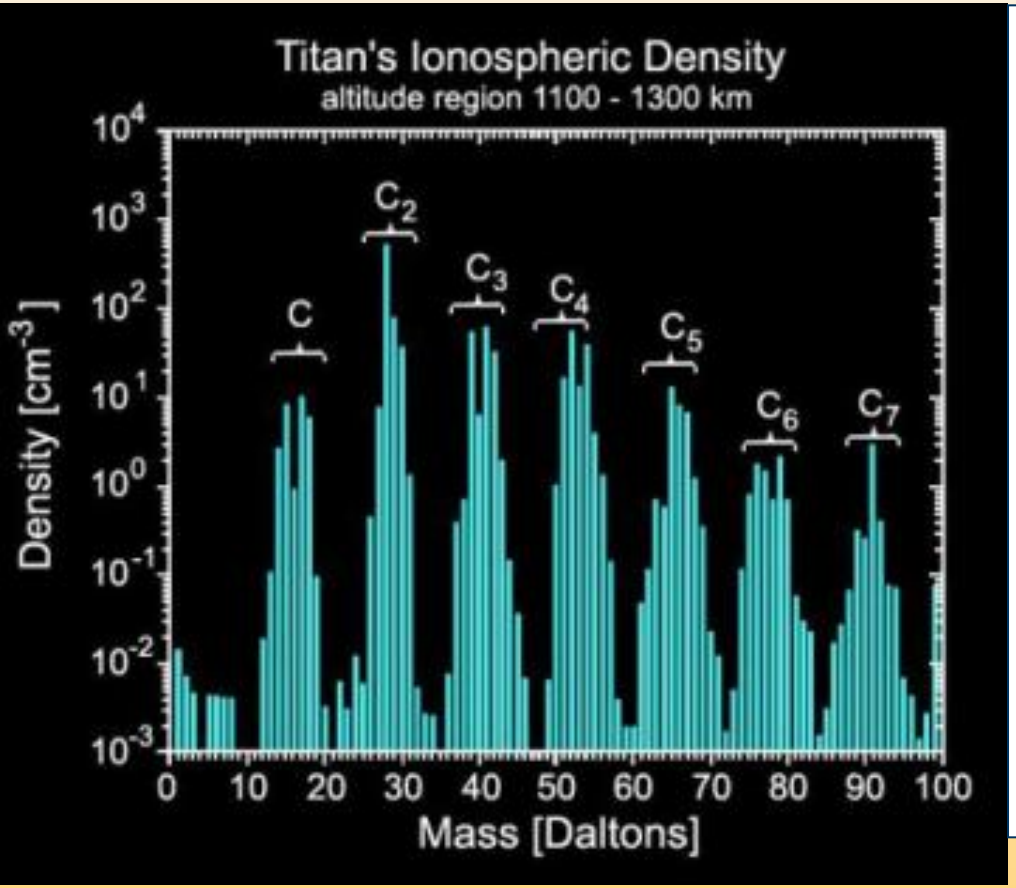
Orbitrap Mass Analyser: a Tool for Titan Complex Molecular Content Exploration

Roland Thissen	Grenoble
Stefano Cornelli	Grenoble
Pascal Puget	Grenoble
Christelle Briois	Orléans
Laurent Thirkell	Orléans
Amirouche Boukrara	Orléans
Jean-Pierre Lebreton	Orléans
Patricia Beauchamp	Pasadena
Evan Neidholdt	Pasadena
Jack Beauchamp	Pasadena
Hervé Cottin	Creteil
Noel Grand	Creteil
Cyril Szopa	Versailles
Nathalie Carrasco	Versailles
Claude Chapuis	Versailles
Abdel Bouabdellah	Versailles
Cécile Engrand	Orsay
Alexander Makarov	Bremen
cnes	Toulouse
	Paris

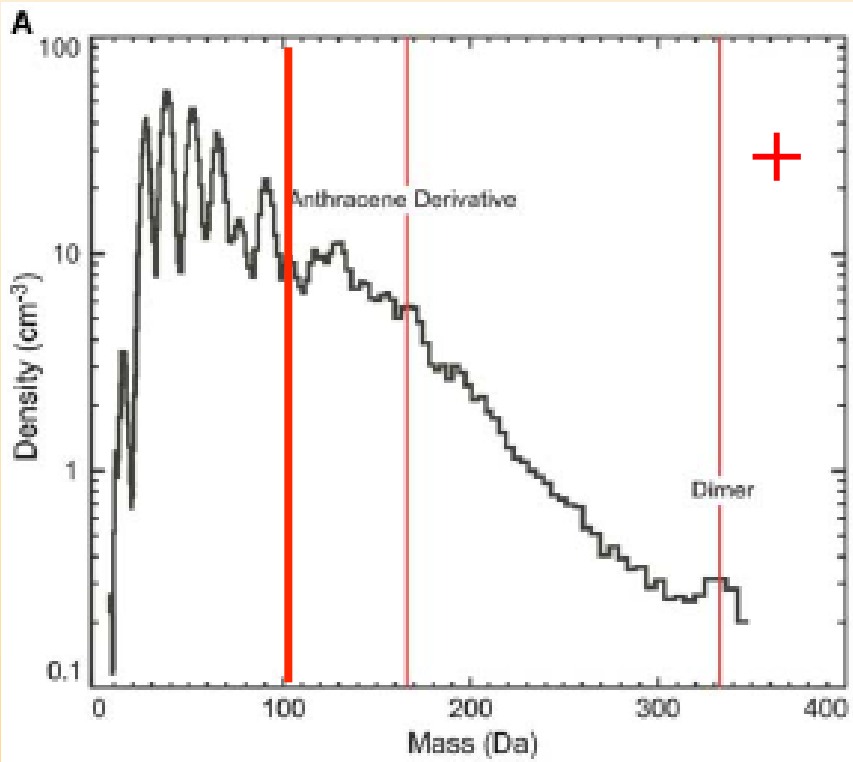
High mass-resolution for Titan?

