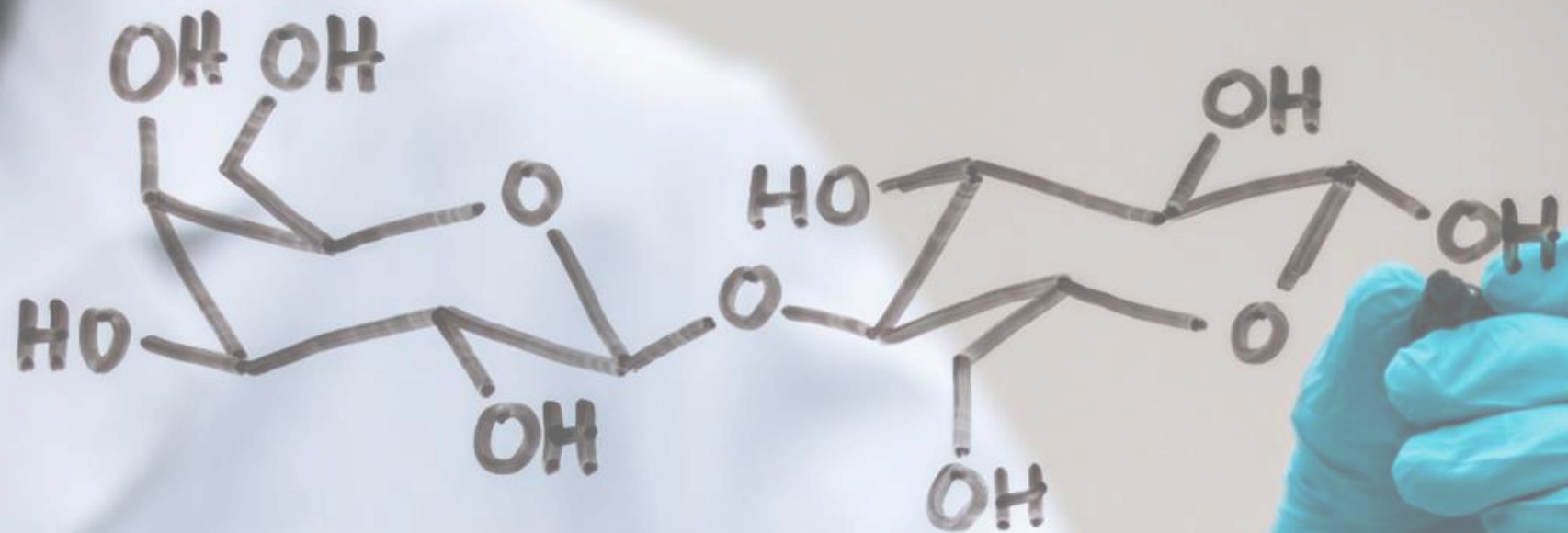


# Mass Spectrometry-Based Techniques to Elucidate the Sugar Code

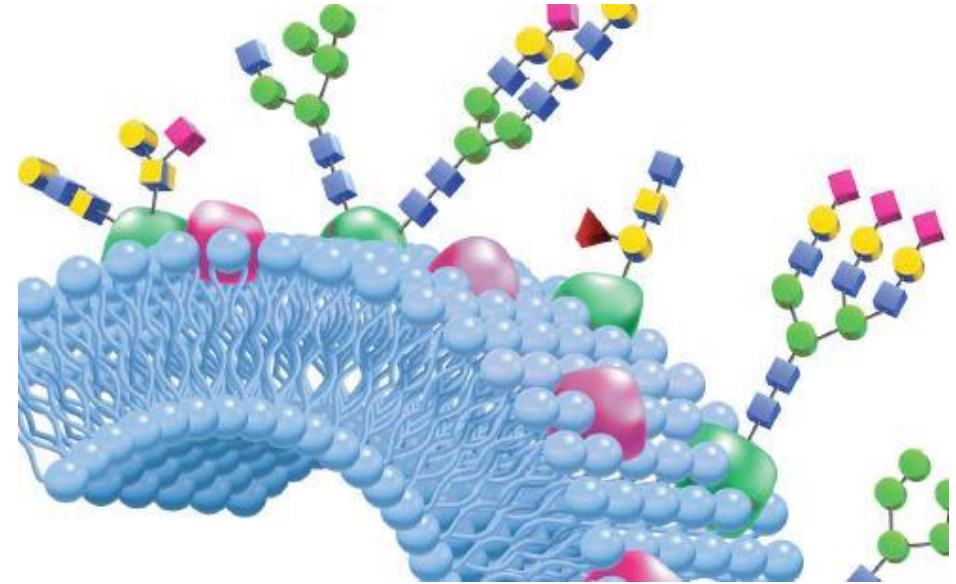


Kevin Pagel

Freie Universität Berlin and Fritz Haber Institute  
of the Max Planck Society, Berlin, Germany

