

An aerial photograph of a coastal landscape. In the foreground, there are white-capped waves crashing against a rocky shore. A prominent feature is a series of steep, light-colored cliffs that form a natural barrier between the ocean and a large, winding river or estuary. The water in the river is a deep blue, reflecting the sky. The surrounding land is green with trees and some buildings, including a large, multi-story building that appears to be a university campus. In the background, there are rolling hills and mountains under a clear blue sky.

Solution Structures Are They Attainable?

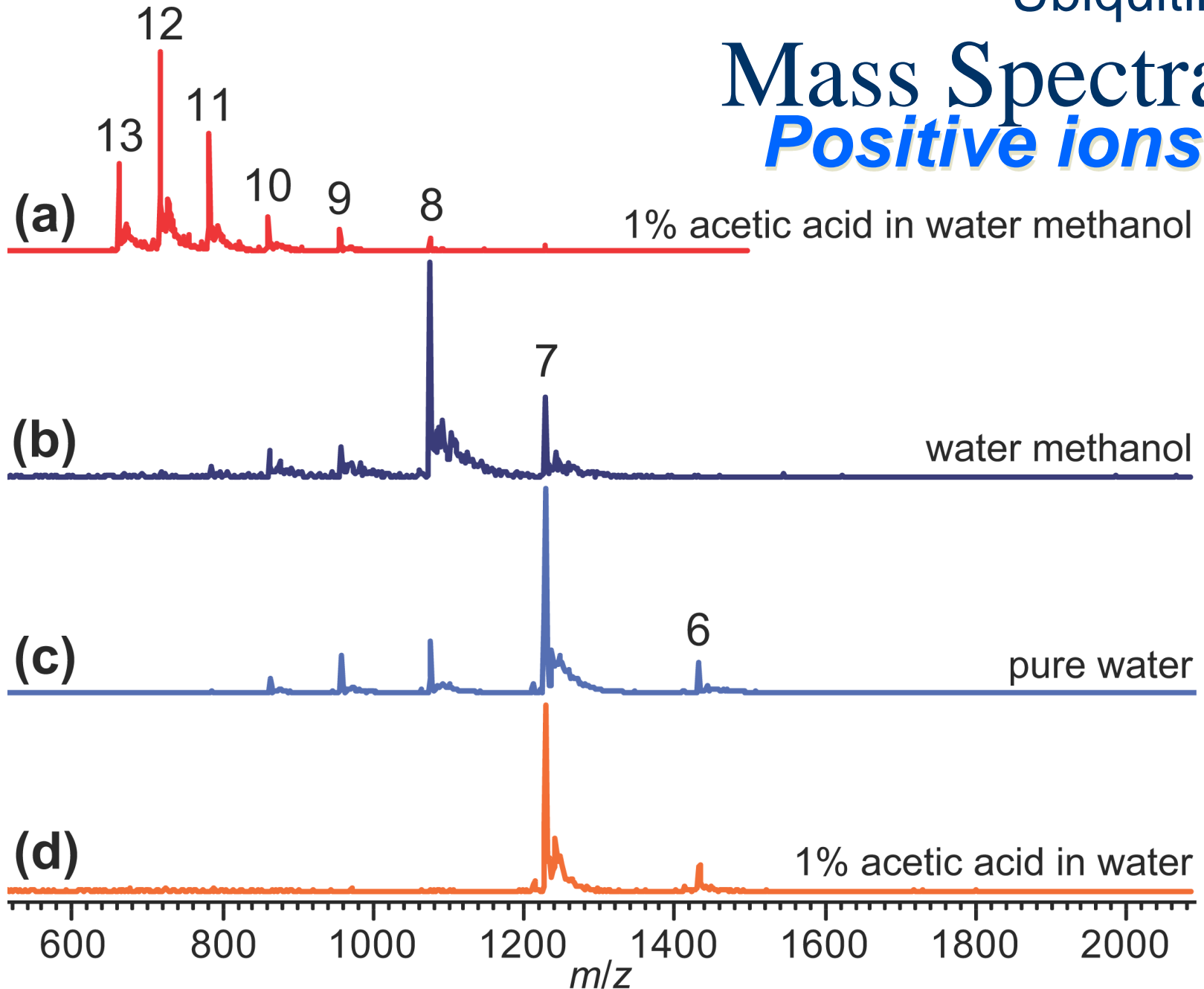
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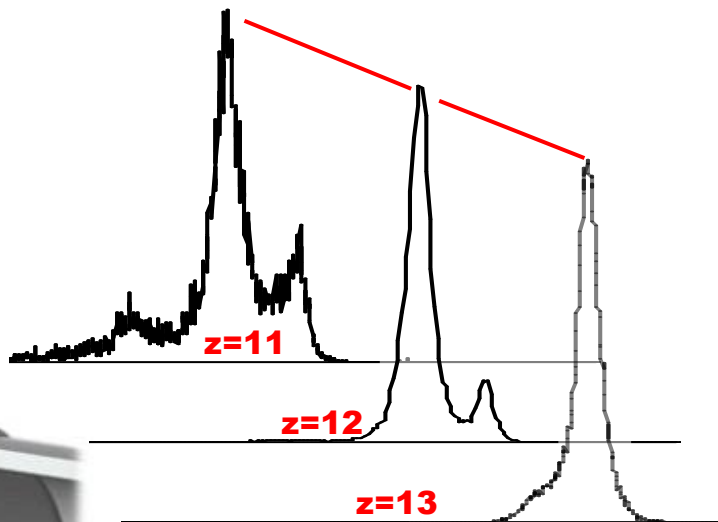
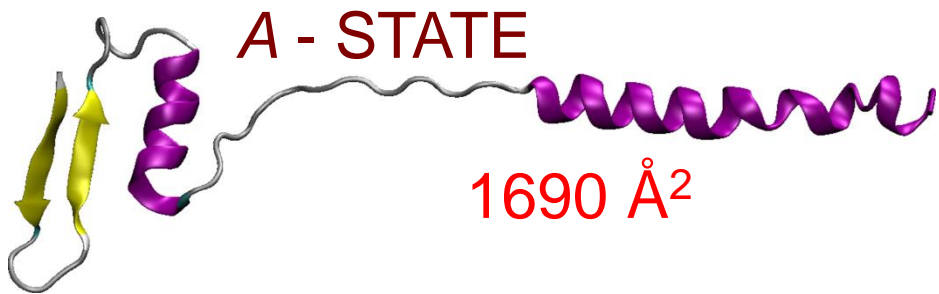
Solution Structures: Are They Attainable?

