Faculty Profile

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Vicki Wysocki

Professor Emerita - Retired

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Honors

- Distinguished Contribution to Mass Spectrometry, ASMS, 2009
- American Society for Mass Spectrometry Research Award, 1992
- Society for Analytical Chemists of Pittsburgh Starter Grant Award, 1990-91

Education and Appointments

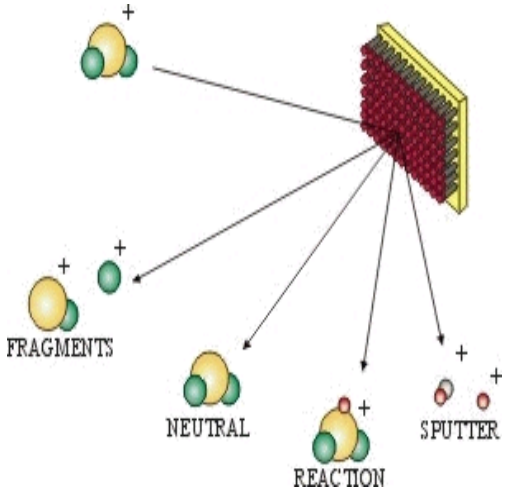
- B.S. 1982, Western Kentucky University
- Ph.D. 1987, Purdue University

Research Interests

- Analytical
- Biochemistry
- Bioanalytical
- Instrument Development
- Spectroscopy/molecular Structure
- Structural Biology

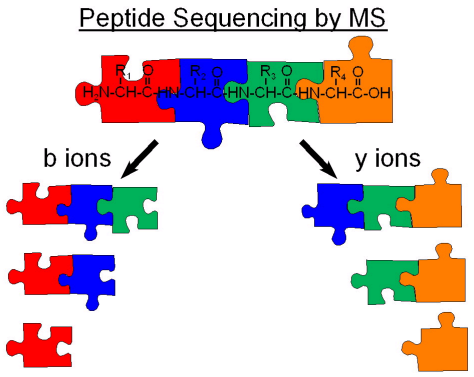
Research Summary

Bioanalytical Mass Spectrometry/Peptide and Protein Sequencing/ Ion-Surface Collisions for Surface Characterization of Organic Thin Films/Biodefense/Mosquito Proteomics and Metabolomics



Research in the Wysocki group is separated into three broad areas: (1) determination of peptide dissociation mechanisms as a means for improving programs used for automated sequencing of

peptides and proteins, (2) surface characterization of organic thin films, and (3) implementation of surface-induced dissociation onto commercial time-of-flight instruments. The research involves collisions of selected reactive and non-reactive ions with well-ordered surfaces (e.g., self-assembled monolayer films of alkanethiols on gold;Langmuir-Blodgett films). The nature of the surface, the type of projectile ion, and the collision energy are the major experimental variables that are explored.



Research in progress on biomolecules is addressing several different questions involving singly and multiply protonated peptides. All of the related projects are designed to increase the current understanding of the hydrogen bonding interactions and fragmentation patterns of activated protonated peptides. The long range goals of this work are to provide additional "rules" that can be used to enhance automated primary sequencing of peptides and proteins by tandem mass spectrometry and, ultimately, to relate information on gas-phase fragmentation patterns and energetics of dissociation to peptide and protein conformation.

Major aims of our surface characterization research are to determine whether the ion/surface chemistry that is detected when low-energy (eV), gas-phase polyatomic ions collide with a well-ordered surface can be used to quantitate the composition of mixed-composition films and to characterize electron transfer through organic thin films in the absence of solvent. Model compounds ("probe ions") are used to define the reactivity of projectile ions with various functional groups at the surface. Projectile ions used include small, odd-spin species such as distonic radical cations and their conventional counterparts; small aromatic compounds with electron-donating and electron-withdrawing groups; large, refractory molecules such as buckminsterfullerene (C_{60}). These different categories of reagents provide distinct types of information on the mechanisms of electron and atom transfer from surfaces to probe ions and on the analytical utility of ion/surface reactions for surface characterization.

A third area of research is the development of improved mass spectrometers for structural characterization of large molecules. Instruments that allow low-energy ion-surface collisions are not available commercially. Commercial MALDI-TOF(matrix-assisted laser desorption time-of-flight) instruments do not have an efficient means of fragmenting the ions. We have recently shown that surface-induced dissociation can be accomplished with good resolution in a sector/time-of-flight instrument and will extend this work to a commercial MALDI system.

