nature

LETTER

doi:10.1038/nature15388

Identification of carbohydrate anomers using ion mobility–mass spectrometry

J. Hofmann[1,2]*, H. S. Hahm[3,4]*, P. H. Seeberger[3,4] & K. Pagel[1,2]

[1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany. [2]Institute for Chemistry and Biochemistry, Free University Berlin, Takustraße 3, 14195 Berlin, Germany. [3]Max Planck Institute of Colloids and Interfaces, Department of Biomolecular Systems, Am Mühlenberg 1, 14476 Potsdam, Germany. [4]Institute for Chemistry and Biochemistry, Free University Berlin, Arnimallee 22, 14195 Berlin, Germany.

*These authors contributed equally to this work.

Abhijit Nag
23/01/2016

Introduction

- Carbohydrates are important biological polymers that are involved in many biological processes.
- Owing to their branched structure and the presence of stereogenic centres at each glycosidic linkage between monomers, carbohydrates are harder to characterize.
- By NMR they can be characterized but it can not detect small amounts of coexisting isomers.
- Mass spectrometry, on the other hand, can provide information on carbohydrate composition and connectivity for even small amounts of sample, but it cannot be used to distinguish between stereoisomers. But combination of mass spectrometry and ion mobility can do the job.
- IM–MS measures the time that ions require to drift through a cell that is filled with an inert neutral gas such as helium or nitrogen, under the influence of a weak electric field. While drifting, compact ions undergo fewer collisions with the gas than more extended ions, and therefore traverse the cell faster.

Chemical Science

ROYAL SOCIETY OF CHEMISTRY

EDGE ARTICLE

Cite this: *Chem. Sci.*, 2014, 5, 3234

Enantiomeric differentiation of aromatic amino acids using traveling wave ion mobility-mass spectrometry†

Virginie Domalain,[a] Marie Hubert-Roux,[a] Vincent Tognetti,[a] Laurent Joubert,[a] Catherine M. Lange,[a] Jacques Rouden[b] and Carlos Afonso*[a]

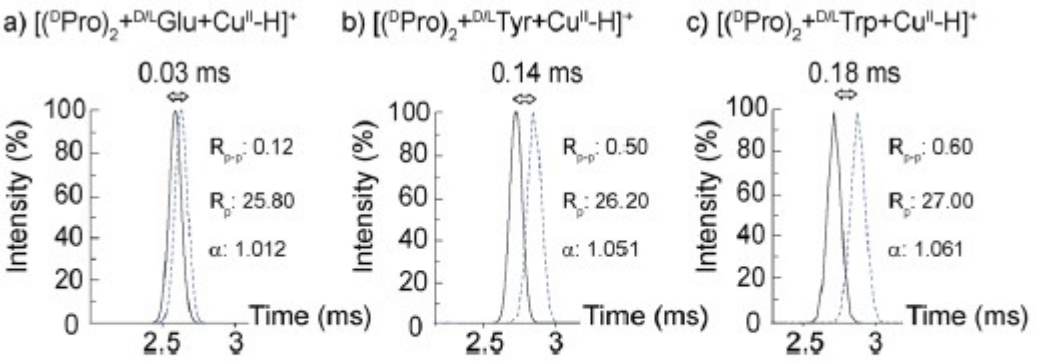


Fig. 5 Overlay of ion mobility spectra for $[(^{D}Pro)_2+^{D/L}M+Cu^{II}-H]^+$ (a) M: glutamic acid; (b) M: tyrosine; (c) M: tryptophan. Solid lines: ion mobility spectra for ^{D}M. Dotted lines: ion mobility spectra for ^{L}M.