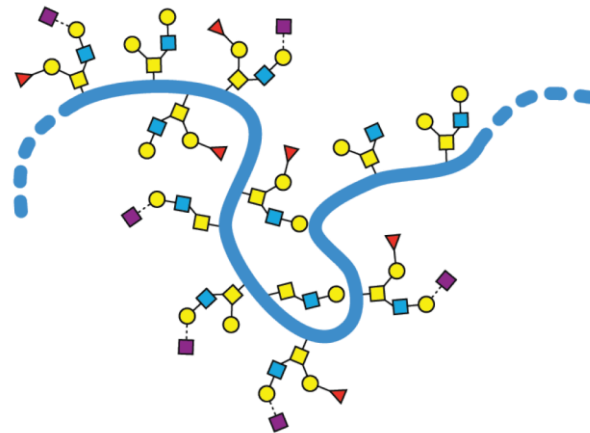
## Biopolymers

Cellulose  
Starch  
Heparin



## Glycosylation of Proteins

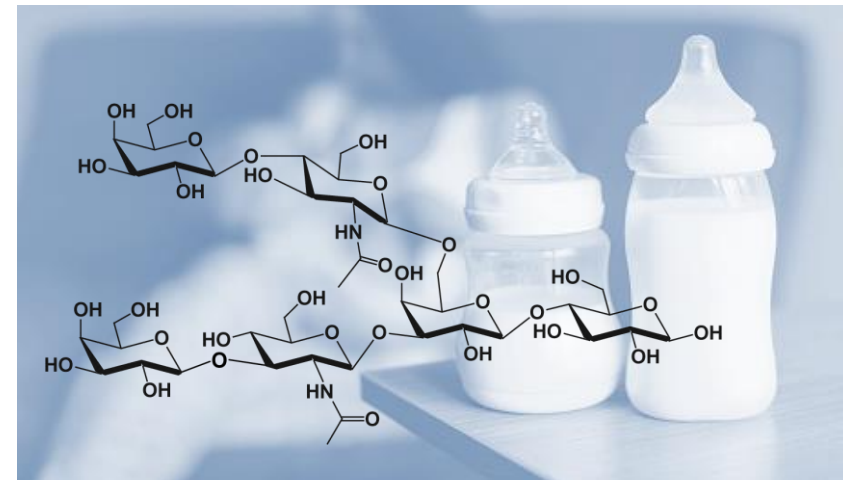
Biomarkers for diseases  
Personalized medicine  
Biopharma



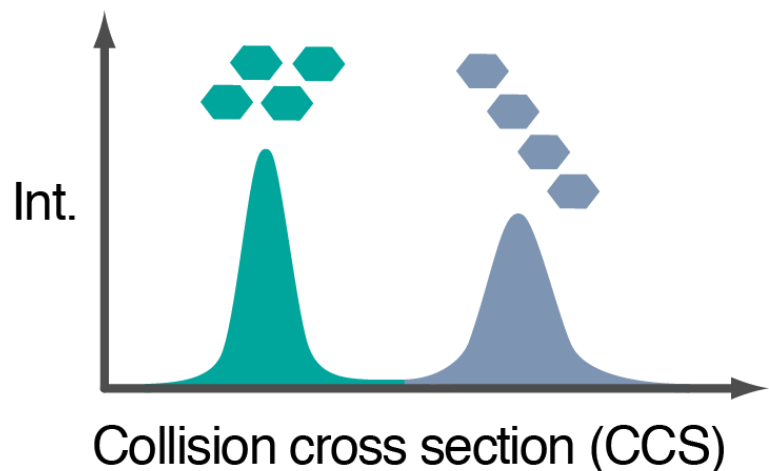
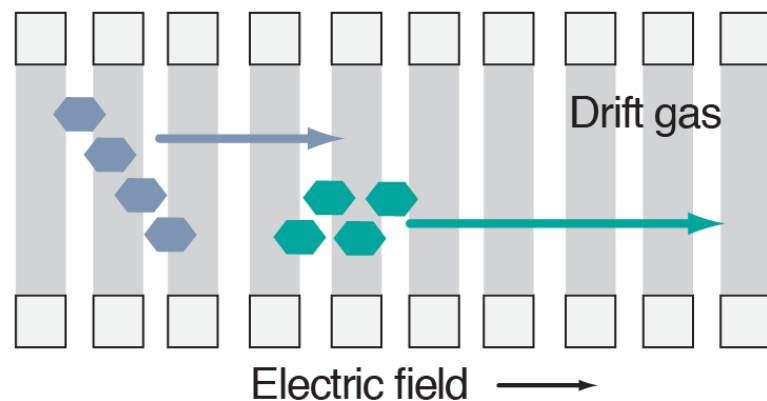
## Free Oligosaccharides