- Lots of evidence from several labs that solution backbone structures can be retained during IMS.
- How the ions are treated all steps is critical.
 - Ubiquitin as an example

Ubiquitin

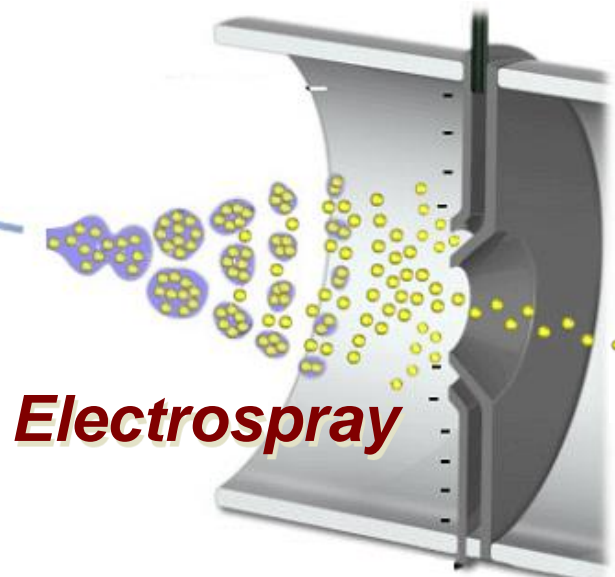
Mass Spectra *Positive ions*





SOLUTION PHASE

Solution

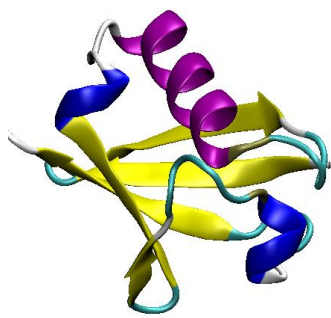


$1700-2000 \text{ \AA}^2$