Vol. 6, No. 1, 2015
ISSN 2233-4203/ e-ISSN 2093-8950
LETTER www.msletters.org | Mass Spectrometry Letters

Amino-β-cyclodextrin Complex Assisted Ionization for Labile Sesamins and their Ion-mobility Separation in ESI Q-TOF MS

Kohtaro Sugahara, Manabu Horikawa, and Tohru Yamagaki*

Suntory Institute for Bioorganic Research, Suntory Foundation for Life Sciences, 1-1-1 Wakayamadai, Shimamoto, Mishima, Osaka, 618-8503 Japan

Received December 01, 2014; Revised February 17, 2015; Accepted March 11, 2015
First published on the web March 31, 2015; DOI: 10.5478/MSL.2015.6.1.17

DOI: 10.1002/cjoc.201500670

Behaviors of Leucine and Isoleucine in Ion Mobility-Quadrupole Time of Flight Mass Spectrometry

Su Guo,[a,c] Fang Zhang,*[,a] Haoyang Wang,[a] Manyu Zhang,[b] Zhixu Zhang,[b] Xiang Zhang,[d] and Yinlong Guo*[,a]

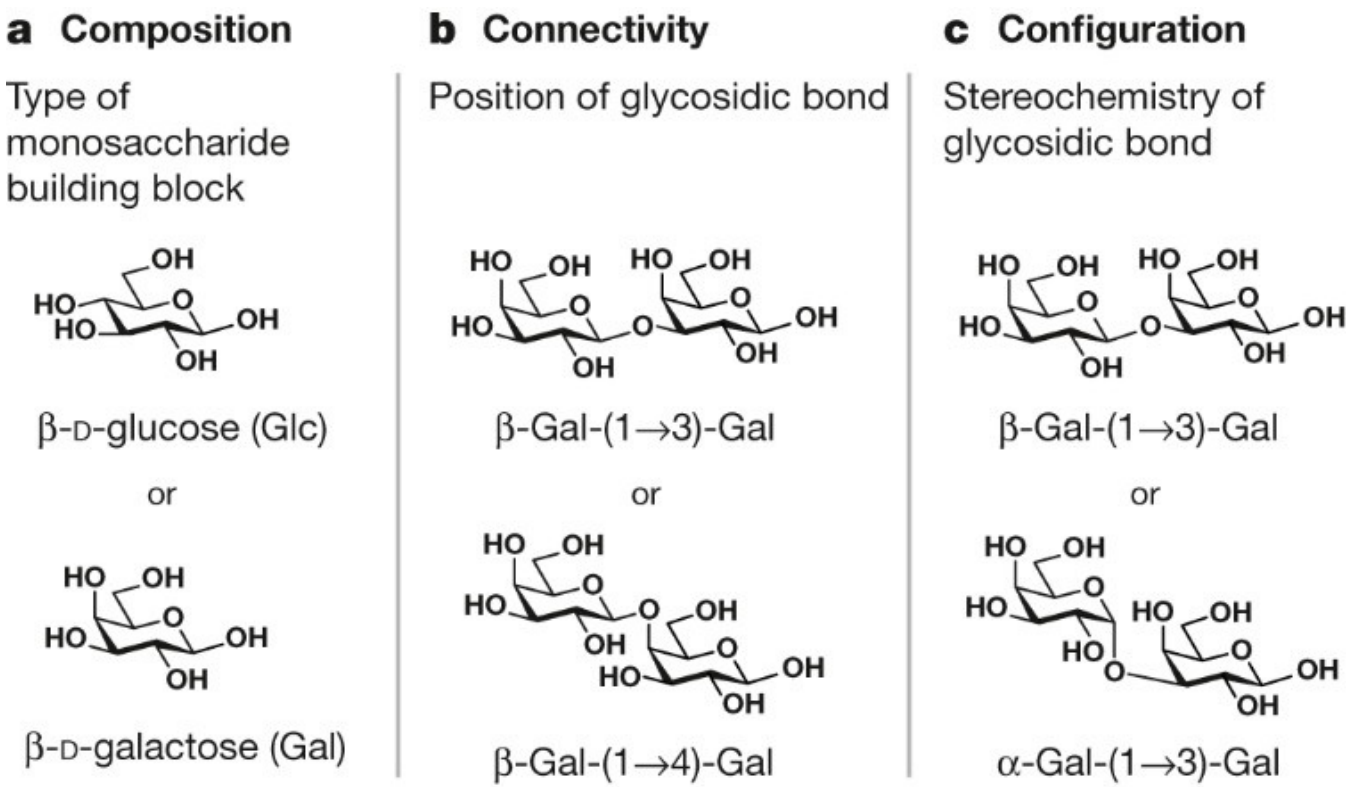
[a] *National Center for Organic Mass Spectrometry in Shanghai, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, China*
[b] *Agilent Technologies (China) CO., Ltd., 1350 North Sichuan Road, Shanghai 200080, China*
[c] *Department of Chemistry, Fudan University, 220 Handan Road, Shanghai 200433, China*
[d] *School of Food Science and Biotechnology, Zhejiang Gongshang University, Hangzhou, Zhejiang 310018, China*