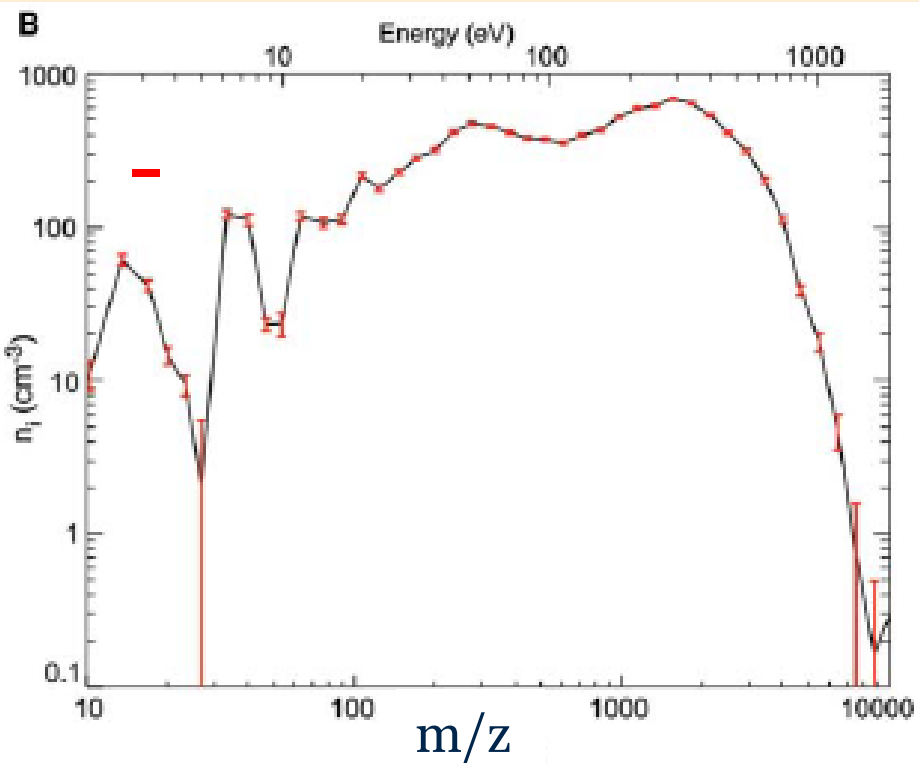
Cassini (INMS)
ionic densities in Titan ionosphere



C_7NH^+	99.0109	resolution
$C_8H_3^+$	99.0235	7857
$C_4N_3H_9^+$	99.0797	1761
$C_5N_2H_{11}^+$	99.0923	7857
$C_6NH_{13}^+$	99.1049	7853
$C_7H_{15}^+$	99.1174	7920

Big molecule synthesis …





Positive ions <350

Negative ions >1000

Bio molecules synthesis…

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Formation of amino acids and nucleotide bases in a Titan atmosphere simulation experiment

				P2CO	P2COi	P5CO	P5COi
			$\%N_2$	96.2	96.2	93.2	93.2
			$\%CH_4$	2	2	5	5
			%CO	1.8	1.8 $C^{18}O$	1.8	1.8 $C^{18}O$
Name	Mass	Formula	Fig				
Nucleotide Base							
cytosine	111	$C_4H_5N_3O$	2	OT	OT	OT/GC-MS	OT
uracil	112	$C_4H_4N_2O_2$		OT	OT	OT/GC-MS	OT
thymine	126	$C_5H_6N_2O_2$		OT	OT	OT/GC-MS	OT
adenine**	135	$C_5H_5N_5$	2	OT		OT/GC-MS	
guanine	151	$C_5H_5N_5O$		OT		OT/GC-MS	
Biological Amino Acid							
glycine	75	$C_2H_5NO_2$		OT		OT/GC-MS	
alanine	89	$C_3H_7NO_2$		OT		OT/GC-MS	
serine	105	$C_3H_7NO_3$		OT		OT	
proline	115	$C_5H_9NO_2$		OT		OT	
valine	117	$C_5H_{11}NO_2$		OT		OT	
threonine	119	$C_4H_9NO_3$		OT			
isoleucine/ leucine	131	$C_6H_{13}NO_2$		OT		OT	
asparagine	132	$C_4H_8N_2O_3$		OT		OT	
glutamine	146	$C_5H_{10}N_2O_3$		OT		OT	
lysine	146	$C_6H_{14}N_2O_2$		OT		OT	
histidine	155	$C_6H_9N_3O_2$	2	OT		OT	OT
phenylalanine	165	$C_9H_{11}NO_2$		OT		OT	
arginine	174	$C_6H_{14}N_4O_2$		OT		OT	

