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Analyzing Viruses using Hydrogen Deuterium Exchange Mass Spectrometry *Hydrogen Deuterium Exchange (HDX) at the Univ. of Texas | Behind the Science* ~~WEBINAR | Hydrogen Deuterium Exchange Coupled with Cyclic Ion Mobility for Higher Quality Analyses~~ **How hydrogen exchange mass spectrometry can**

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Chemistry **Facilitating Drug Discovery with HDX-Mass Spectrometry** ~~Hydrogen or deuterium exchange~~

1HNMR spectroscopy: D2O exchange

Hydrogen-Deuterium Exchange of Phosphorylated Phosphomannomutase

Hydrogen Deuterium Exchange M Spectrometry

Electrospray mass spectrometry can provide detailed insights into ... We will then proceed to discuss hydrogen/deuterium exchange techniques that can decipher the inner workings of soluble and ...

Dr. Lars Konermann

By using finely-tuned photons instead of traditional broad spectrum heat sources ... only the lighter hydrogen atoms could tunnel through the activation barrier to dissociation while the deuterium ...

5. Activated Chemisorption of Methane

Our activities include various areas of modern mass and ion mobility spectrometry, ion-molecule reaction ... on utilizing gas-phase ion-molecule reaction kinetics such as hydrogen-deuterium exchange ...

Dr. Touradj Solouki

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Journal of the American Society for Mass Spectrometry

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Journal of chromatography. A
Kolappan, S, Lo, KY. Shen, CLJ, Guttman, J.A., and Craig, L. Structure of a conserved Francisella virulence protein FvfA. Acta Cryst

D73, 814-821. Wang, F, Coureuil ...

Molecular Biology and Biochemistry

Because such beams can be polarized, have low emittance, and small energy bandwidth, they are applicable to a broad spectrum of commercial and medical uses. They can also be used to provide compact, ...

ABSTRACTS - Phase I

and the Wbl protein (Figure), which uses an Fe-S cluster to sense NO in M. tuberculosis and hence evade host defences. We have studied how proteins recognize polysaccharides such as starch, cellulose, ...

Professor Mike

Williamson

M.O. Alfred , M.O. Omorogie, O. Bodede, R. Moodley, A. Ogunlaja, O. G. Adeyemi, C. G ü nter, A. Taubert, I. Iermak, H. Eckert, I. D.A. Silva, A.S.S. de Camargo, A. de ...

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Hydrogen exchange mass spectrometry is widely recognized for its ability to probe the structure and dynamics of proteins. The application of this technique is becoming widespread due to its versatility for providing structural information about challenging biological macromolecules such as antibodies, flexible proteins and glycoproteins. Although the technique has been around for 25 years, this is the first definitive book devoted entirely to the topic. Hydrogen Exchange Mass Spectrometry of Proteins: Fundamentals, Methods and Applications brings into one comprehensive volume the theory, instrumentation and applications of Hydrogen Exchange Mass

Spectrometry (HX-MS) - a technique relevant to bioanalytical chemistry, protein science and pharmaceuticals. The book provides a solid foundation in the basics of the technique and data interpretation to inform readers of current research in the method, and provides illustrative examples of its use in bio- and pharmaceutical chemistry and biophysics In-depth chapters on the fundamental theory of hydrogen exchange, and tutorial chapters on measurement and data analysis provide the essential background for those ready to adopt HX-MS. Expert users may advance their current understanding through chapters on methods including membrane protein analysis, alternative proteases, millisecond hydrogen exchange, top-down mass spectrometry, histidine exchange and method validation. All readers can explore the diversity of HX-MS applications in areas such as ligand binding, membrane proteins, drug discovery, therapeutic protein formulation, biocomparability, and intrinsically disordered proteins.

The application of hydrogen/deuterium exchange mass spectrometry (HDX-MS) to investigating protein-carbohydrate interactions is described. Proteins from three bacterial toxins, the B subunit homopentamers of Cholera toxin (CTB5) and Shiga toxin type 1 (Stx1B5) and a fragment of Clostridium difficile toxin A (TcdA-A2), and their interactions with native carbohydrate receptors, GM1 pentasaccharide (GM1-os), Pk trisaccharide and CD-grease, respectively, were first served as model systems for this study.

The results suggested that HDX-MS can serve as a useful tool for localizing the ligand binding sites in carbohydrate-binding proteins. Following this, HDX-MS measurements were applied to explore the existence of distinct HMOs binding sites on toxins. Altogether, two toxins were studied, CTB5 and TcdA-A2, and their interactions with

HMOs, 2'-fucosyllactose (2'-FL) and lacto-N-tetraose (LNT), respectively. For CTB5 and its interaction with 2'-FL, a novel binding site was localized for 2'-FL, different from the one for native receptor GM1-os. For TcdA-A2 and its interaction with LNT, however, the localized binding site was the same as its native carbohydrate receptor CD-grease. A HDX-MS based titration method Protein-Ligand Interactions in solution by Mass Spectrometry, Titration and hydrogen/deuterium Exchange (PLIMSTEX), was also applied to CTB5 and its interactions GM1-os, to test the reliability of using peptides as indicators to obtain the protein-carbohydrate binding affinities. The average apparent association constant measured for the addition of GM1-os to CTB at pH 7.0 and 20 °C was found to be (1.6 ± 0.2) * 106 M-1. This is in reasonable agreement with the reported value of (3.2 ± 0.2) * 106 M-1, which was measured using direct ESI-MS assay at pH 6.9 and room temperature.