* E-mail: ylguo@sioc.ac.cn; Tel.: 0086-021-54925300
Received September 17, 2015; accepted September 28, 2015; published online XXXX, 2015.
Supporting information for this article is available on the WWW under http://dx.doi.org/10.1002/cjoc.201500670 or from the author.

Chin. J. Chem. **2015**, *XX*, 1—6

In this paper

Structural features of complex carbohydrates.



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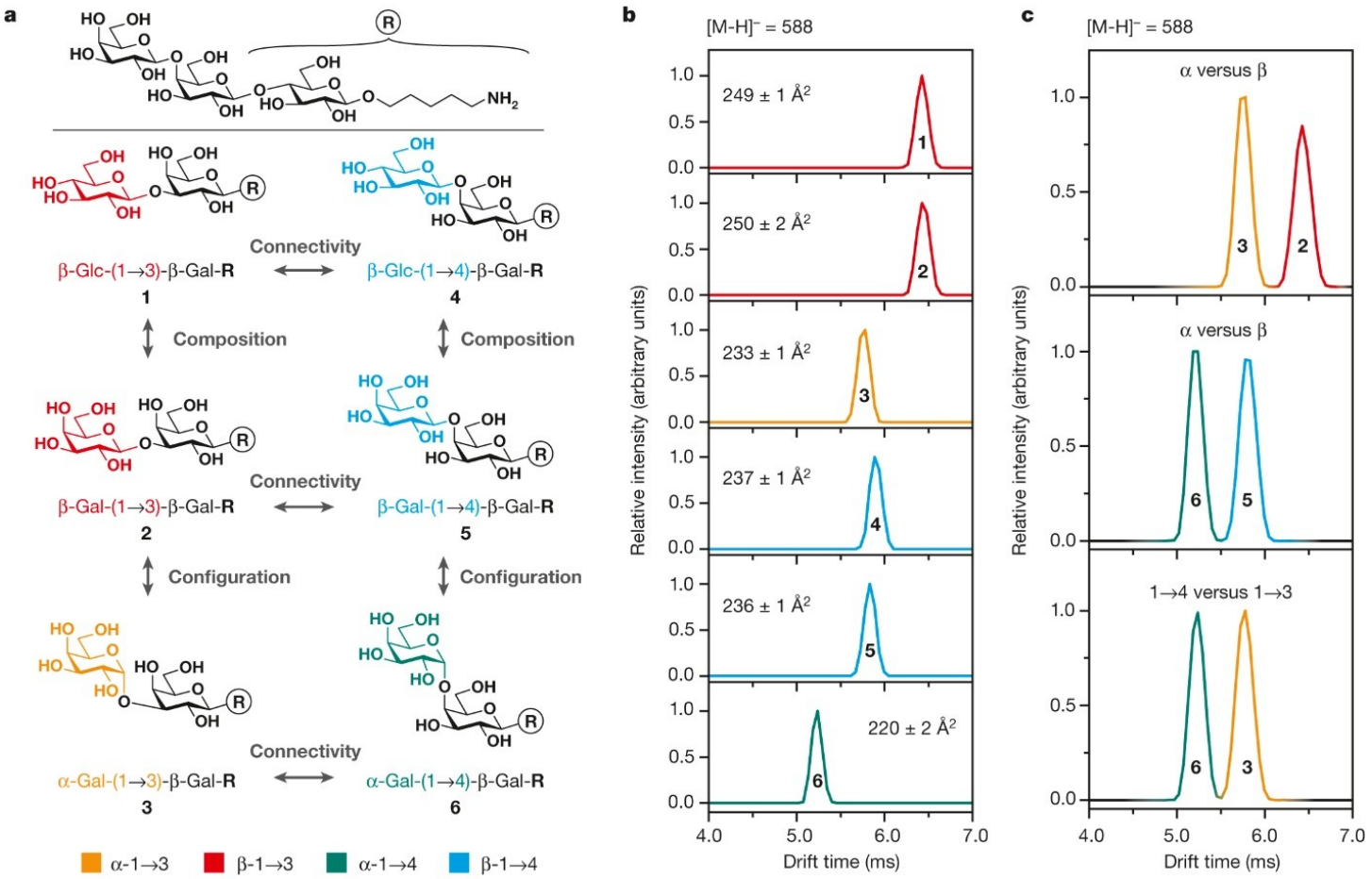
Structure and IM–MS data of trisaccharides 1–6.