Horst et al. Accepted in Astrobiology

Tholins mass spectrum at high resolution

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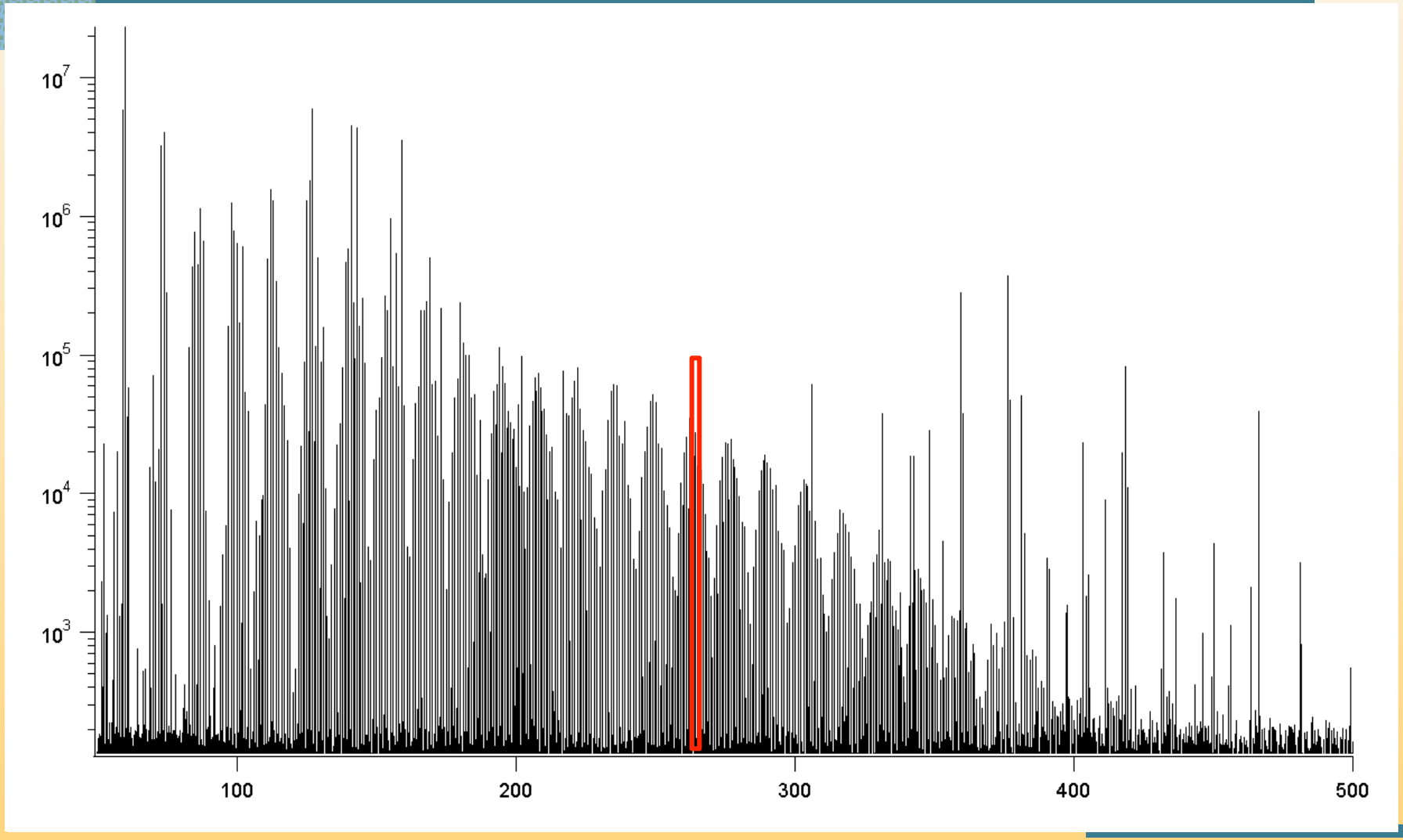
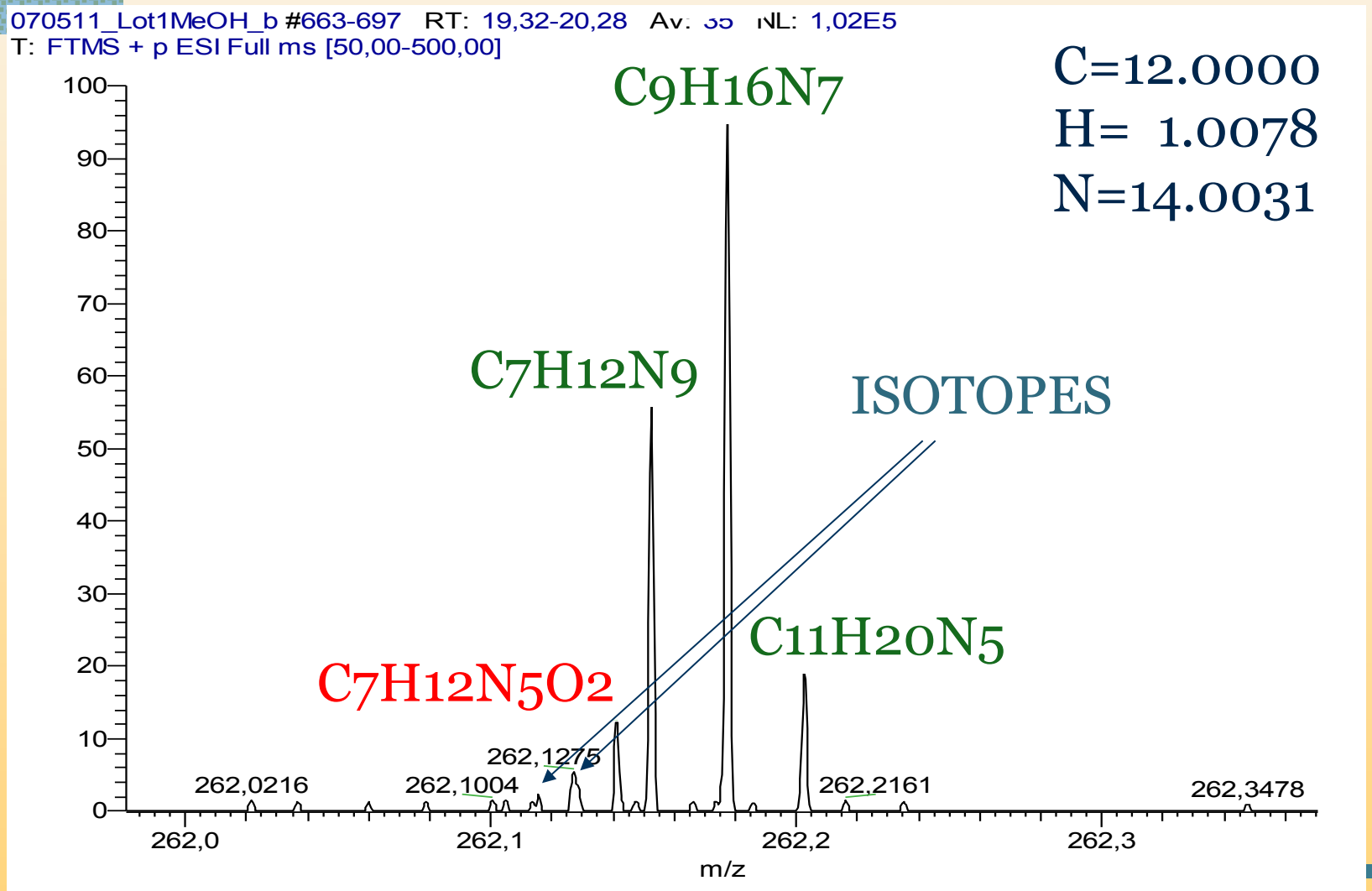