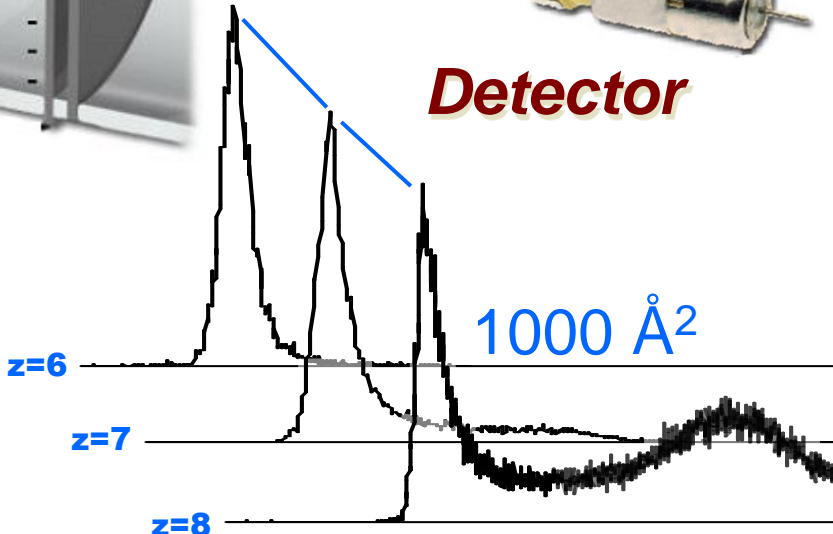
GAS PHASE



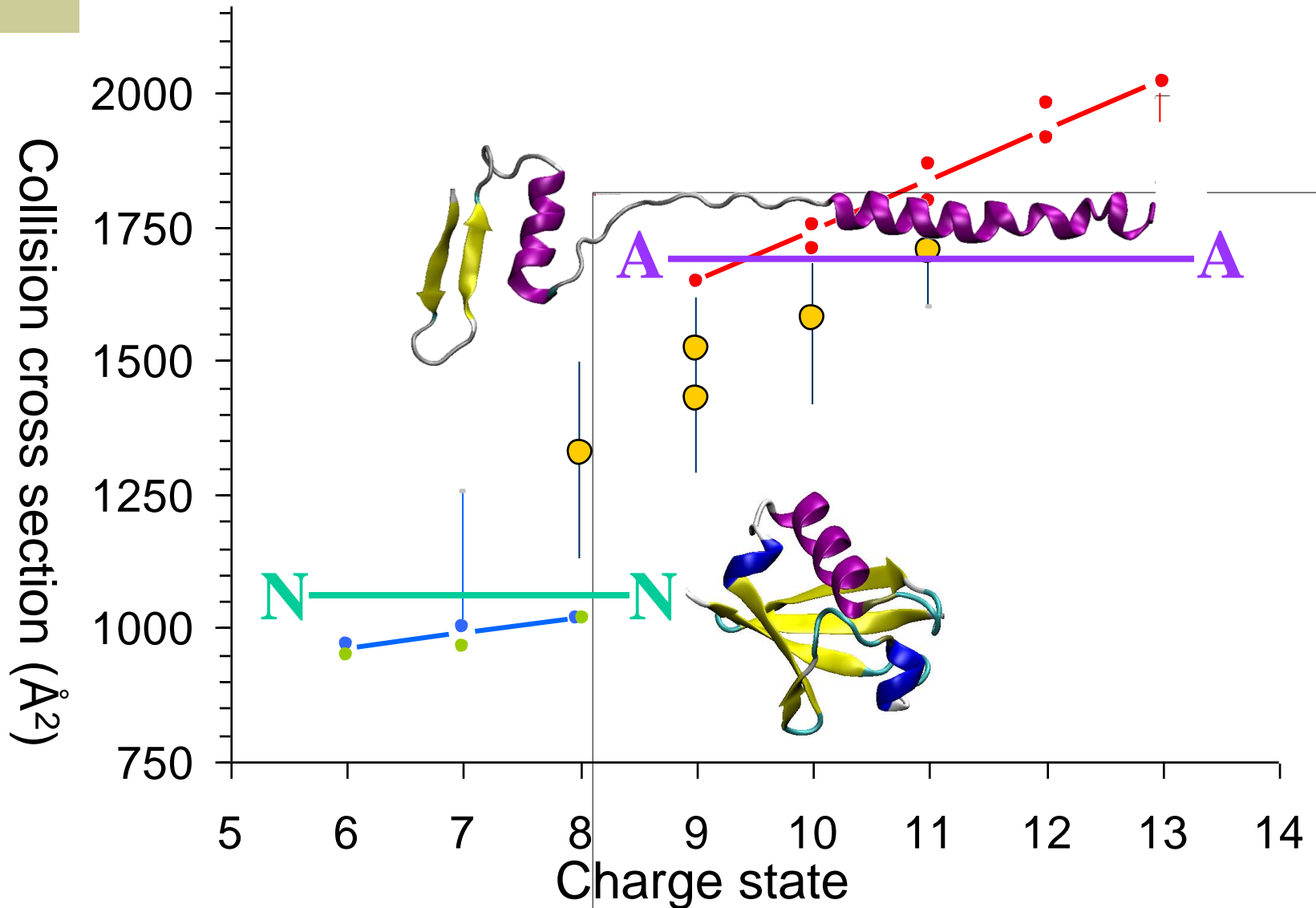
Detector



NATIVE STATE



Cross sections

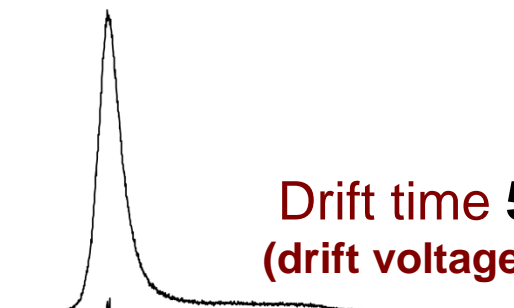


z=7

No trapping



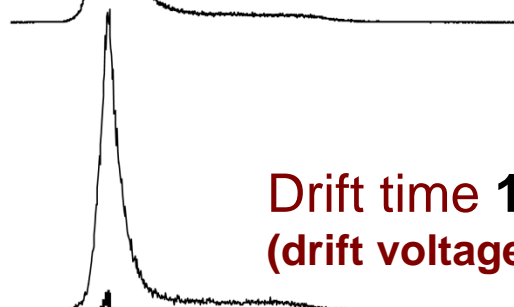
Drift time **50 ms**
(drift voltage 3.5 kV)



No trapping



Drift time **120 ms**
(drift voltage 1.5 kV)