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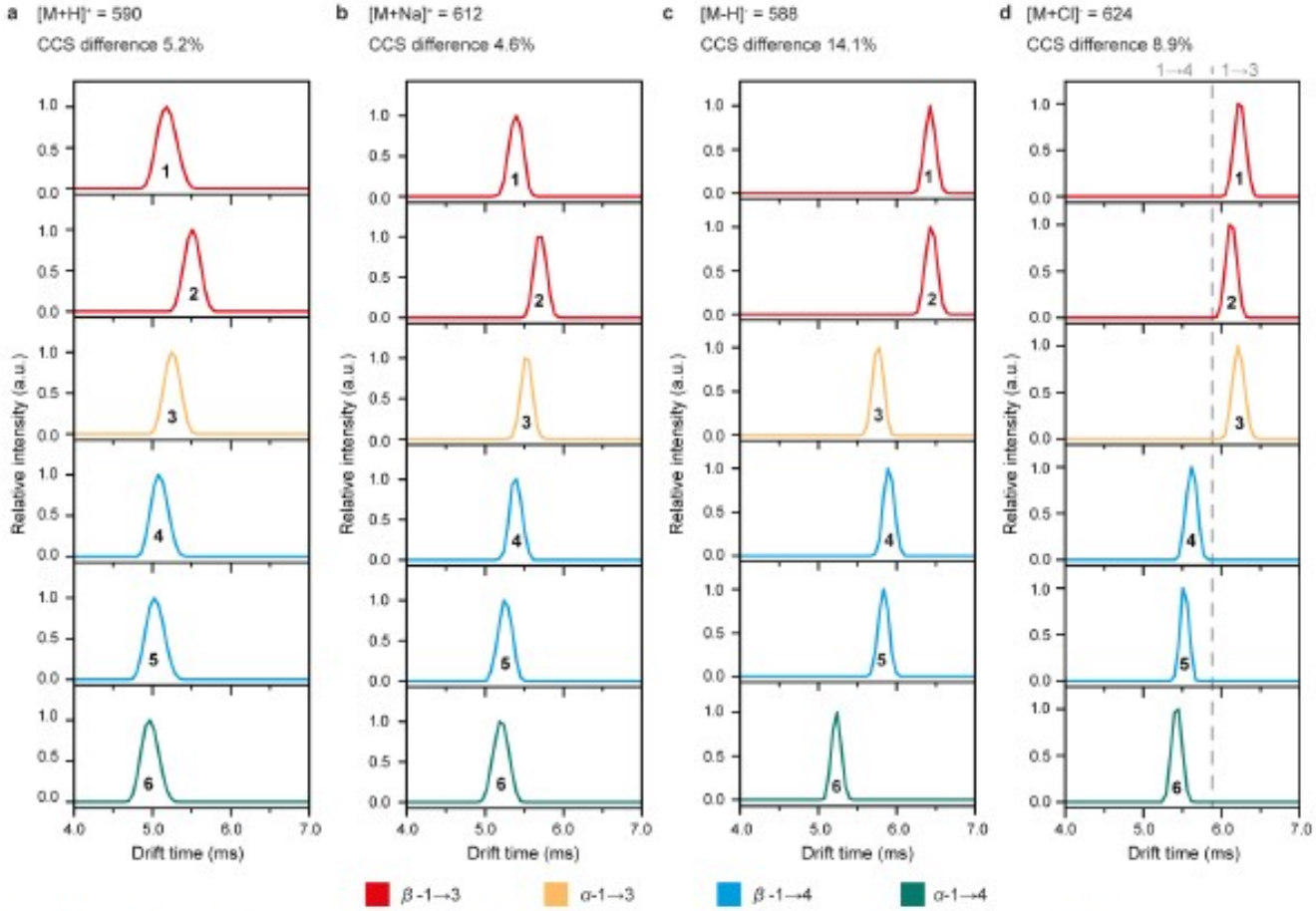
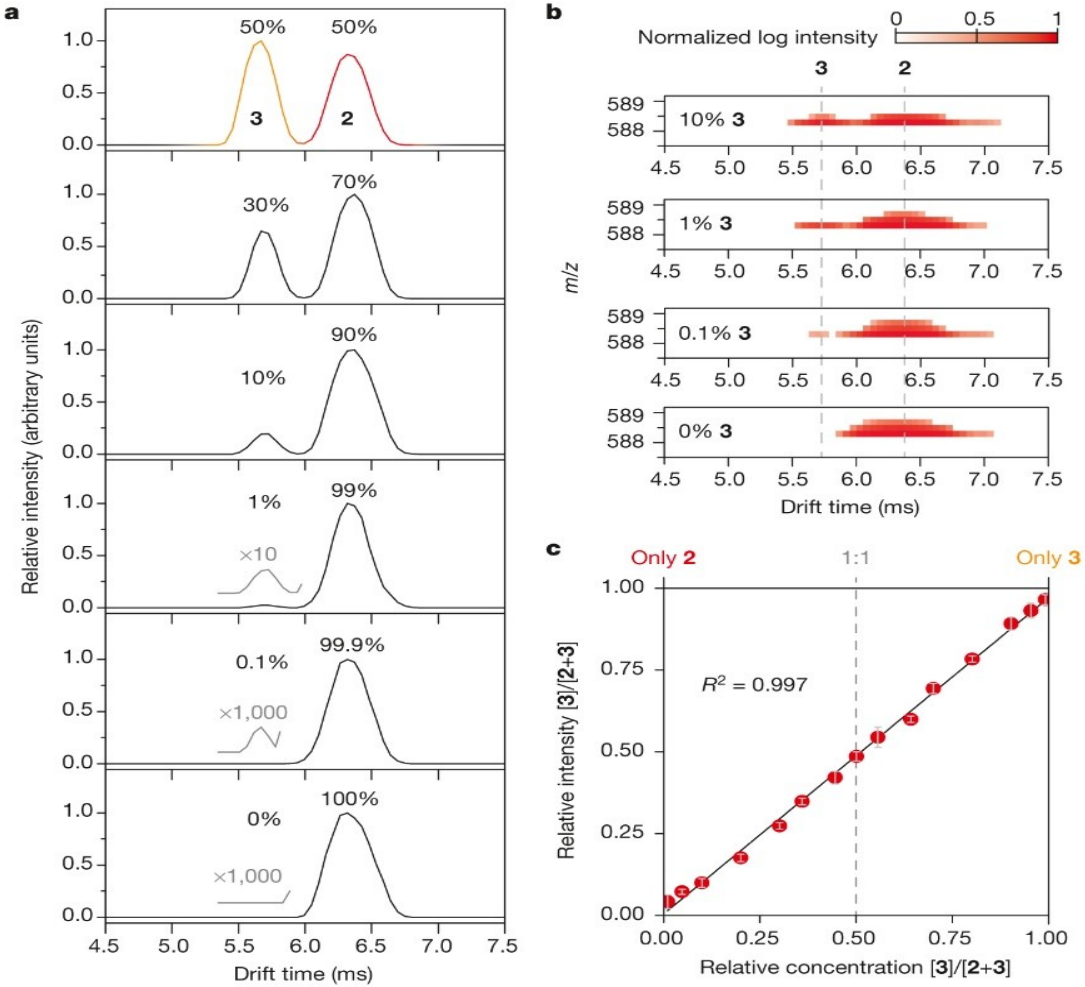