Zoom on mass 262



Isotopical abundancies, example on complex mixture…

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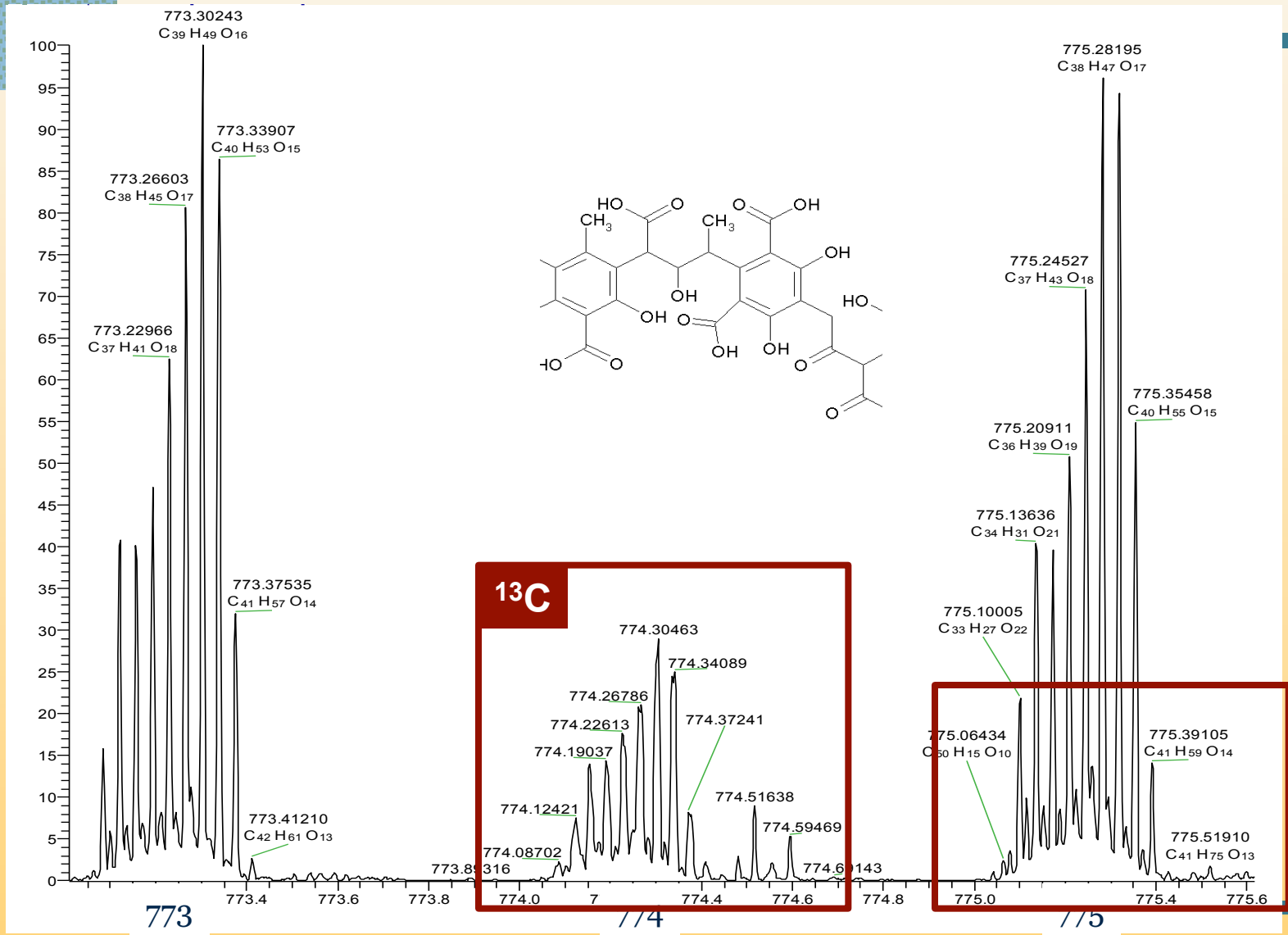

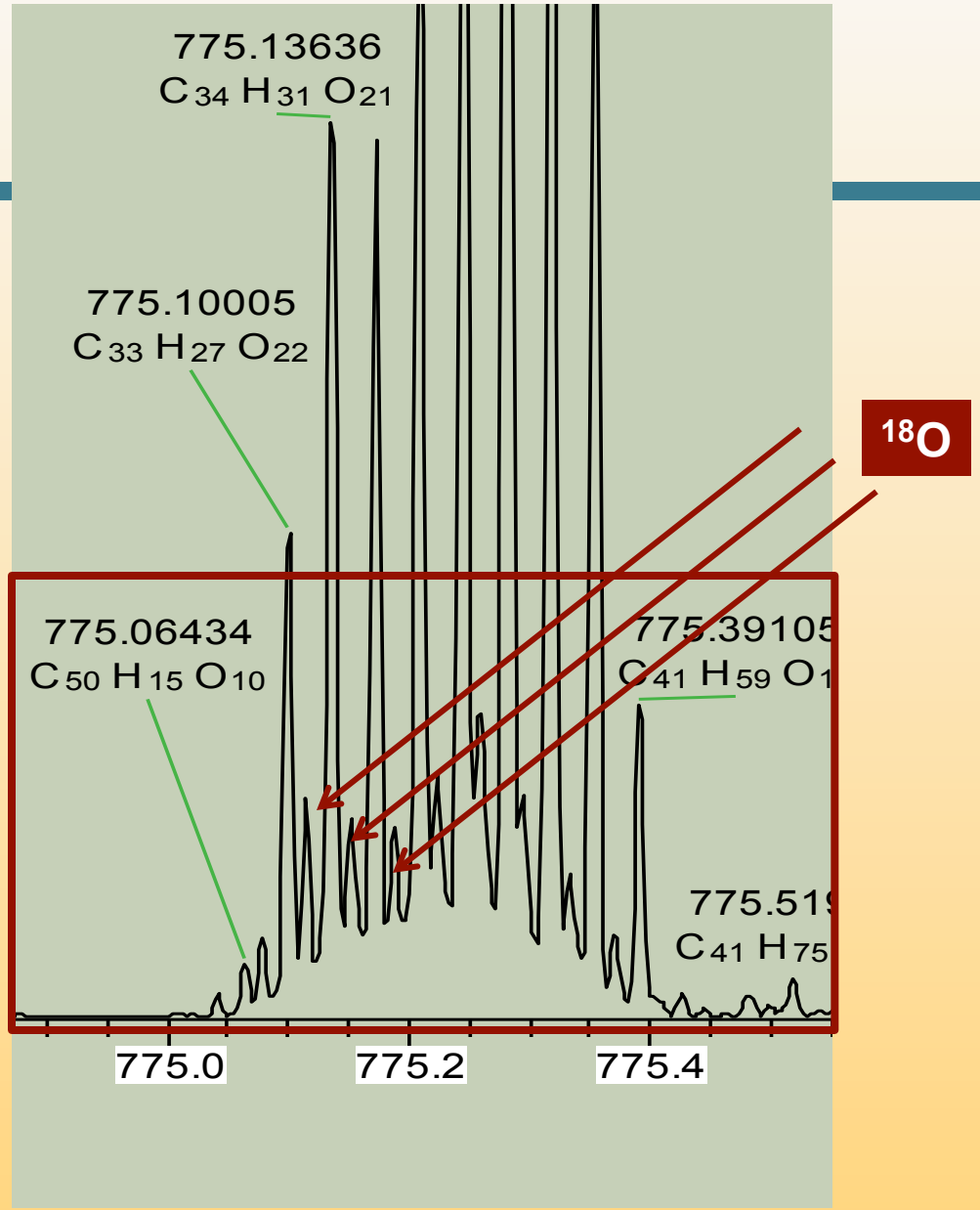

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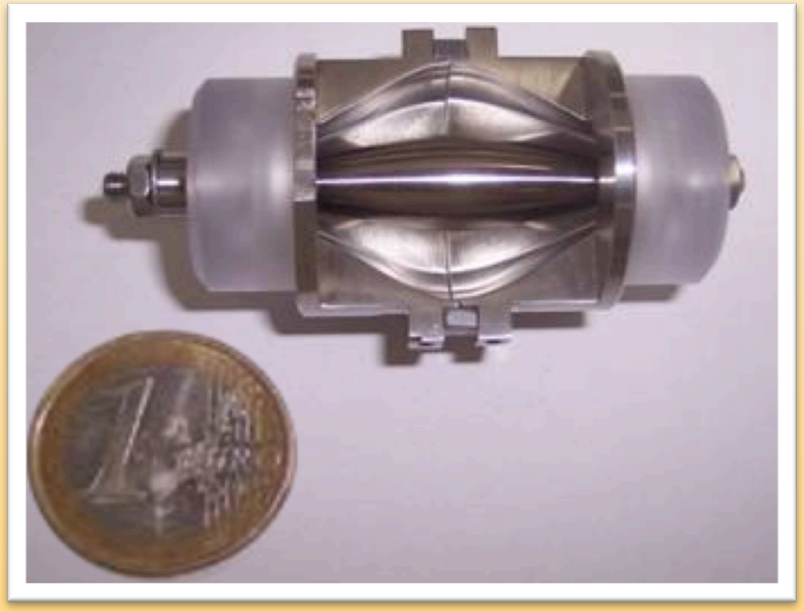
Orbitrap mass Analyser ?



