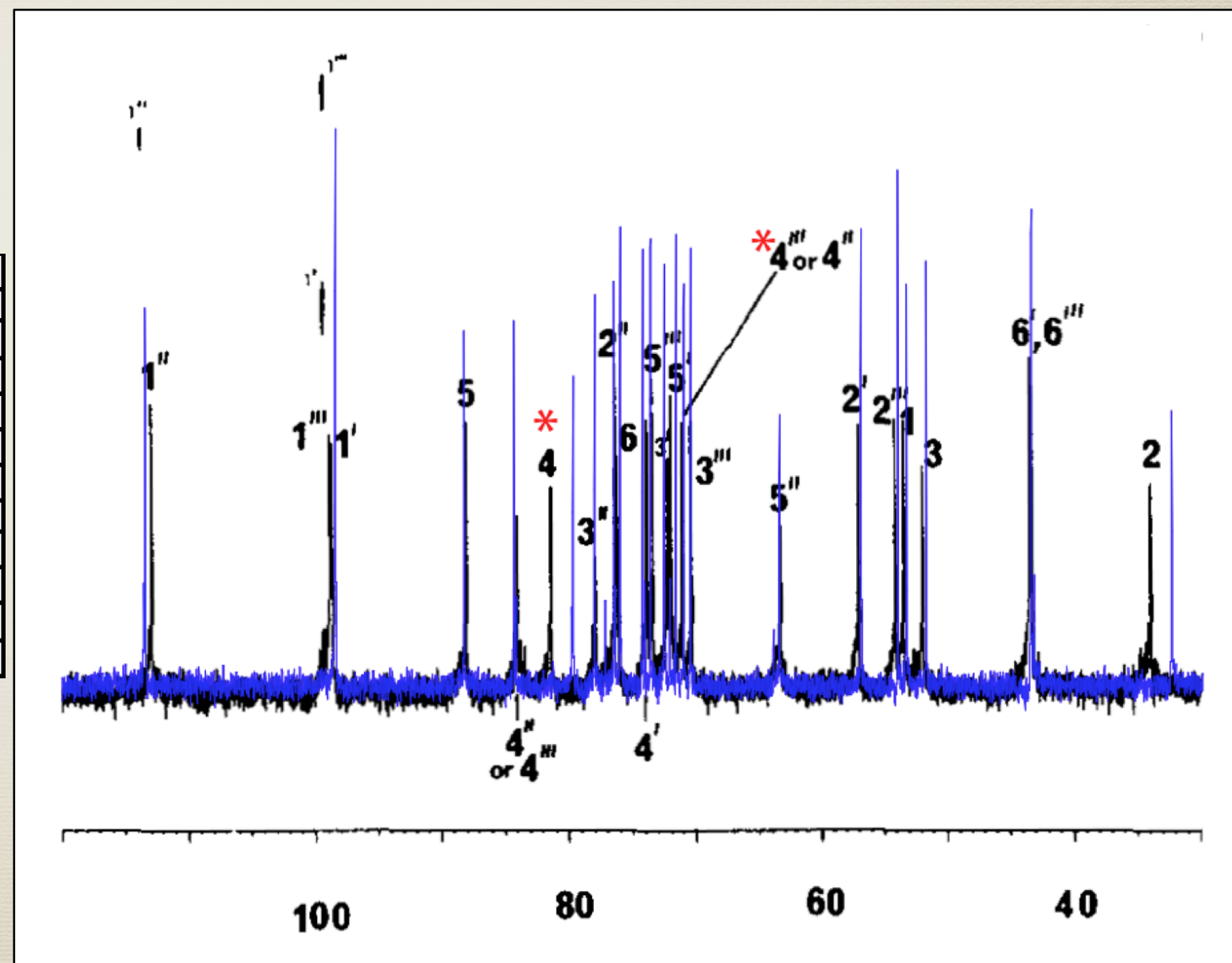
- \* **A** and **B** were published based on NMR
- \* **A** and **B** can not be distinguished by NMR with theoretical data!
- \* More information needed