Detection of diseases  
Microbiota  
Pharma

→ **Isomer problem**



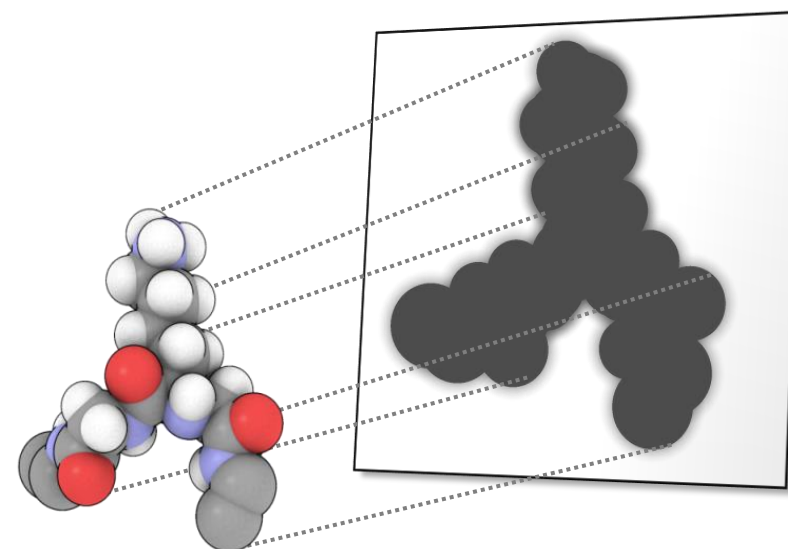
## Ion mobility cell



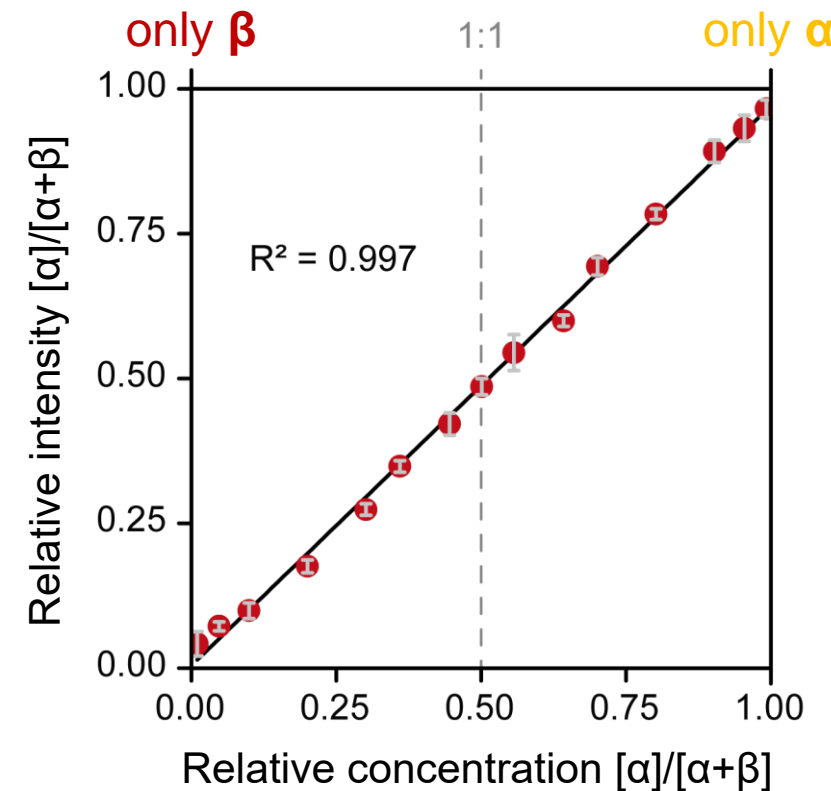
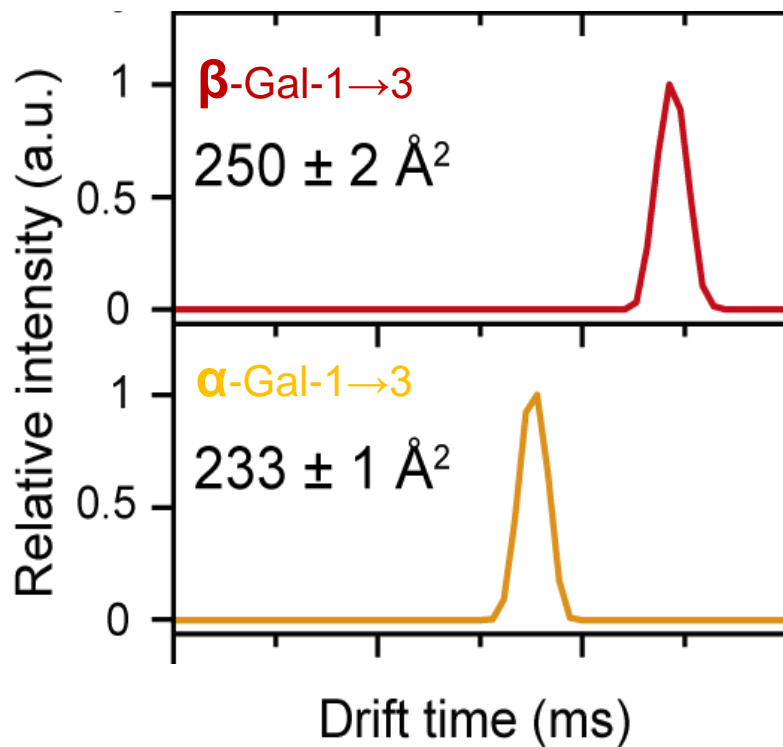
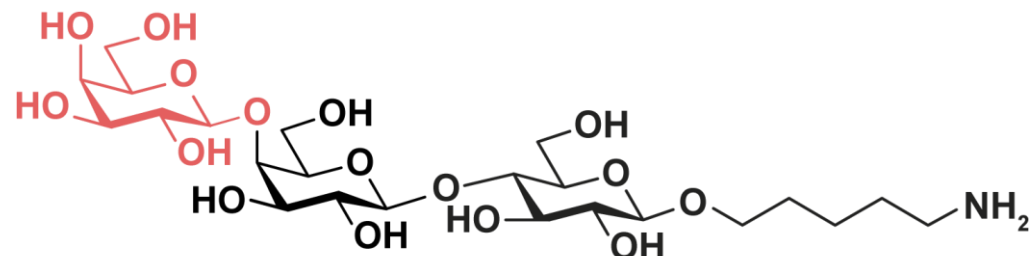
**Size and shape information**