Preliminary remark, what is orbitrap…

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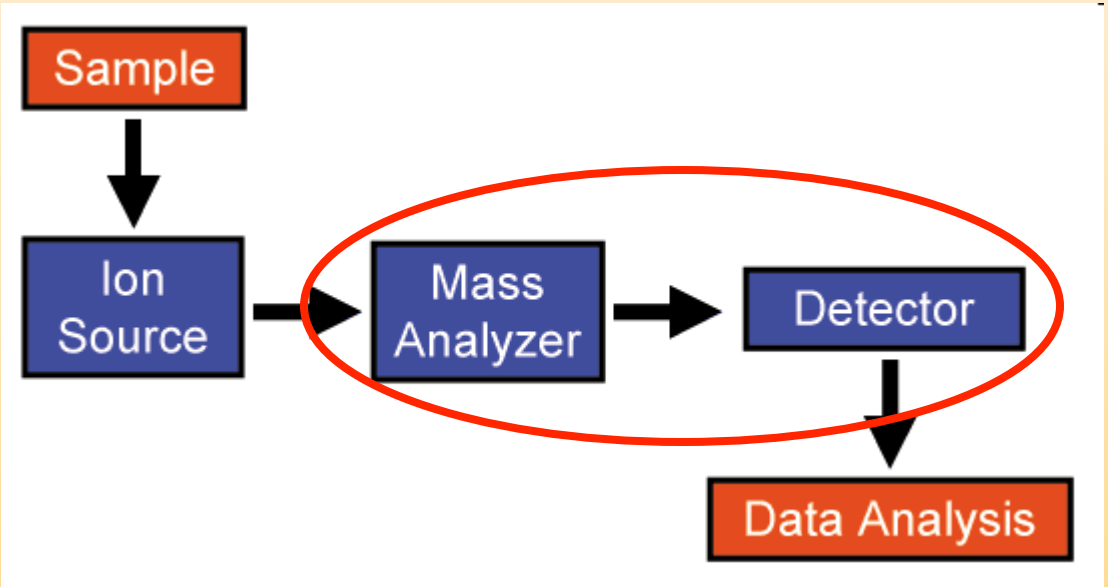
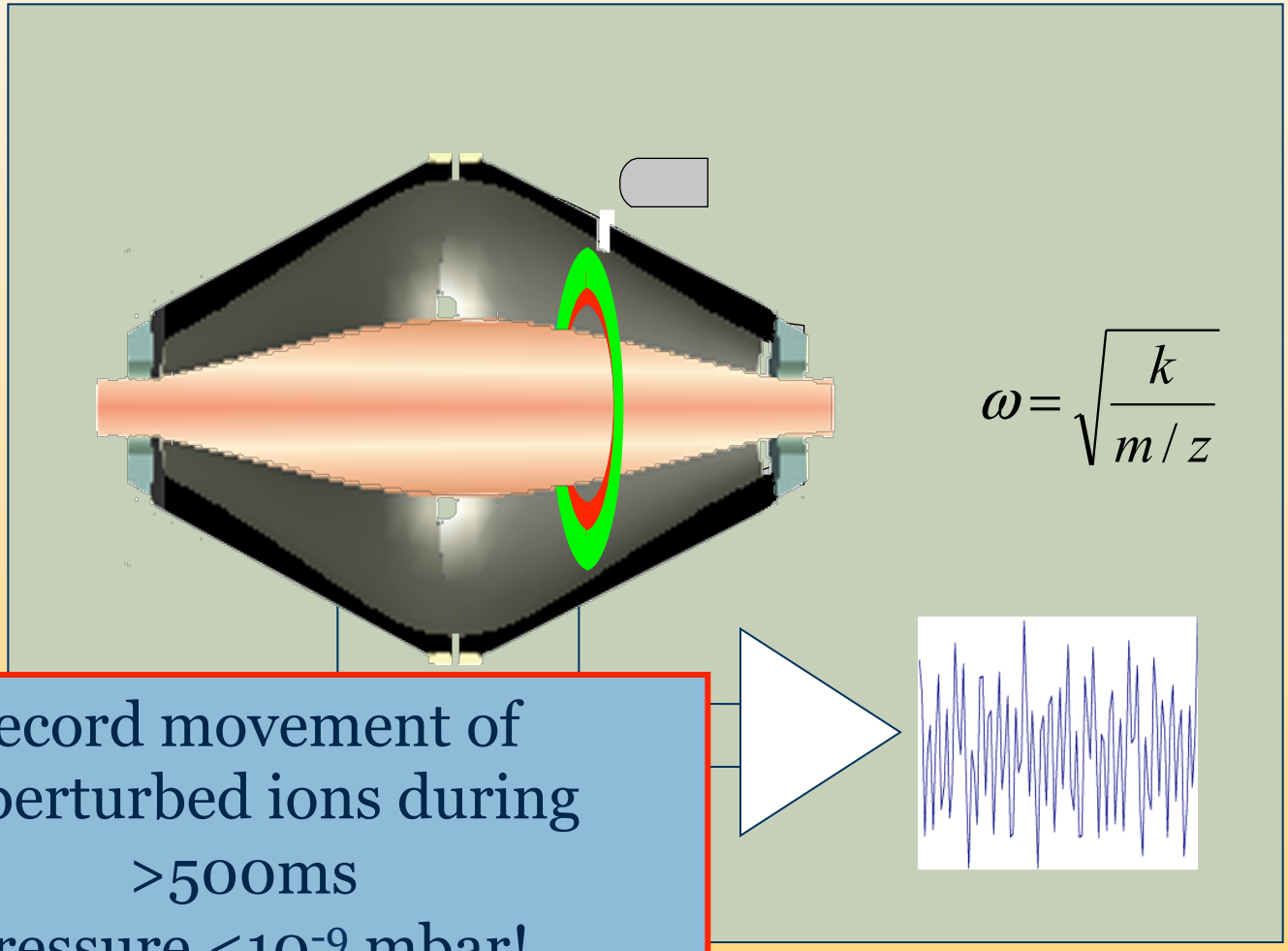
Mass Spectrometry :



Perfect quadro logarithmic potential



record movement of unperturbed ions during >500ms
pressure $<10^{-9}$ mbar!