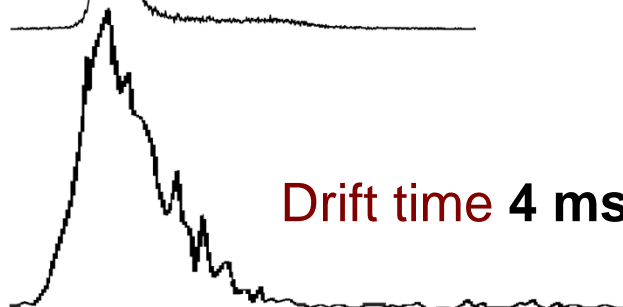


Wytttenbach, Bowers
J. Phys. Chem. B **2011**, 115, 12266

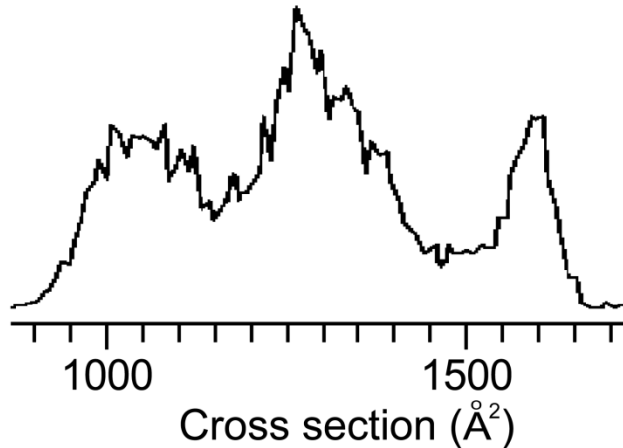
Ion trap **20 ms**



Drift time **4 ms**



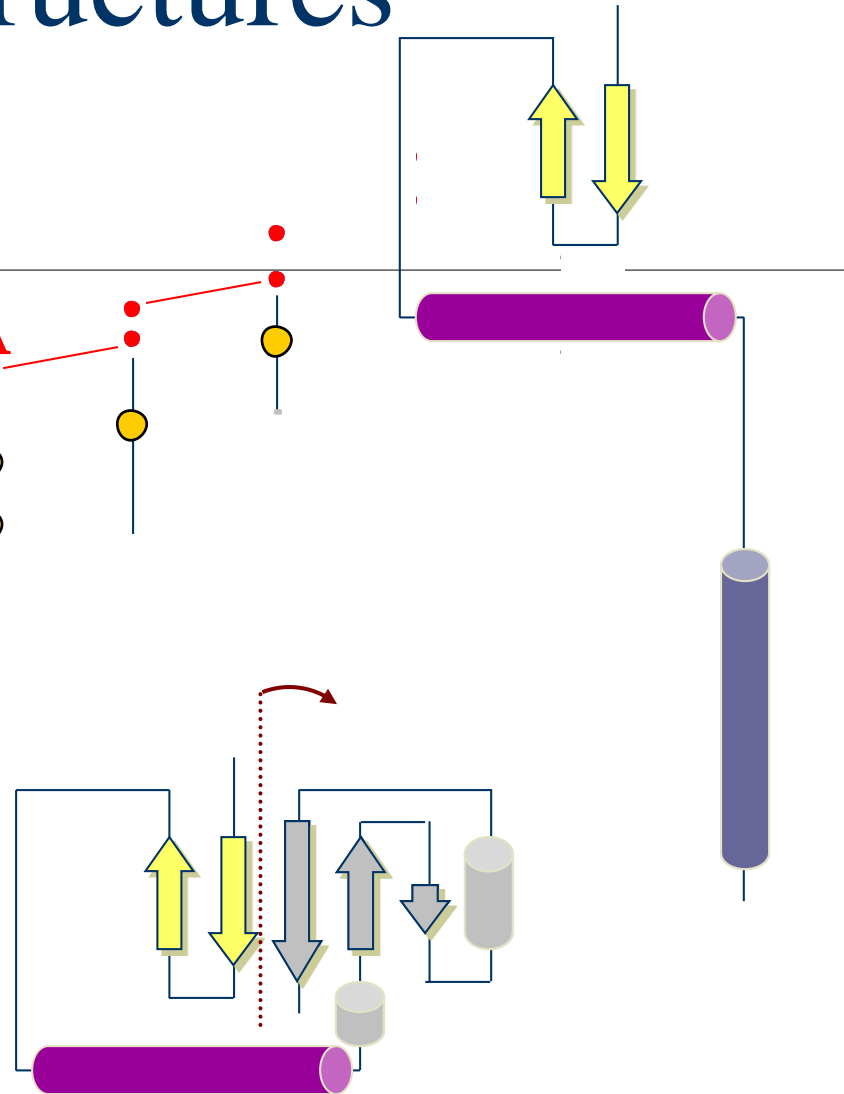
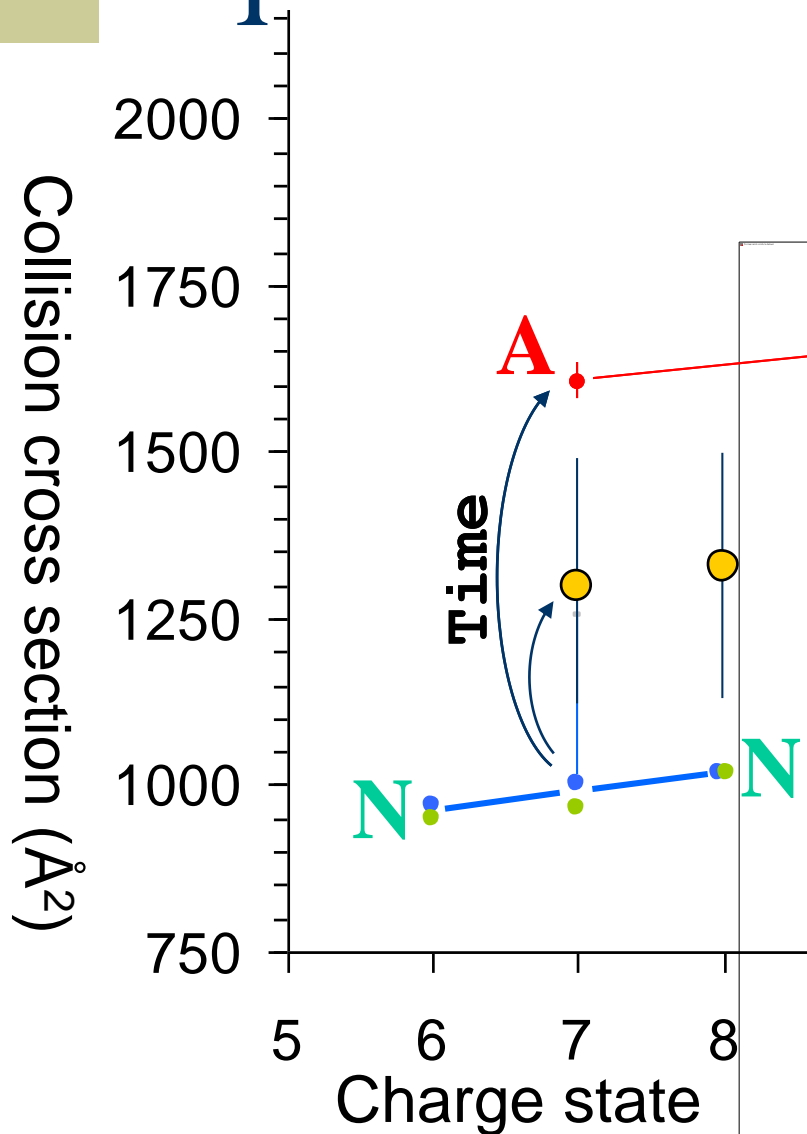
Ion trap **100 ms**



Myung, Badman, Lee, Clemmer
J. Phys. Chem. A **2002**, 106, 9976

1000 1500
Cross section (Å²)