## Collision Cross Section

- CCS is a molecular property
- Corresponds to the area that collides with the drift gas
- Can be calculated theoretically
- Can be implemented in databases



# IM-MS of Synthetic Glycans

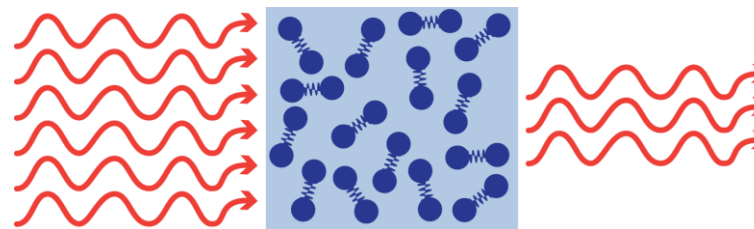


**Identification and quantification of glycan isomers**

## Absorption Spectroscopy

Measures the influence of the molecule on the light

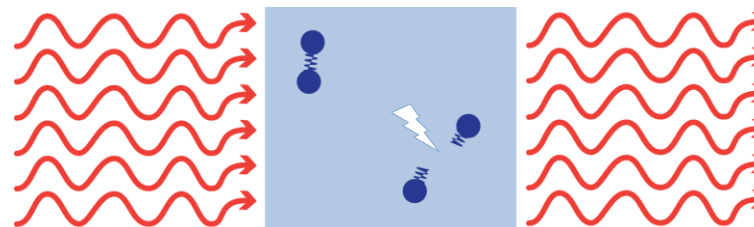
- Many molecules needed  
(but not many photons)



## Action Spectroscopy

Measures the influence of the light on the molecule

- Many photons needed  
(but not many molecules)