Extended Data Figure 3 | Drift-time distributions of trisaccharides 1–6 as different species in positive- and negative-ion mode. The CCS difference between the most compact and the most extended isomer of each set is given as a percentage. Small CCS differences are observed in positive-ion mode (**a**, **b**), which makes an unambiguous identification of the trisaccharides difficult. The largest CCS differences are observed using deprotonated ions (**c**), allowing the identification of linkage isomers (for example, **3** + **6**) and stereoisomers (for example, **2** + **3**). A clear identification of regioisomers with a terminal 1→3 or 1→4 glycosidic bond can be obtained for chloride adducts (**d**).

Relative quantification of configurational trisaccharide isomers.



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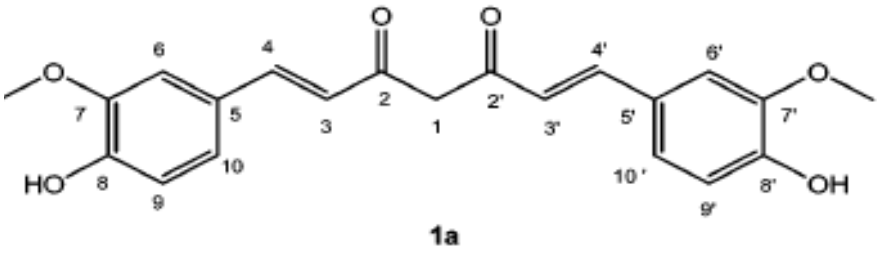
Summary

- In summary, they demonstrate that IM–MS is a powerful tool for the structural analysis .
- Connectivity and configurational isomers can be separated efficiently.
- The relative content of isomeric impurities can be determined quickly and easily.
- No other experimental technique can provide the same structural information as quickly and with such minimal sample consumption.

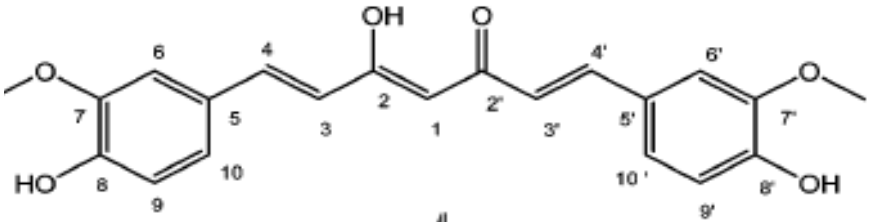
Future Plan

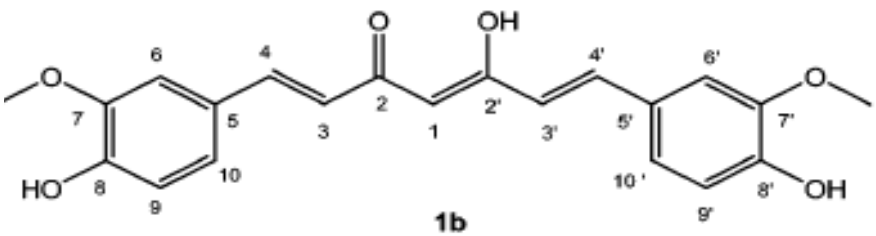
❖ Tautomers can be separated by ion mobility mass spectrometry.



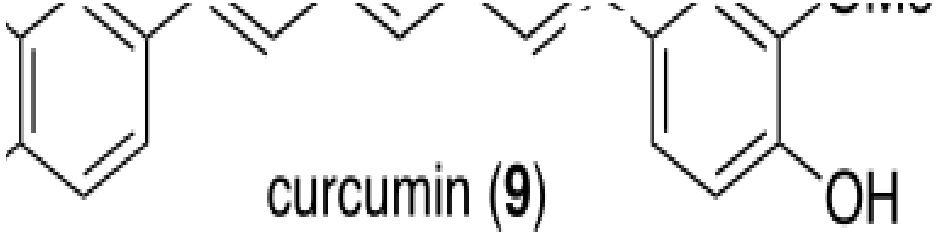
1a

Beta-Diketone Tautomer





1b



Future Plan

- Different silver and gold clusters and cyclodextrin inclusion complexes can be studied by ion mobility mass spectrometry.
- If one can separate the racemic mixtures of a cluster (silver, gold), that will be a good work.


Thank you!