Towards gas-phase equilibrium structures

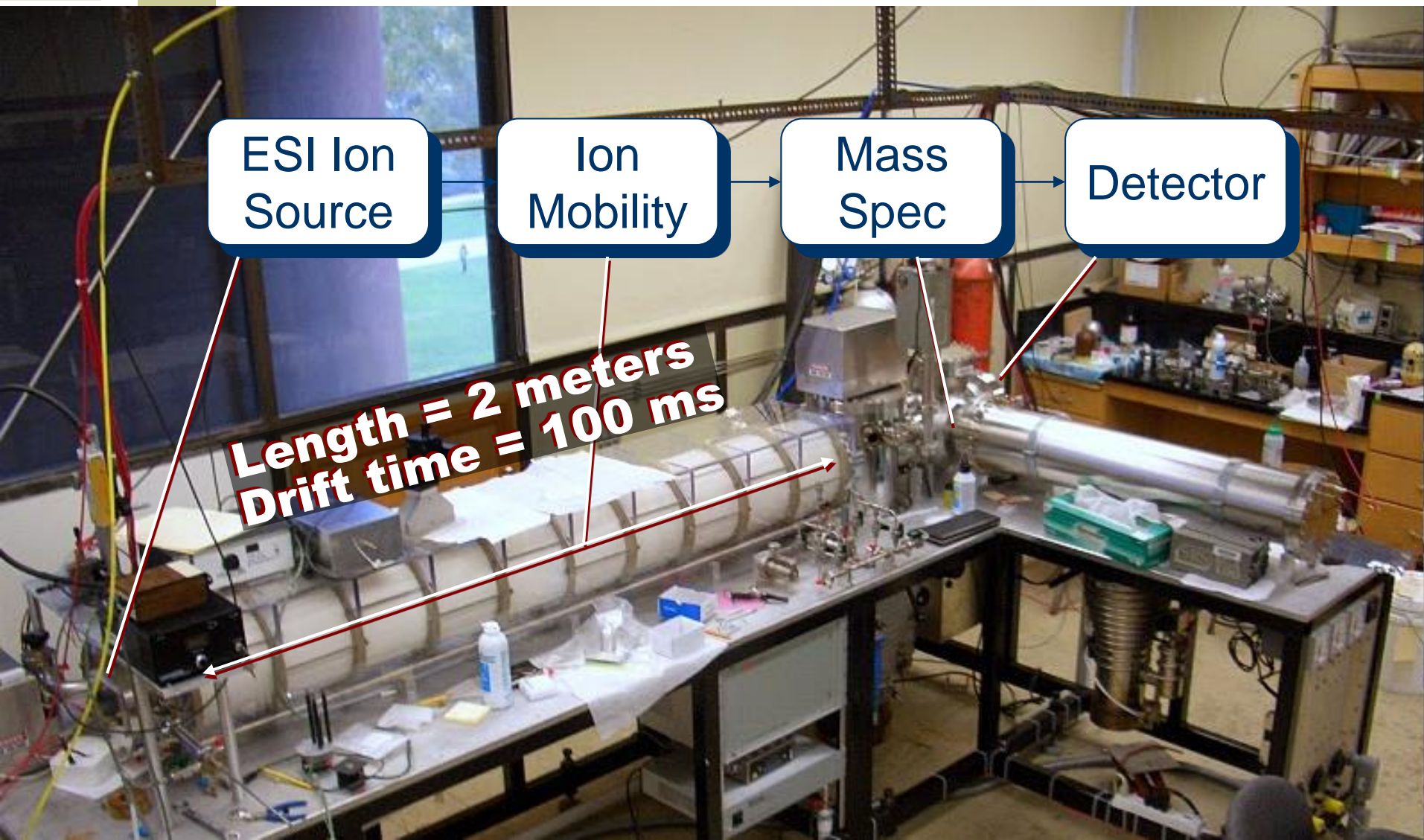




The Effect of Energy on Conformation

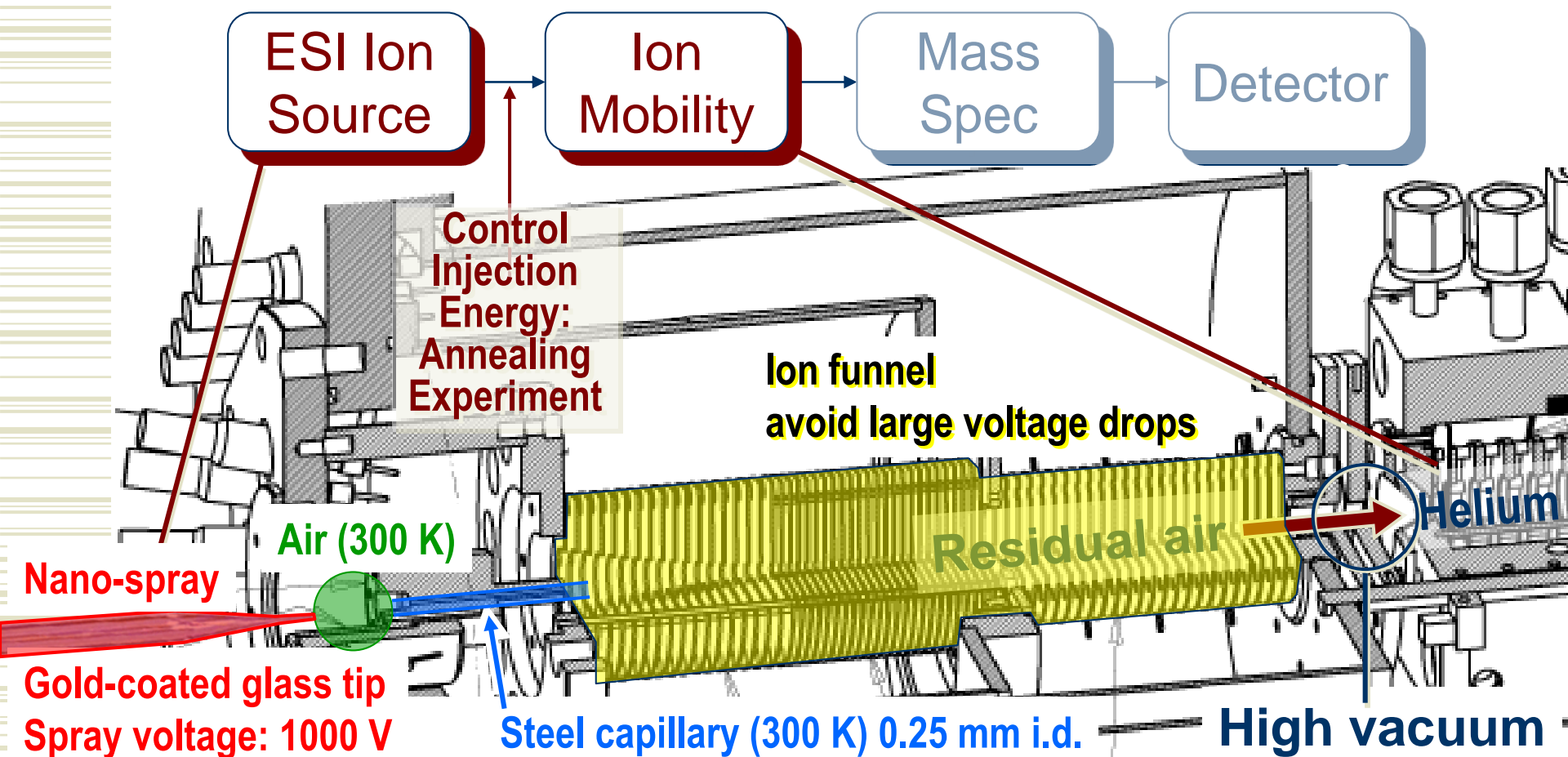
A New, Higher Resolution, Ion Mobility Mass Spectrometer