# Gas-Phase IR Spectroscopy

**nESI source**  
Ionization

**Quadrupole**  
Mass selection

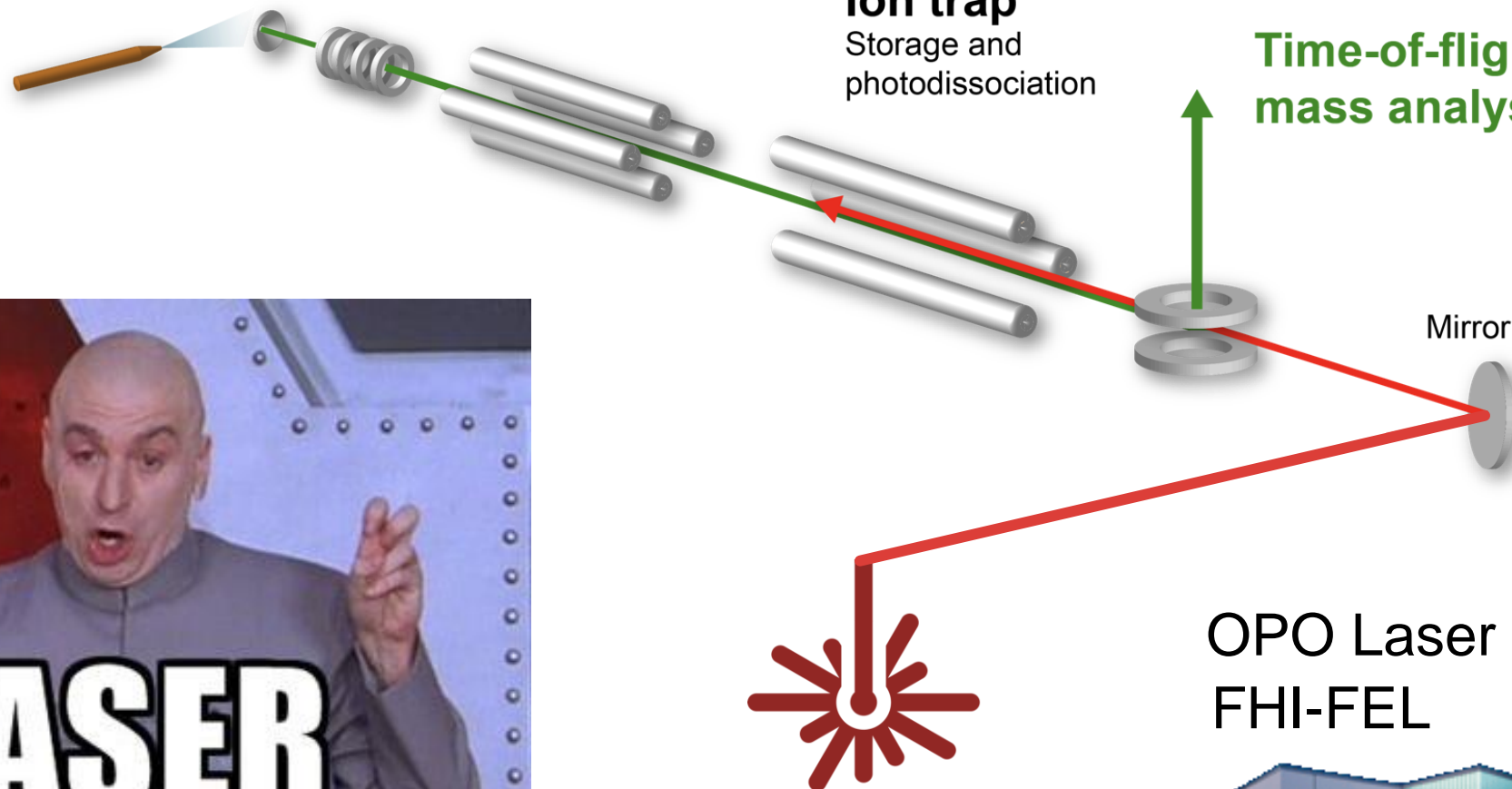
**Ion trap**  
Storage and  
photodissociation