How to inject and stabilize ions in this perfect potential? "Electrodynamic squeezing"

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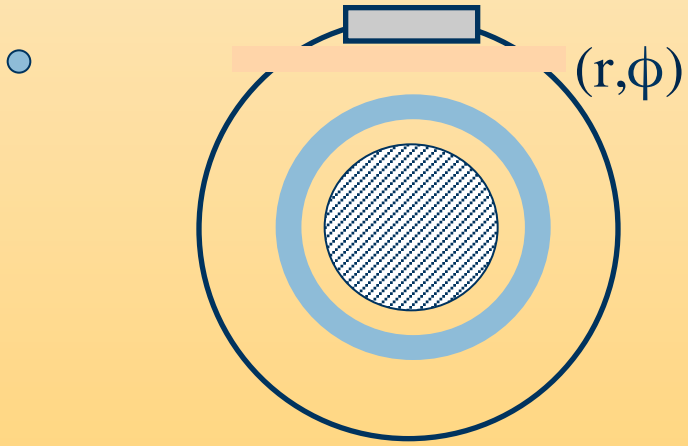
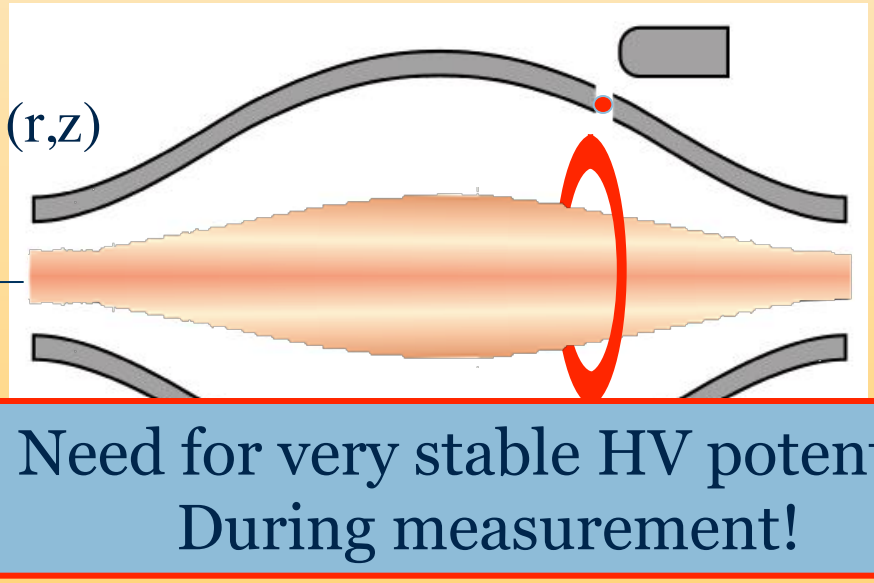
- a bunch of ions enters in the field, tangentially
- ions are squeezed towards central electrode by variation of its potential (deepening of well)
- The excitation of quadratic movement is inherent to "off axis" injection

Need to pulse ions in the trap!





Need for very stable HV potential During measurement!

Orbitrap, potential

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- Ultra high resolution: 100 000 at mass 400, adjustable during mission, as it depends only on the integration time
- Very small volume, lightweight : l=4 , f= 4 cm
- Good detection Dynamic : 50 000 per spectrum
- Positive or negative Ions as only one potential to invert
- All ions are analysed simultaneously
- No detector, no saturation, …
- no RF, no moving part
- Ideal for solids or aerosols

Orbitrap for Titan

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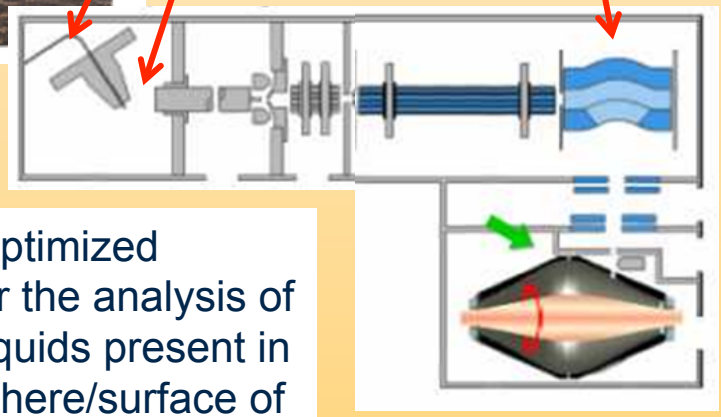
Sample handling