# Quality Control

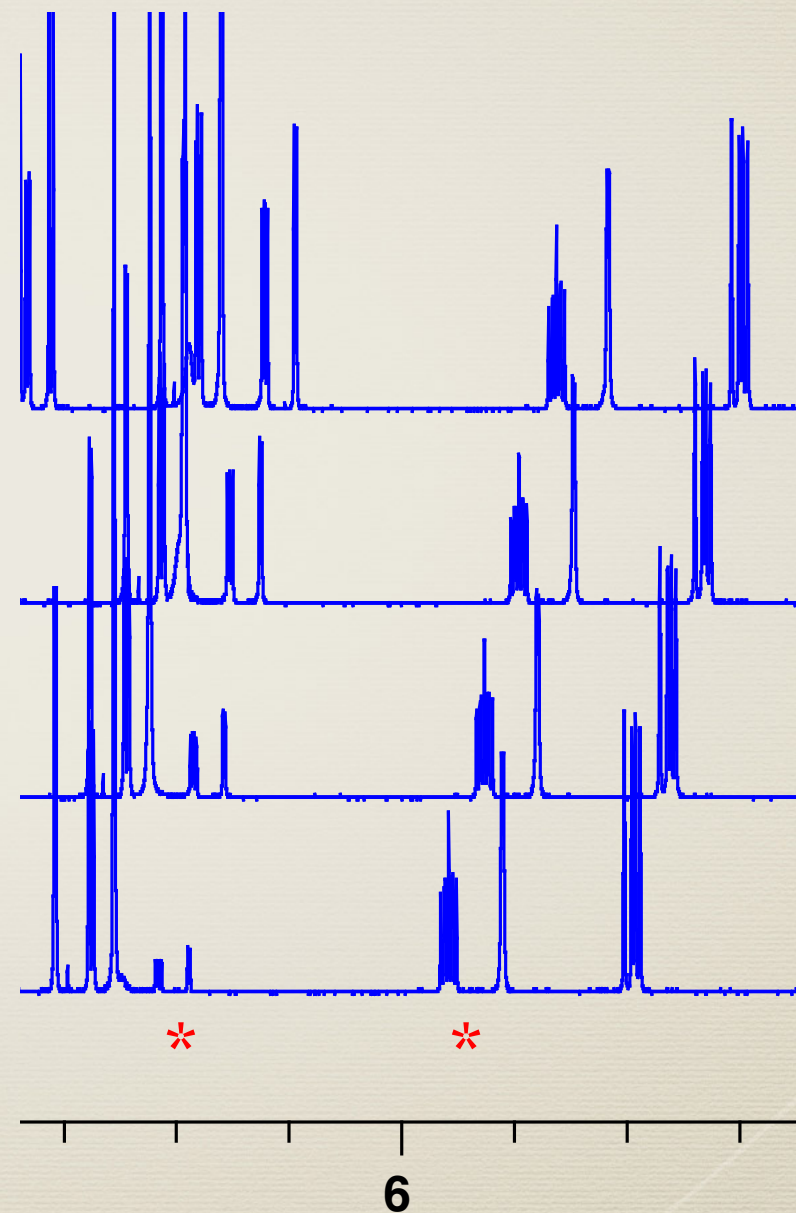
	Neomicina B sulfato		Neomicina B sulfato, REID (1987)	
Átomos	<sup>13</sup> C (ppm)	<sup>1</sup> H (ppm)	<sup>13</sup> C (ppm)	<sup>1</sup> H (ppm)
4 CH*	70,3	4,4	81	3,74
5 CH	76,6	4	88	3,84
1' CH	95,2	5,3	98	5,89
3' CH	74	4,4	72	3,88
4' CH	69,2	3,9	75	3,21
4'' CH	85,1	3,9	71 / 84	4,2
1''' CH	95,3	6	98	5,24
3''' CH	67,8	4,3	71	3,79
4''' CH*	67,2	3,8	84 / 71	4,2
5''' CH	71	3,5	74	4,3