P. R. Kemper, N. F. Dupuis, M. T. Bowers *Int. J. Mass Spectrom.* **2009**, 287, 46-57

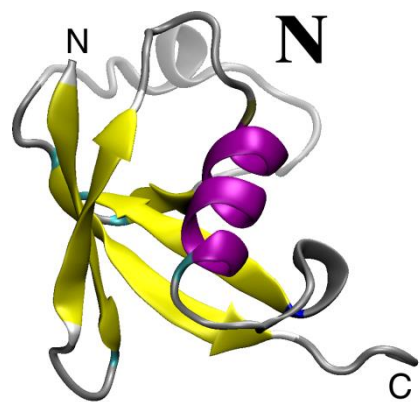


Design of a New Electrospray Ion Mobility Mass Spectrometer

T. Wytttenbach, P. R. Kemper, M. T. Bowers *Int. J. Mass Spectrom.* **2001**, *212*, 13-23



Ubiquitin ATDs
(HiRes vs. ESI)
 $z = 6$

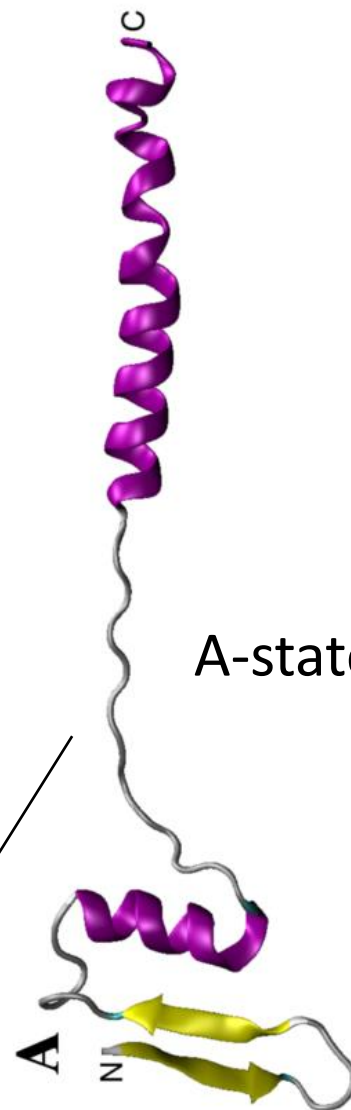


Native
state

HiRes

ESI

A-state



750

1000

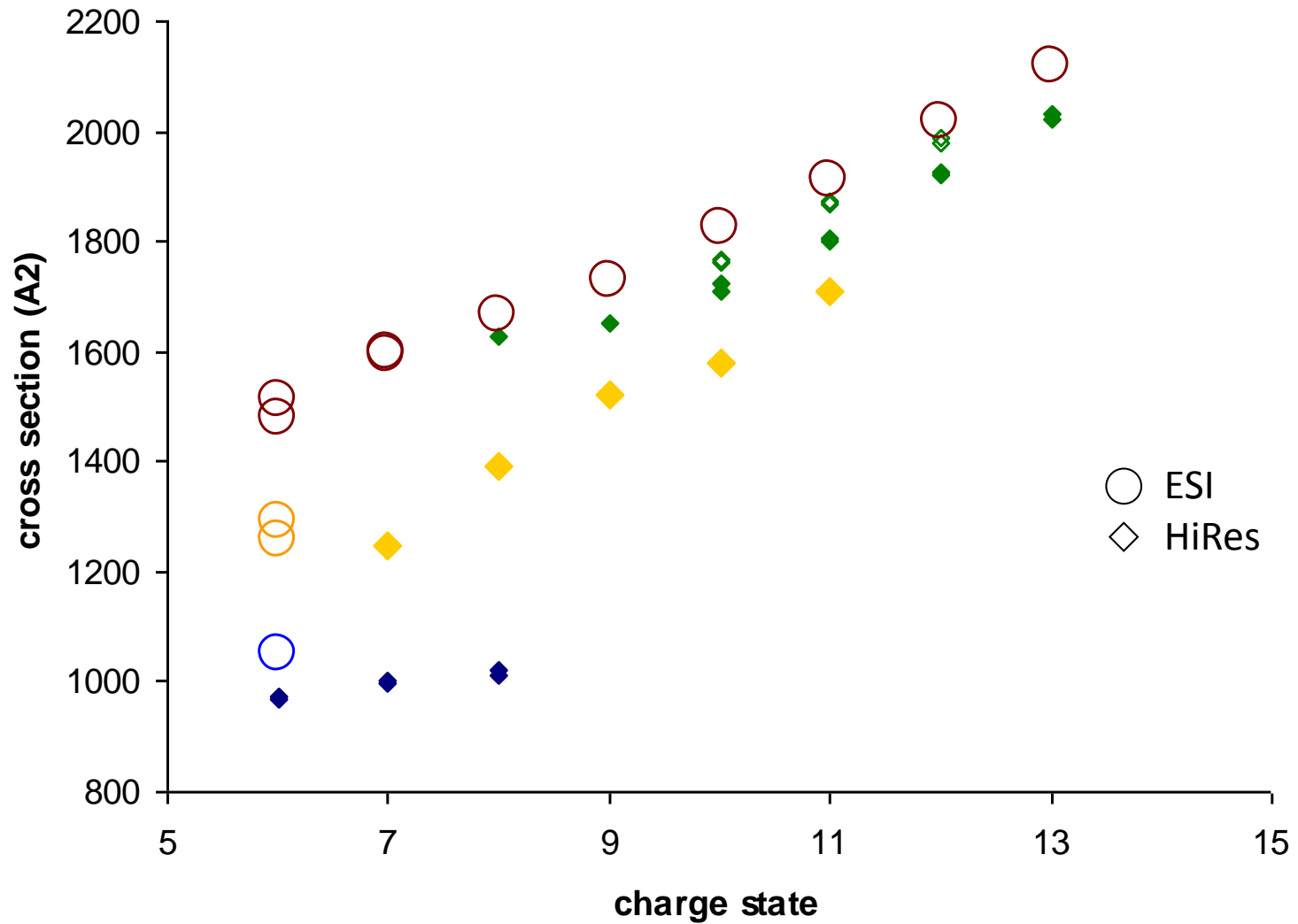
1250

1500

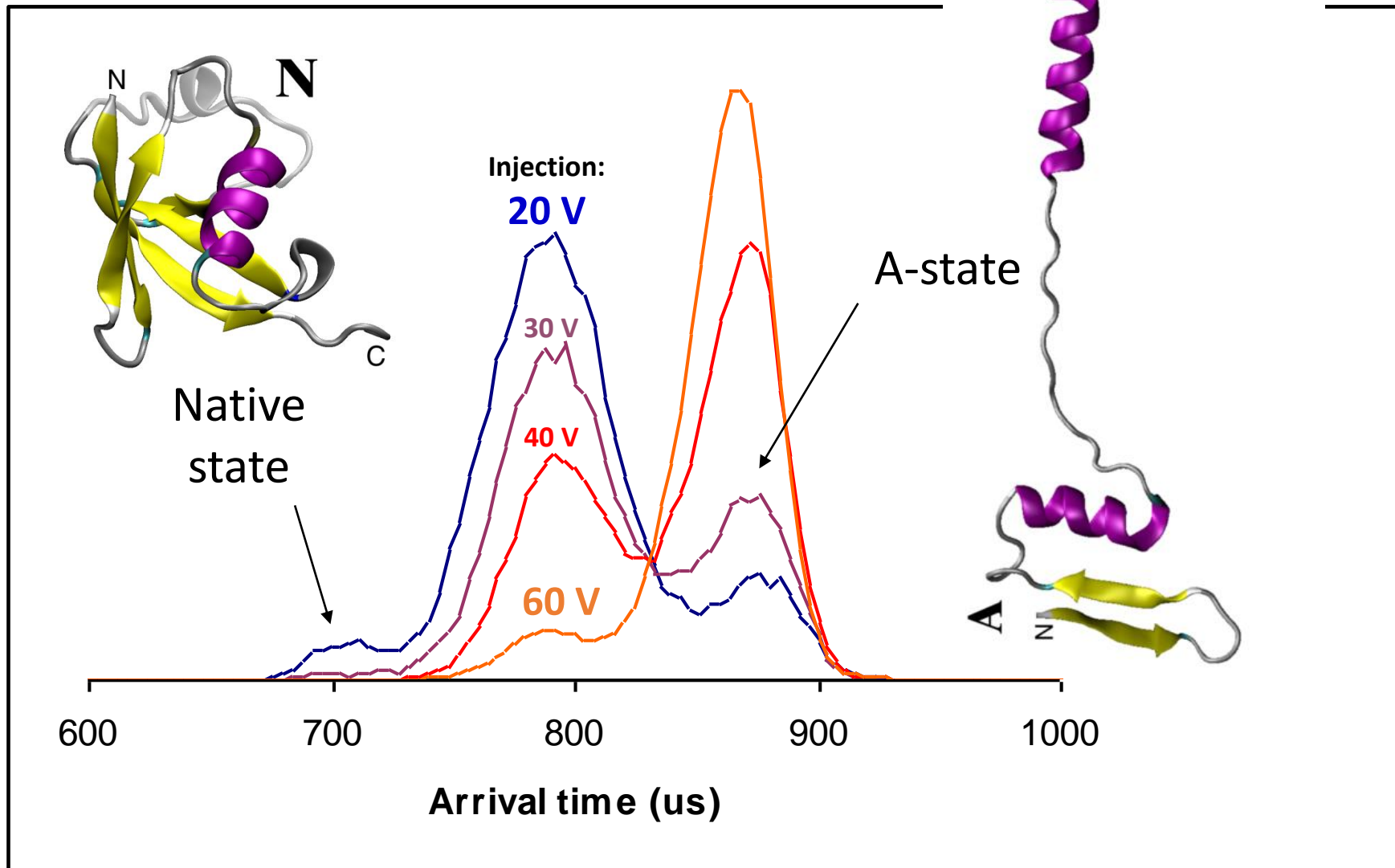
1750

cross section (\AA^2)

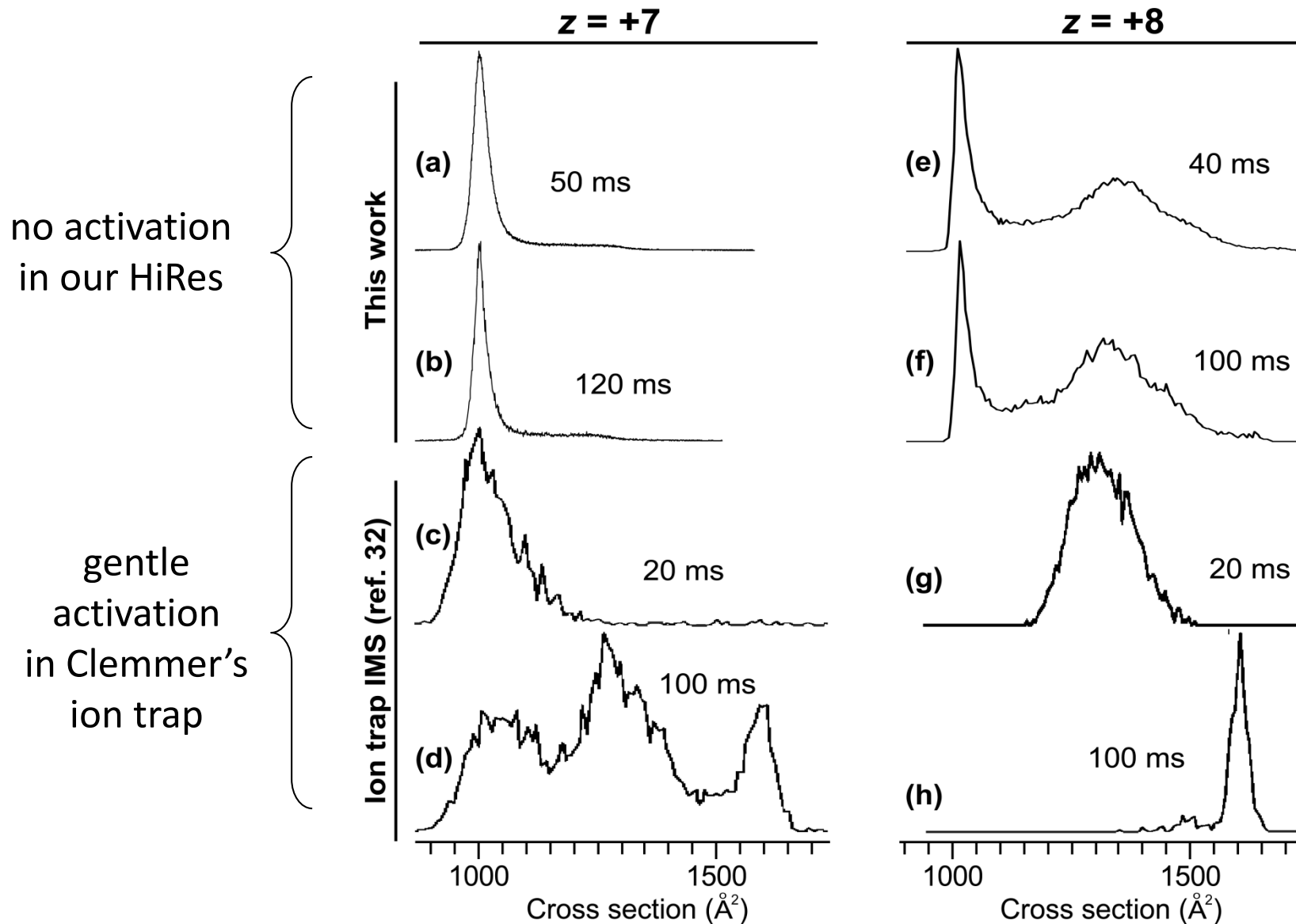
Ubiquitin cross sections (HiRes vs. ESI) z = 6 to 13