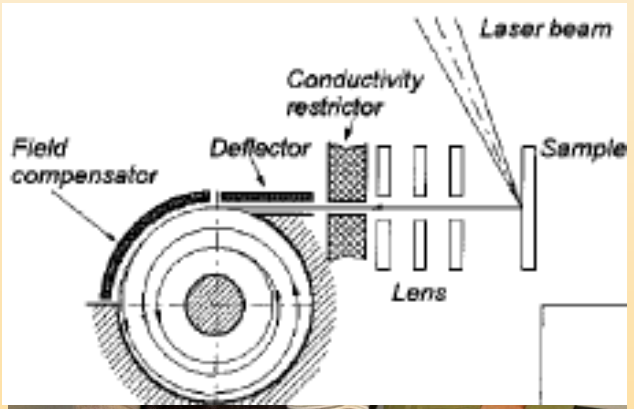
ionization

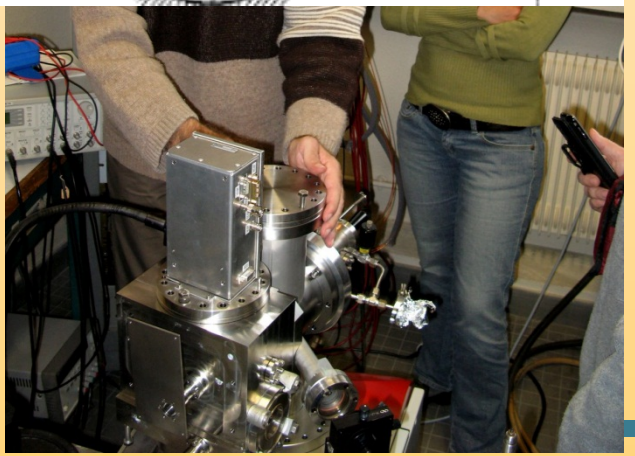
Ion accumulation



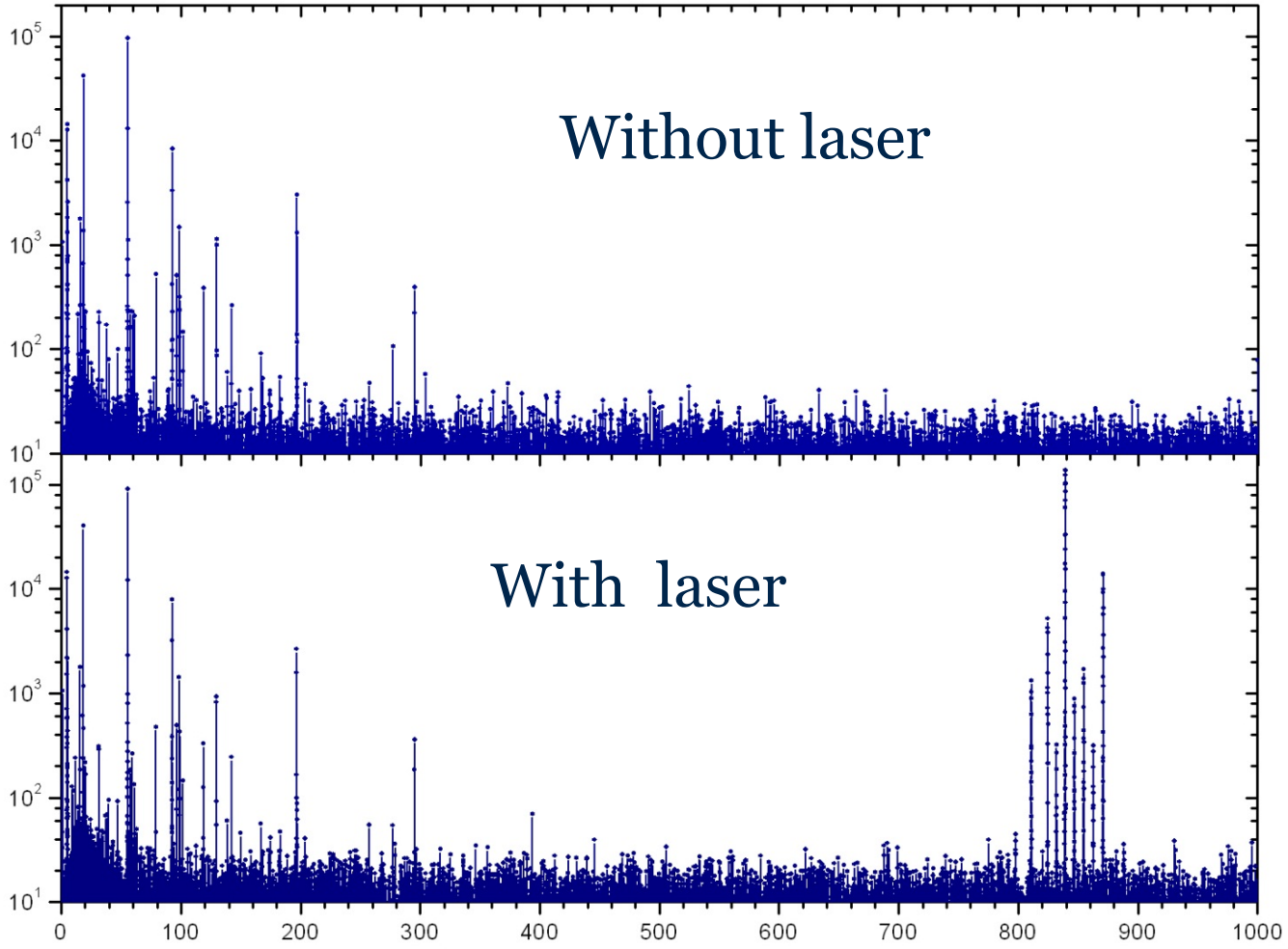
Study of optimized MS instrument for the analysis of aerosols/solids/liquids present in the deep atmosphere/surface of Titan

Orbitrap prototype in Orléans





Performances of prototype…



1 laser shot on Stainless steel

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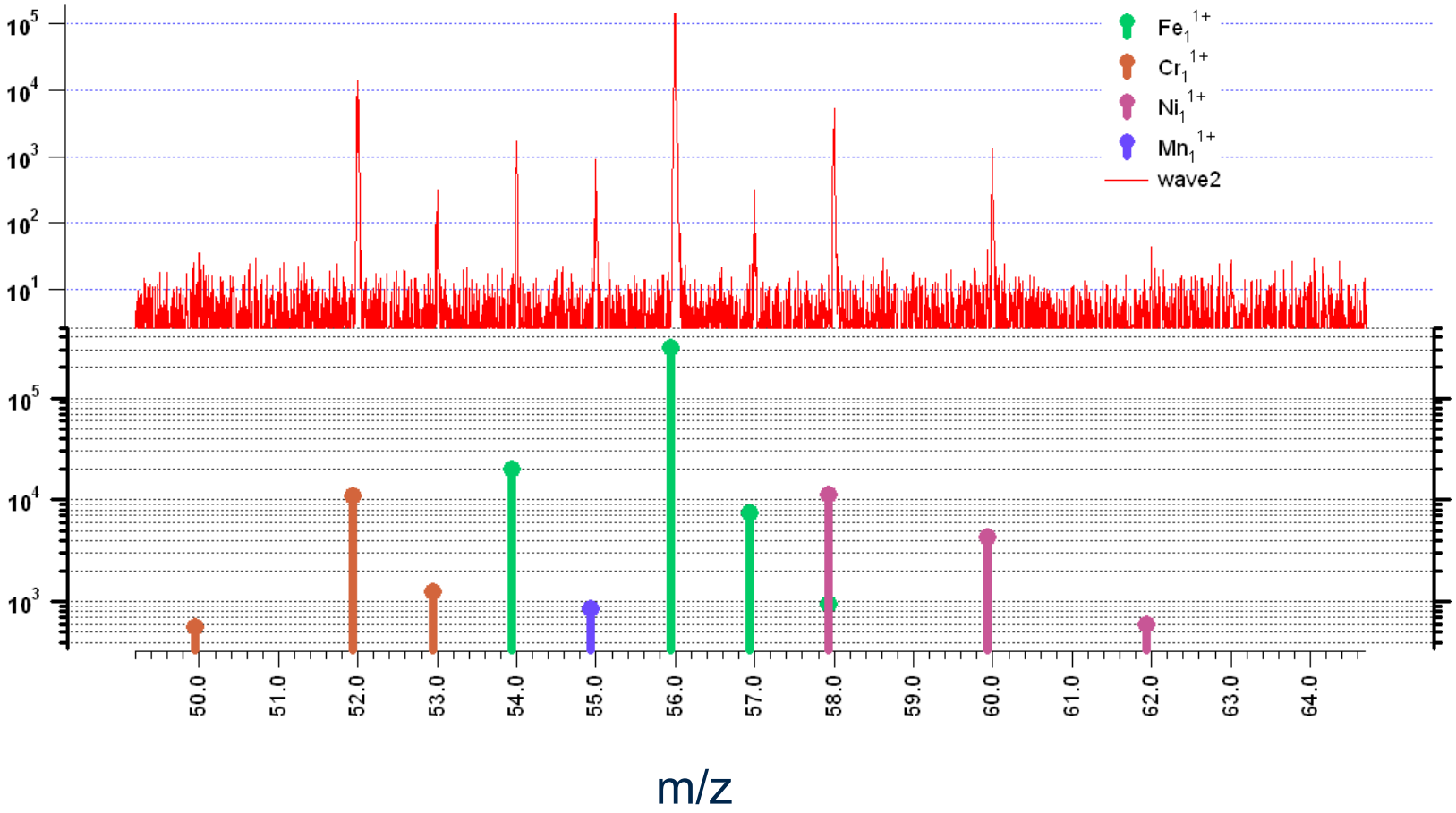
R=280 000