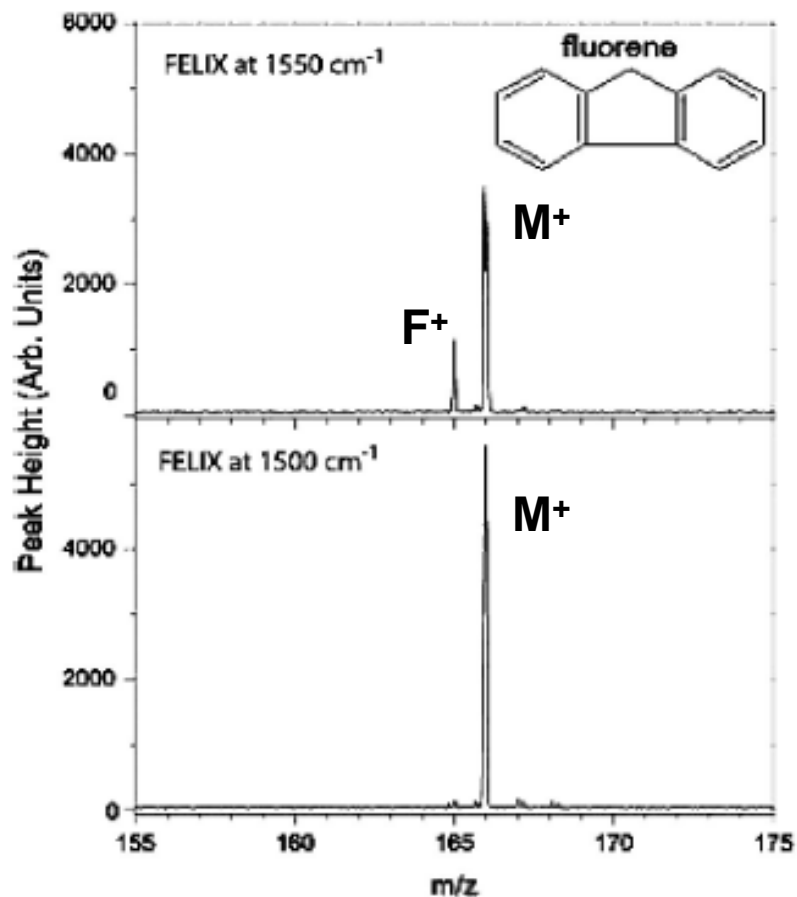
**Mass Spectrometer**

**Time-of-flight  
mass analysis**

Mirror

OPO Laser  
FHI-FEL





1550cm<sup>-1</sup>

Resonant – dissociation

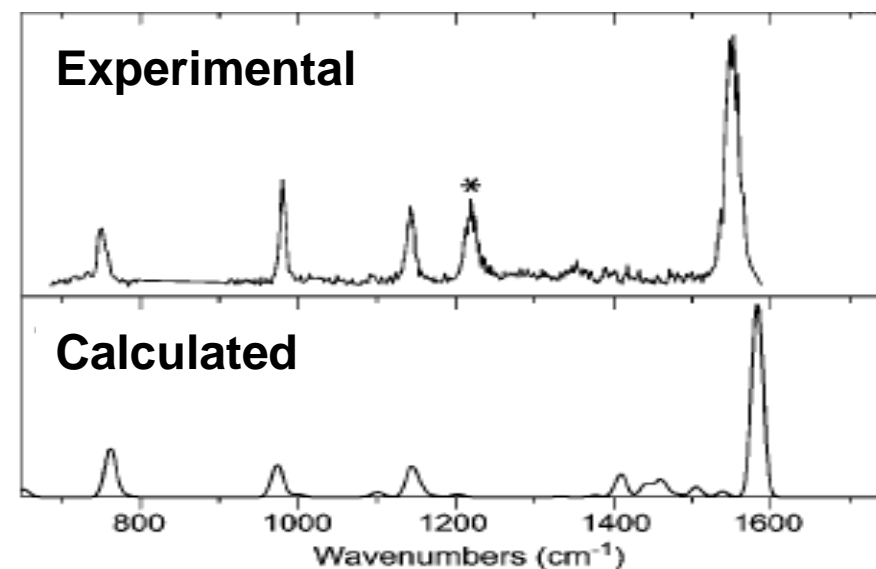
- depletion of precursor ions M<sup>+</sup>
- emerging fragment ions F<sup>+</sup>

1500cm<sup>-1</sup>

Off-resonant – no dissociation

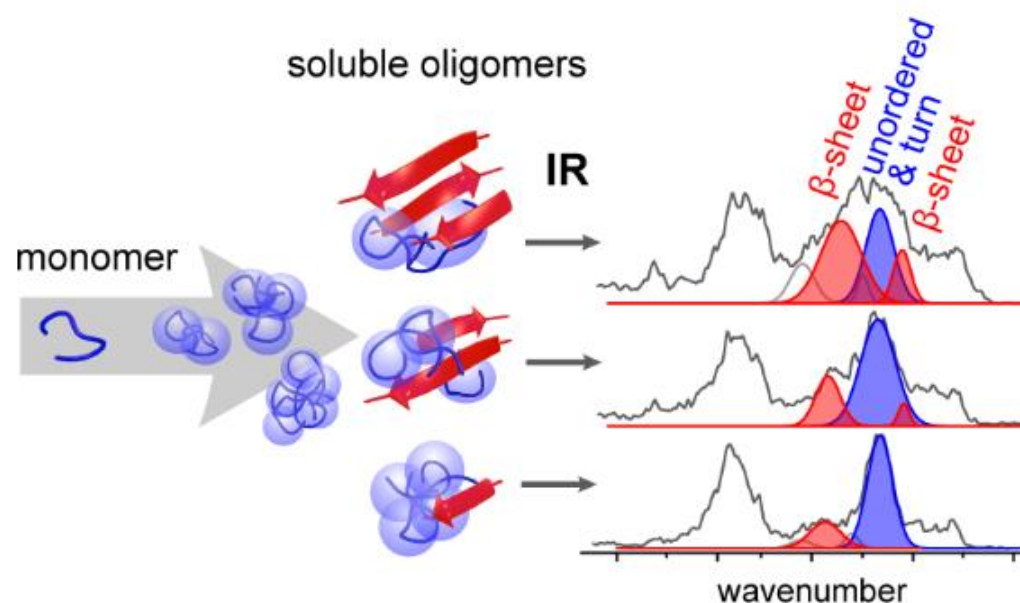
record mass spectra as a function of the IR wavelength