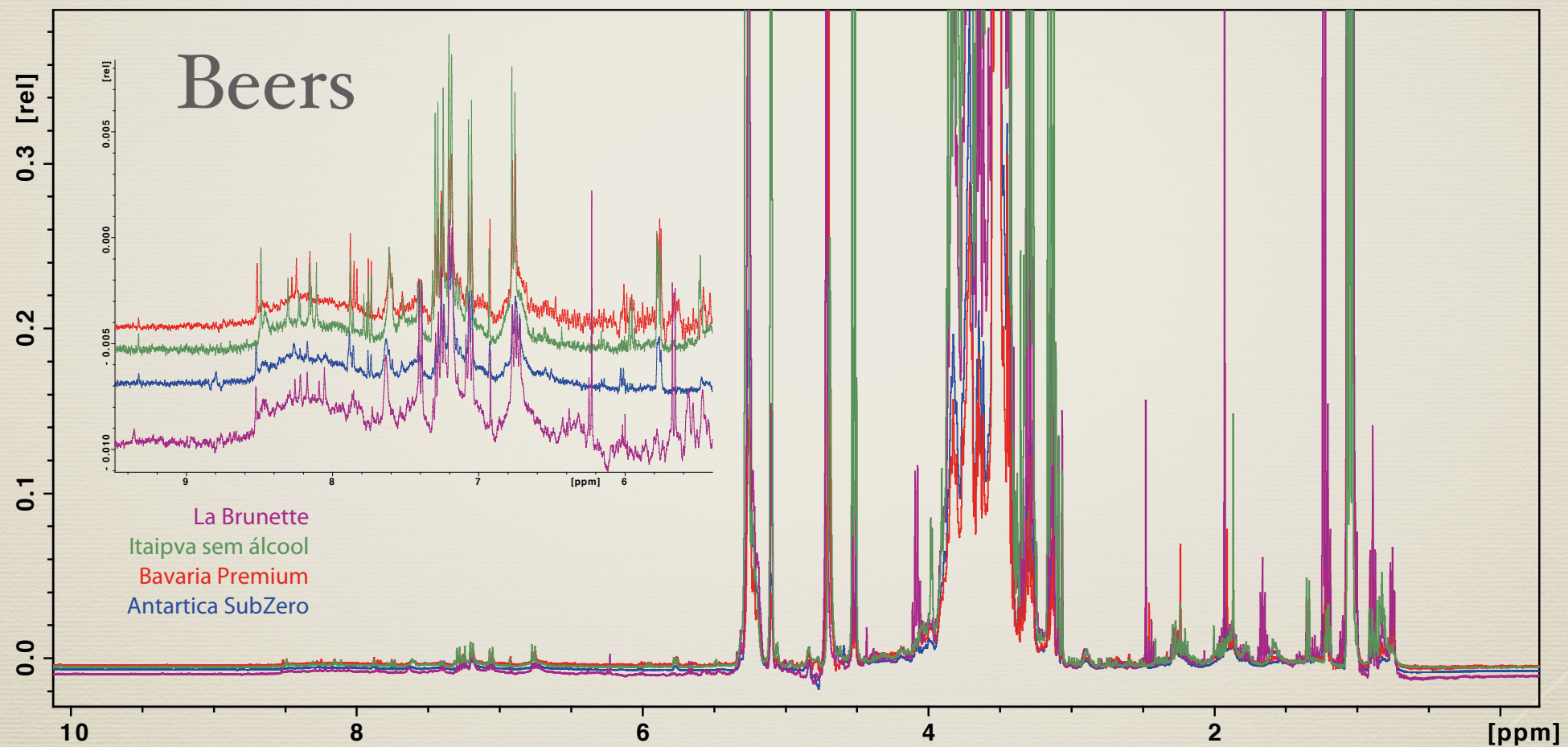
# Other NMR Uses

- \* Quantitative
- \* Analysis of mixtures
- \* fast
- \* error  $< 10\%$



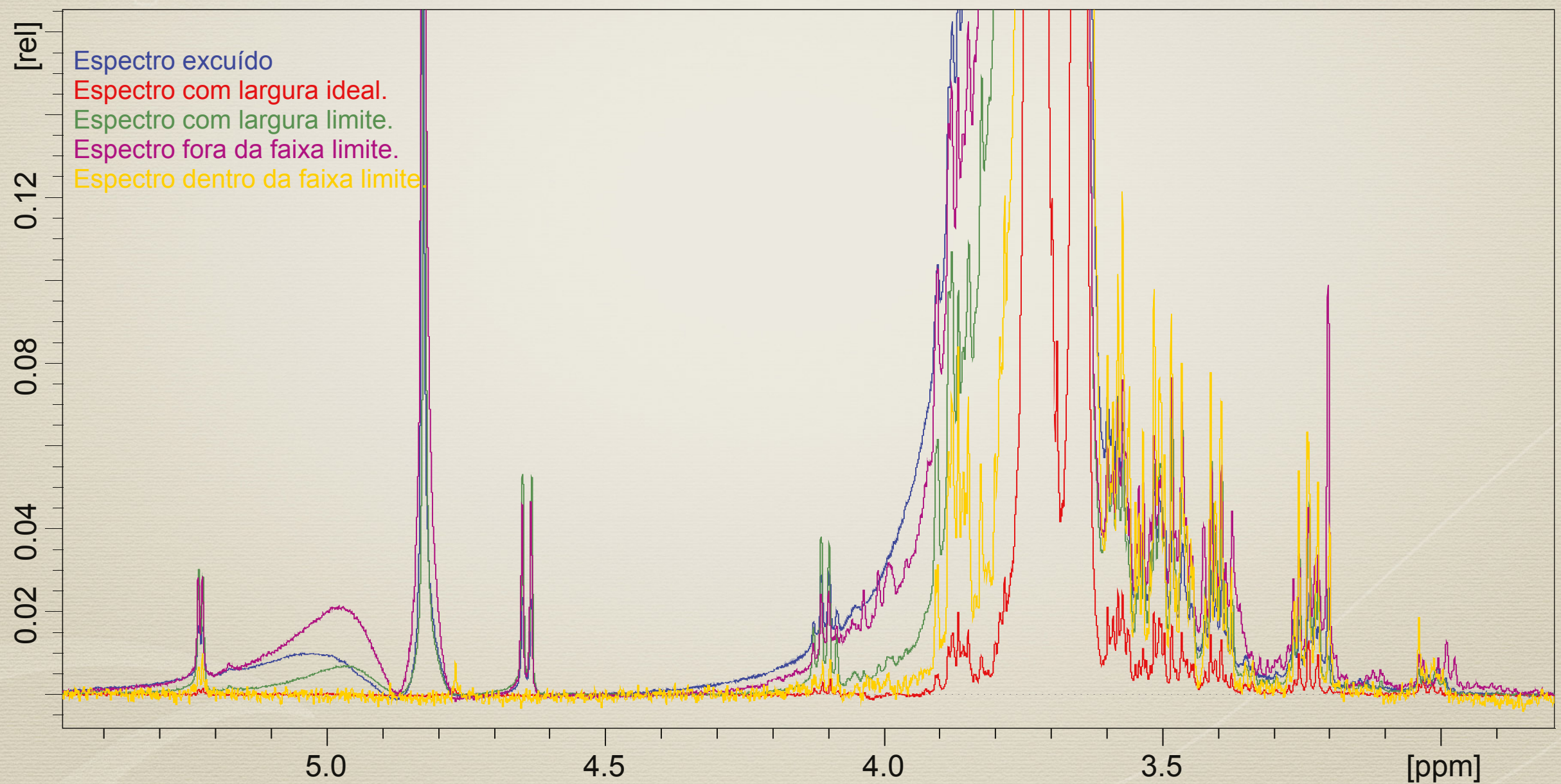


# Beer, Honey, Coffee, ...



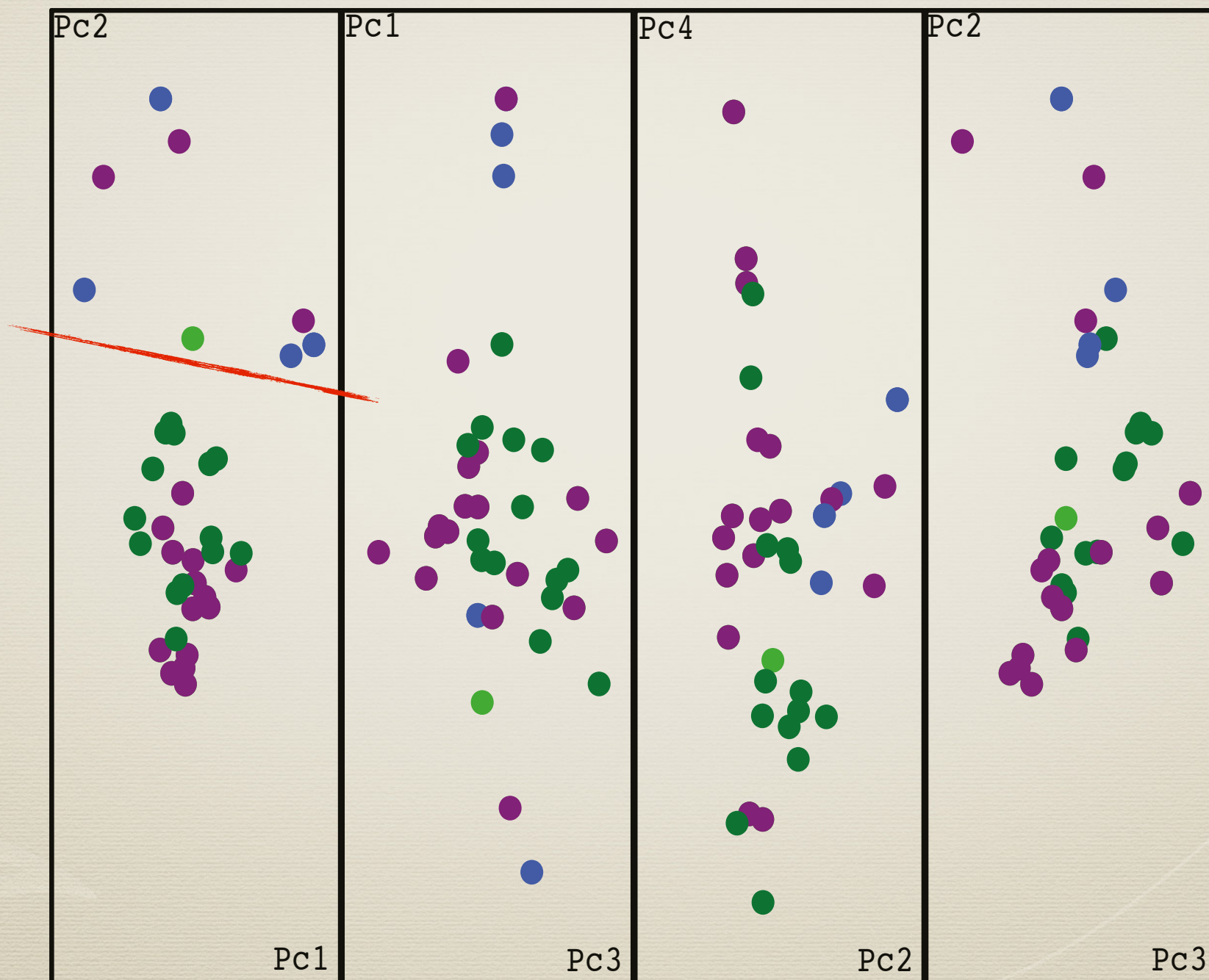


# Chemometrics with Blood Plasma





# Chemometrics with Blood Plasma





# Acknowledgements



- \* Charles Amaral
- \* Eliane Gonçalves

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- \* Thomas Lindel



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- \* Raquel Rodrigues
- \* Marcela Oliveira
- \* Camilla Bernardo
- \* Emanuelle Felix
- \* Amanda Lima
- \* Ana Azevedo
- \* Priscila Santana





Thank you!