Tholins survive the laser desorption/ionization

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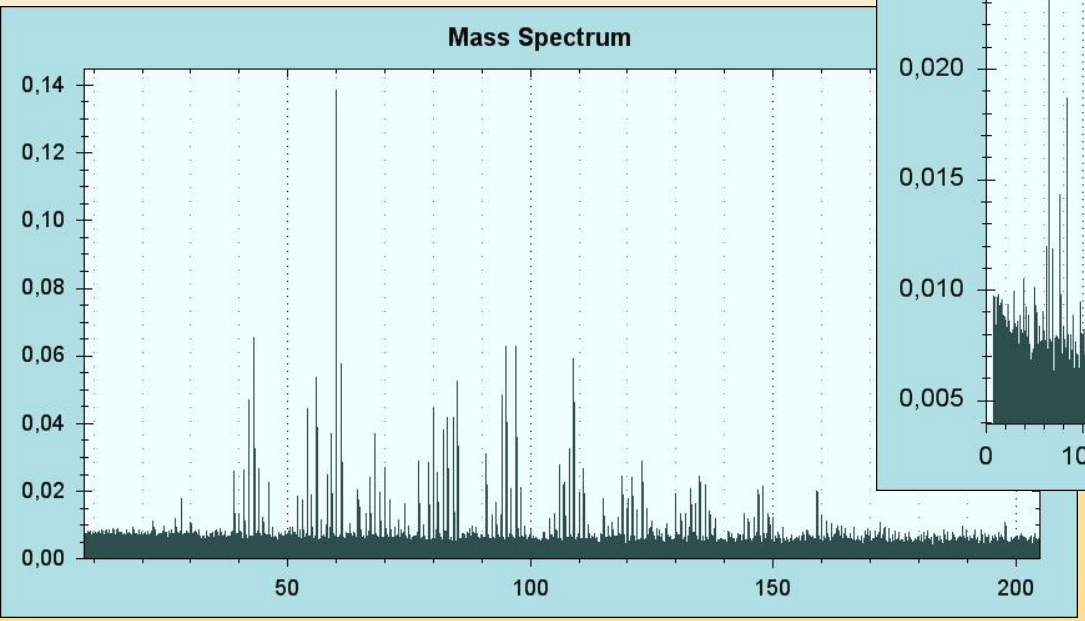

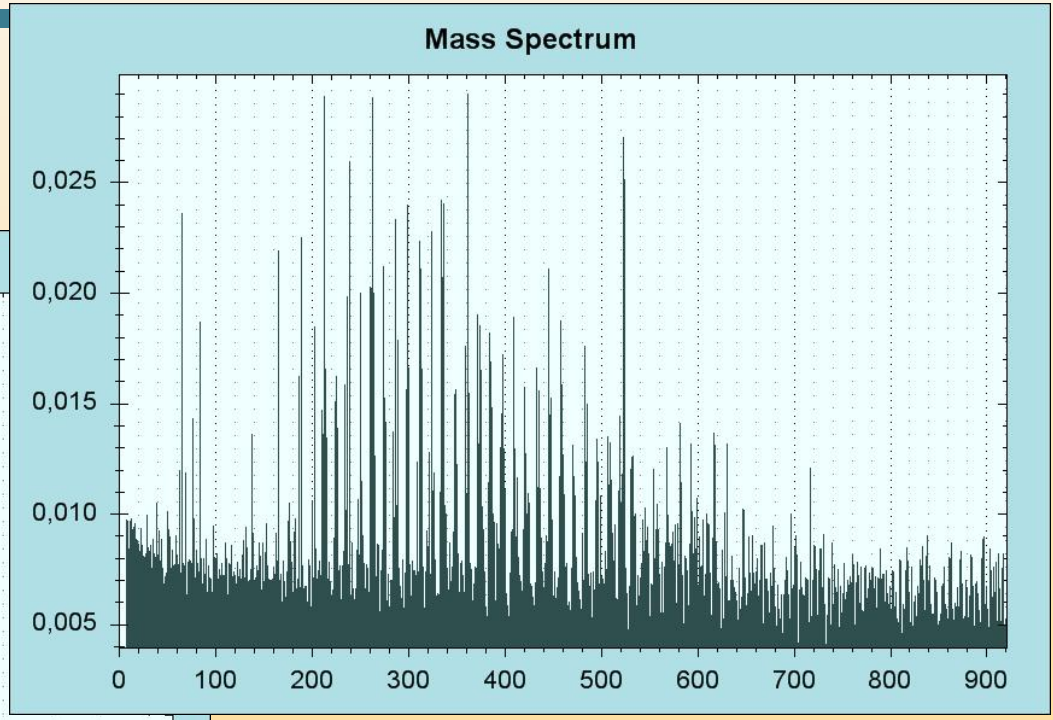

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Conclusions

- Going back to Titan, we need to do much better than Cassini.
- We know that very large (bio)organic molecules are produced/ present in
  - Atmosphere Aerosols
  - Surface Liquids / solids
- Request for very high resolution mass spectrometry to be characterized.
- Orbitrap is a very promising analyser/detector for this purpose.
- However big challenges remain:
  - Sample handling ?
  - Ionization method ?
  - High-Vacuum generation/maintenance ?
  - Beyond formulas, what about structural analysis ?
  - …
- Further info ? Come & visit posters 7A/B
  Briois, Cornelli and Thirkell