→ **Gas-phase IR spectrum**



## Proteins and Peptide Oligomers

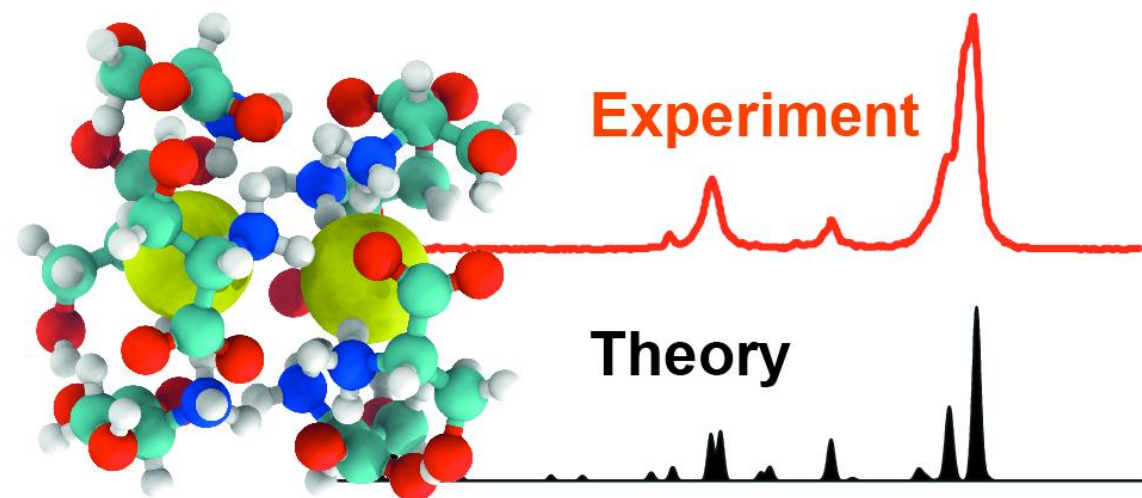
Challenge: polydispersity



## Serine Octamer

$(\text{Ser}_8\text{Cl}_2)^{2-}$

highly symmetric, stable, homochiral



Seo, J. et al. *Nature Chem.* **2017**, 9, 39

Hoffmann, W. et al. *J. Am. Chem. Soc.* **2018**, 140, 244

Seo, J. et al. *Angew. Chem. Intl. Ed.* **2016**, 55, 14173

Seo, J. et al. *Nature Chem.* **2017**, 9, 1263



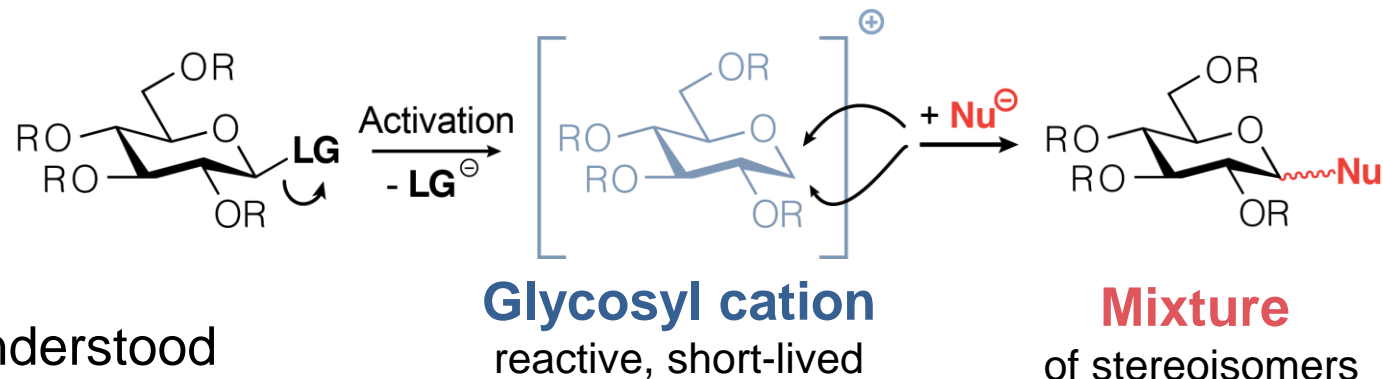
## Mitteilungen.

464. Emil Fischer: Ueber die Glucoside der Alkohole<sup>1)</sup>.

[Aus dem I. Berliner Universitäts-Laboratorium.]