Selected Publications

E.J. Kaleta, A.E. Clark, Cherkaoui, V.H. Wysocki, E.L. Ingram, J. Shcrenzel & D.M. Wolk, "Comparative Analysis of PCR-Electrospray Ionization/Mass Spectrometry (MS) and MALDI-TOF/MS for the identification of Bacteria and Yeast from Positive Blood Culture Bottles," *Clin Chem* doi:10.1373/clinchem.2011.161968.

E. Dodds, A. Blackwell, CM Jones, KL Holso, DJ O'brien, MH Cordes & VH Wysocki, "Determinants of gas-phase disassembly behavior in homodimetric protein complexes with related yet divergent structures", *Anal. Chem.* 83 (10), 3881-9 (2011). PMCID: PMC3094495

A. Blackwell, E. Dodds, V. Bandarian & V.H. Wysocki, " Revealing the Quaternary Structure of a Heterogeneous Noncovalent Protein Complex through Surface-Induced Dissociation", *Anal. Chem.* 83(8), 2862-2865, (2011).

W. Li, L. Ji, J. Goya, G. Tan & V.H. Wysocki, "SQID: An Intensity-Incorporated Protein Identification Algorithm for Tandem Mass Spectrometry ," *J. Proteome Res* 10(4), 1593-1602.

A.C. Gucinski, A. Somogyi, J. Chamot-Rooke & V.H. Wysocki, "Separation and Identification of Structural Isomers by Quadrupole Collision-Induced Dissociation- Hydrogen/Deuterium Exchange-Infrared Multiphoton Dissociation (QCID-HDX-IRMPD)", *J Am Soc Mass Spectrom*, 21(8), 1329-1338 (2010).

B. Perkins, J. Chamot-Rooke, S.H. Yoon, A. Gucinski, A. Somogyi & V.H. Wysocki, "Evidence of Diketopiperazine and Oxaxolone Structures for HA b2+Ion", *J. Am. Chem. Soc.,* 131(48), 17528-17529 (2009).

E.M. Johnson, W.R. Ellis, Jr., L. Powers & V.H. Wysocki, "Affinity Capture Mass Spectrometry of Biomarker Proteins Using Peptide Ligands from Biopanning", *Anal. Chem.*, 81(15), 5999-6005 (2009). PMCID: PMC2846195

R.L. Beardsley, C.M. Jones, A.S. Galhena, V.H. Wysocki, et al. "Noncovalent Protein Tetramers and Pentamers with 'n' Charges Yield Monomers with n/4 and n/5 Charges ", *Anal. Chem.,* 81(4), 1347-1356 (2009).

G. Cheng, E. Basha, V.H. Wysocki & E. Vierling, "Insights into Small Heat Shock Protein and Substrate Structure During Chaperone Action Derived from Hydrogen/Deuterium Exchange and Mass Spectrometry", *J. Bio. Chem.* 283(39), 26634-26642 (2008).

V.H. Wysocki, C.M. Jones, A. Galhena & A. Blackwell, "Surface-Induced Dissociation Shows Potential to be More Informative than Collision-Induced Dissociation for Structural Studies of Large Systems", *J Am Soc Mass Spectrom* 19(7), 903-913 (2008).

A.S. Galhena, S. Dagan, C. Jones., R.L. Beardsley & V.H. Wysocki, "Surface-Induced Dissociation of Peptides and Protein Complexes in a Quadrupole/Time-of-Flight Mass Spectrometer", *Anal. Chem. - Washington DC* 80 (5), 1425-1436 (2008).

V.H. Wysocki, K.E. Joyce, C.M. Jones & R.L. Beardsley, "Surface-Induced Dissociation of Small Molecules, Peptides, and Non-covalent Protein Complexes", *J Am Soc Mass Spectrom* 19 (2), 190-208 (2008).

Y. Huang, G.C. Tseng, S. Yuan, L. Pasa-Tolic, M.S. Lipton, R.D. Smith & V.H. Wysocki, "A Data-Mining Scheme for Identifying Peptide Structural Motifs Responsible for Different MS/MS Fragmentation Intensity Patterns", *J. Prot. Res.*7 (1), 70-79 (2008).

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