Ion mobility-mass spectrometry (IM-MS), gas-phase hydrogen/deuterium (H/D) exchange ion molecule reactions and molecular modeling provide complimentary information and are used here for the characterization of peptide ion structure, including fine structure detail (i.e., cation-[pi] interactions, [Beta]-turns, and charge solvation interactions). IM-MS experiments performed on tyrosine containing tripeptides show that the collision cross-sections of sodiated, potassiated and doubly sodiated species of gly-gly-tyr are smaller than that of the protonated species, while the cesiated and doubly cesiated species are larger. Conversely, all of the alkali-adducted species of try-gly-gly have collision cross-sections that are larger than that of the protonated species. The protonated and alkali metal ion adducted (Na, K and Cs) species of bradykinin and bradykinin fragments 1-5, 1-6, 1-7, 1-8, 2-7, 5-9 and 2-9 were also studied using IM-MS and the alkali metal ion adducts of these species were found to have cross-sections very close to those of the protonated species. Additionally, multiple peak features observed in the ATDs of protonated bradykinin fragments 1-5, 1-6 and 1-7 are conserved upon alkali metal ion adduction. It was observed from gas-phase H/D ion molecule reactions that alkali adducted species exchange slower and to a lesser extent than protonated species in the tyrosine- and arginine-containing peptides. Experimental and computational results are discussed in terms of peptide ion structure, specifically the intra-molecular interactions present how those interactions change upon alkali salt adduction, as well as with the sequence of the peptide. Additionally, IM-MS data suggests the presence of a compact conformation of bradykinin fragment 1-5 (RPPGF) when starting from organic solvent conditions. As water is added stepwise to methanolic solutions, a more extended conformation is populated. When the starting solution is composed of [approximately]90% water, two distinct mobility profiles are observed as well as a shoulder, indicating the presence of three gas-phase conformations for RPPGF. Gas-phase H/D exchange of [M+H]+ ions prepared from aqueous solvents show a bi-exponential decay, whereas samples prepared from organic solvents show a single exponential decay. The effect of solvent on gas-phase peptide ion structure, i.e., solution-phase memory effects, is discussed and gas-phase structures are compared to know solution-phase structures.

This Brief summarizes the current research on the novel BRICHOS domain, which is a chaperone domain found in a variety of proteins and is shown to exhibit anti-amyloidogenic chaperone-like functions. The BRICHOS domain is defined from sequence similarities, lacks established physiological function(s) and is found about 10 distantly related pro-protein families, several of which are associated with human disease. In this work, the authors review the mechanism by which BRICHOS inhibits A β aggregation and examine recent results from in vivo experiments where BRICHOS inhibits A β aggregation and toxicity in Drosophila melanogaster. BRICHOS is one of nature ́s (more specific) ways to protect against fibril formation, and exploring the potential of using the BRICHOS domain in the fight against Alzeimer's Disease and other amyloid diseases seems highly relevant. This brief is useful for newcomers to this field or researchers in related fields wishing to gain a quick overview of the latest findings.

Isotope Labeling of Biomolecules:

Applications, the latest in the Methods in Enzymology series, focuses on stable isotope labeling methods and applications for biomolecules. This practical guide to biomolecular labeling looks at new techniques that are becoming widely used. Continues the legacy of this premier serial with quality chapters authored by leaders in the field Focuses on stable isotope labeling of biomolecules, which is important for structural studies of proteins and nucleic acids

The book highlights the current practices and future trends in structural characterization of impurities and degradants. It begins with an overview of mass spectrometry techniques as related to the analysis of impurities and degradants, followed by studies involving characterization of process related impurities (including potential genotoxic impurities), and excipient related impurities in formulated products. Both general practitioners in pharmaceutical research and specialists in analytical chemistry field will benefit from this book that will detail step-by-step approaches and new strategies to solve challenging problems related to pharmaceutical research.

Introduce your students to the latest advances in spectroscopy with the text that has set the standard in the field for more than three decades: INTRODUCTION TO SPECTROSCOPY, 5e, by Donald L. Pavia, Gary M. Lampman, George A. Kriz, and James R. Vyvyan. Whether you use the book as a primary text in an upper-level spectroscopy course or as a companion book with an organic chemistry text, your students will receive an unmatched, systematic introduction to spectra and basic theoretical concepts in spectroscopic methods. This acclaimed resource features up-to-date spectra; a modern presentation of one-dimensional nuclear magnetic resonance (NMR) spectroscopy; an introduction to biological molecules in mass spectrometry; and coverage of modern techniques alongside DEPT, COSY, and HECTOR. Important Notice: Media content referenced within the product description or the product text may not be available in the ebook version.

Due to its enormous sensitivity and ease of use, mass spectrometry has grown into the analytical tool of choice in most industries and areas of research. This unique reference provides an extensive library of methods used in mass spectrometry, covering applications of mass spectrometry in fields as diverse as drug discovery, environmental science, forensic science, clinical analysis, polymers, oil composition, doping, cellular research, semiconductor, ceramics, metals and alloys, and homeland security. The book provides the reader with a protocol for the technique described (including sampling methods) and explains why to use a particular method and not others. Essential for MS specialists working in industrial, environmental, and clinical fields.

This volume details the importance of multiple experimental techniques and computational methods needed to obtain the comprehensive picture of protein complex structure, dynamics and assembly afforded by the emerging field of integrative structural biology. Chapters guide readers through the broad spectrum of approaches required for a complete representation of protein complexes, including expression and purification, experimental characterization of structure and assembly, and computational methods for identifying protein complexes and modelling their assembly. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Authoritative and cutting-edge, Protein Complex Assembly: Methods and Protocols aims to ensure successful results in the further study of this vital field.