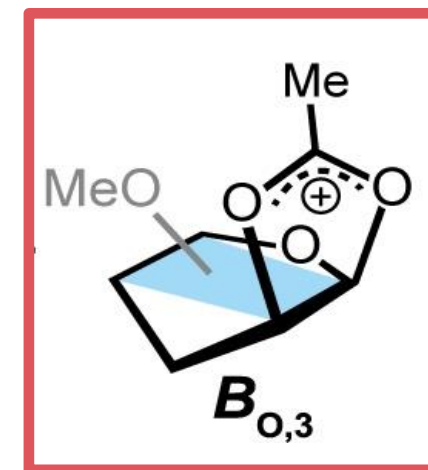
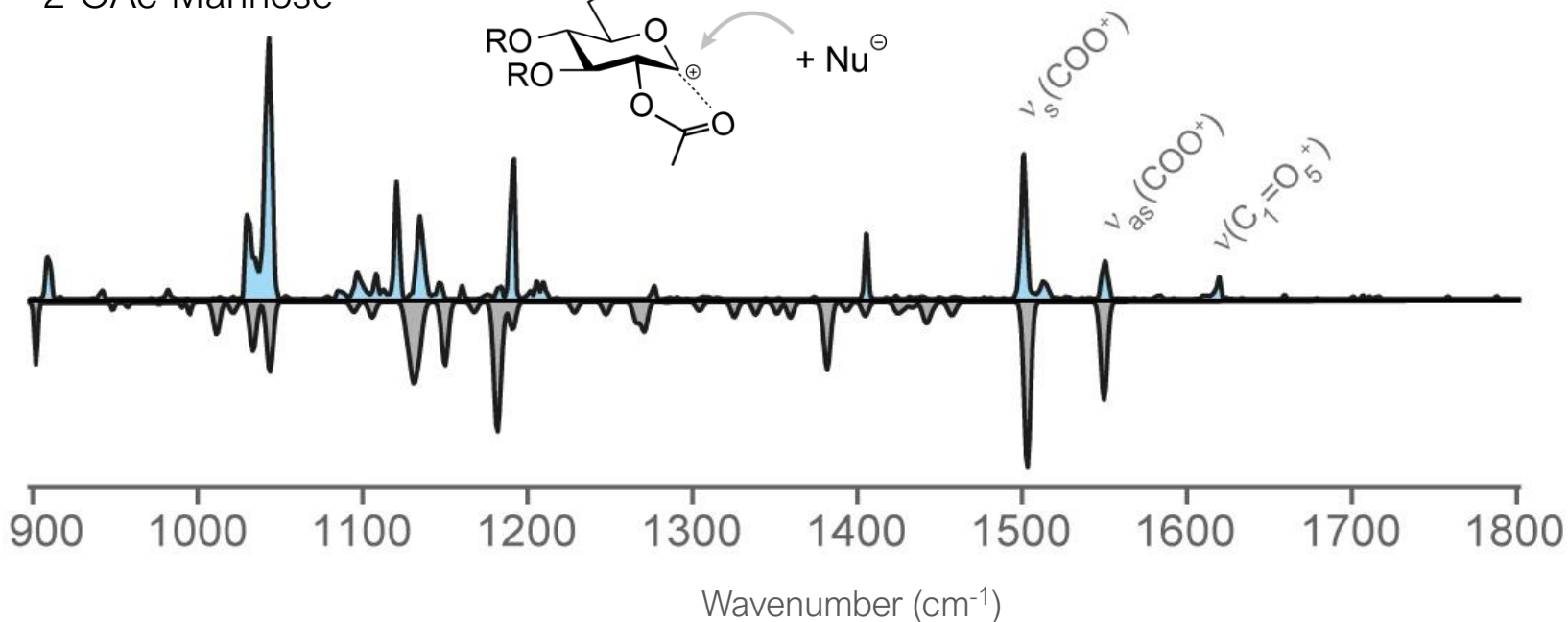
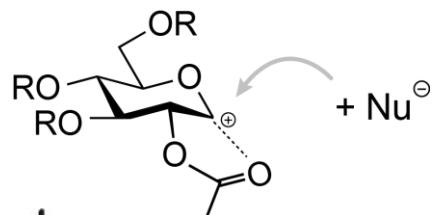
(Eingegangen am 9. October; vorgetragen in der Sitzung vom Verf.)

Für die künstliche Bereitung von Glucosiden ist zur Zeit nur die



→ Cationic intermediate is crucial but not understood

2-OAc-Mannose



Covalent bond!  
Conserved pucker

*Nature Commun.* **2018**, 9, 4147  
*Angew. Chem.* **2020**, 59, 6166  
*Nat. Synth.* **2024**

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