Ubiquitin z = 6 ATD:
ESI injection energy



Ubiquitin collisional activation

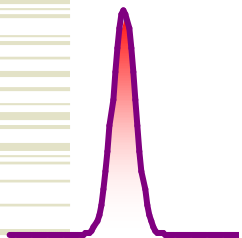


Conclusions

Low energy ESI-MS–based methods have the potential to reveal molecular **SOLUTION STRUCTURE** information.

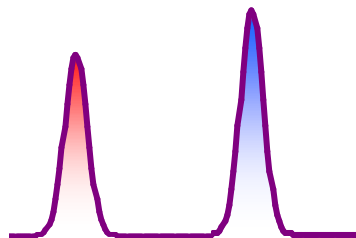
Tremendous potential for biochemical and other applications

Arginine
0.2 kDa



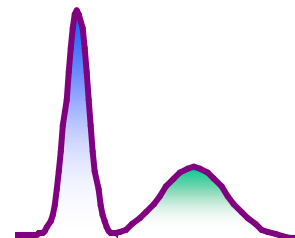
GAS PHASE

**Amyloid
 β -Protein**
5 kDa



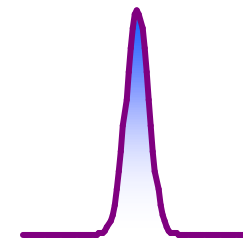
**SOLUTION
GAS PHASE**

Ubiquitin
9 kDa



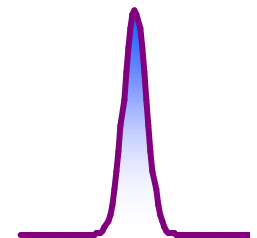
**SOLUTION
INTERMEDIATE?**

Calmodulin
17 kDa



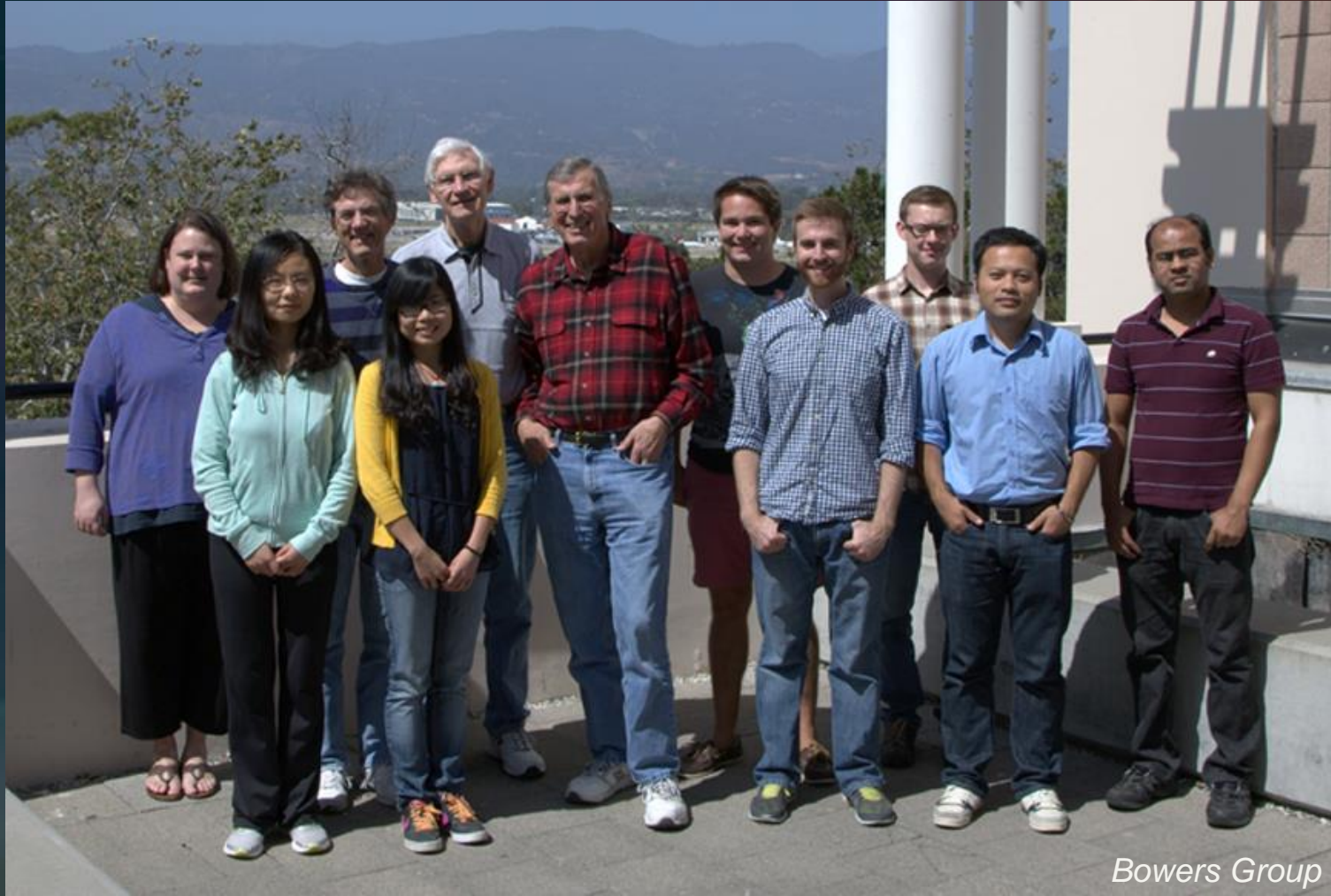
SOLUTION

**Protein
complex**
>1 MDa



SOLUTION

Acknowledgements



Bowers Group

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von Humboldt
Foundation



Waters



bowers.chem.ucsb.edu

Thanks for your attention!

